Density, Viscosity, Speed of Sound, Bulk Modulus, and Surface Tension of Binary Mixtures of *n*-Heptane + 2,2,4-Trimethylpentane at (293.15 to 338.15) K and 0.1 MPa

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S *Supporting Information*

ABSTRACT: In this work, the physical properties of binary mixtures of *n*-heptane and 2,2,4-trimethylpentane were measured. Density and speed of sound were measured at temperatures ranging from (293.15 to 338.15) K, and viscosity was measured at temperatures ranging from (293.15 to 333.15) K. At 298.15 K, pure component values for heptane of 679.61 kg·m^{-3}, 0.389 mPa·s, and 1130.1 m·s^{-1} for density, viscosity, and speed of sound, respectively, agree with literature values. Similarly for 2,2,4-trimethylpentane, the values of 687.70 kg·m^{-3}, 0.501 mPa·s, and 1081.7 m·s^{-1} for density, viscosity, and speed of sound, respectively, agree with literature values. Density mole fraction and temperature data were fit to a second-order polynomial. Bulk moduli ranged from (551.7 to 907.1) MPa over (293.15 to 338.15) K. Viscosity mole fraction data were fit using the three-body McAllister model, while the viscosity deviations were fit to a Redlich–Kister type equation. For the mixtures, an increase in mole fraction of 2,2,4-trimethylpentane resulted in an increase in density and viscosity and in a decrease in speed of sound, bulk modulus, and surface tension. Increases in temperature decreased density, viscosity, speed of sound, and bulk modulus. At room temperature, the surface tension values ranged from (18.7 to 20.3) mN·m^{-1}. These data can be used by researchers who are modeling the combustion process of mixtures of primary reference fuels and are modeling the physical properties of fuels.
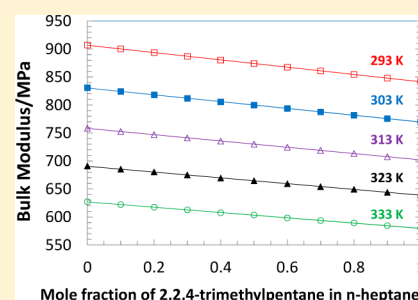
1. INTRODUCTION

The chemical compounds *n*-heptane and 2,2,4-trimethylpentane are the primary reference fuels (PRFs) that are used to define the octane reference scale for fully blended gasoline.[1] The combustion processes for the pure PRFs and their blends have been studied in variable-pressure flow reactors,[1] flow and burner assemblies,[2] shock tubes,[3,4] rapid compression machines,[5] and high-pressure jet-stirred reactors,[6] and the kinetic mechanisms for the combustion process have been modeled.[1,2,7−9] By understanding the combustion of these compounds, mechanisms can be developed for other mixtures that can act as "surrogates" for other petroleum-based and alternative fuels.[1] The combustion process and the delivery of the fuel to the engine are related to the physical and chemical properties of the fuels such as density, viscosity, speed of sound, and surface tension. The bulk modulus, which is calculated from density and speed of sound measurements, directly effects fuel injection time.[10] The viscosity, surface tension, and density have been used as input parameters in the simulation of the vaporization of multicomponent fuel droplets.[11,12] Having measurements of these properties at various temperatures for PRFs would be useful in modeling their transport and combustion.

In this work, the density, viscosity, surface tension, and speed of sound were measured for binary mixtures of 2,2,4-trimethylpentane with *n*-heptane. Density values and excess molar volumes of these mixtures have been reported at 298.15 K[13,14] and 313.15 K,[14] and for 0.5223 mole fraction of heptane in 2,2,4-trimethylpentane at 338.15 K.[14] Excess molar volumes alone without the density data have also been reported at 298.15 K.[15] Viscosity values for binary mixtures have only been reported at 298.15 K.[13] The current study expands the temperature range for the viscosity measurements of these mixtures, examines more mixtures at higher temperatures for density measurements, and also measures speed of sound and surface tension. Using the speed of sound and density measurements, bulk modulus is calculated. The goal of this work is to provide physical property measurements for computer modeling purposes.

2. MATERIALS

The *n*-heptane and 2,2,4-trimethylpentane were used as received from the supplier (Table 1). Mixtures of *n*-heptane and 2,2,4-trimethylpentane were prepared at 293.15 K by weighing each component on a Mettler Toledo AG204 analytical balance with an error of 0.0004 g. The error in mole fraction of the 2,2,4-trimethylpentane in *n*-heptane as given by the combined expanded uncertainty is 0.0001, which is

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Table 1. Sample Information

chemical name	molar mass (g/mol)	source/lot number	mole fraction purity	analysis method
n-heptane	100.2019	Alfa Aesar/ N07A522	0.999	GC[a]
2,2,4-trimethylpentane	114.2285	Alfa Aesar/ L27Z752	0.996	GC[a]

[a]Gas−liquid chromatography.

the same as found for other mixtures prepared the same way.[16−19]

3. METHODS

The speed of sound and density of the n-heptane, 2,2,4-trimethylpentane, and their mixtures was measured using an Anton Paar DSA 5000 density and sound analyzer. The viscosity of the compounds and mixtures was measured using an Anton Paar SVM 3000 Stabinger viscometer. The DSA 5000 was cleaned and calibrated with degassed distilled water each day as specified by the manufacturer. For this instrument, samples of each individual liquid or liquid mixture were measured at 10 temperatures between (293.15 and 338.15) K, and replicate samples (two or more samples at each temperature) were used to determine the precision of the measurement. The accuracy of the density measurements was tested using a NIST certified toluene liquid density standard-extended range (211d) and a NIST certified isooctane (2,2,4-trimethylpentane) liquid density standard (standard reference materials 2214). The accuracy of the SVM 3000 was tested and calibrated using two NIST certified/traceable viscosity/density reference standards (Standard S3 and N.4 from Cannon Instrument Company). Deviations from reference values resulted in cleaning and additional analysis of the standards. Using this device, two or more samples of each individual liquid or liquid mixture were measured at eight temperatures between (293.15 and 333.15) K, and these replicate measurements were used to determine the precision of the measurement.

A Kruss DS100 drop shape analyzer was used to measure the surface tension of the liquids. This instrument records the magnified image of an organic liquid droplet formed in air using a syringe with a needle whose diameter had been measured using a micrometer. Using input parameters of the needle diameter, air density, and organic liquid density, the software fit the shape of the droplet to the Young−LaPlace equation to determine the surface tension.[16,17,19] Using this instrument, more than 15 surface tension measurements were taken for a minimum of three droplets of each liquid, and these values were used to calculate the standard deviation of each measurement.

To determine the combined expanded uncertainty of density, viscosity, speed of sound, and surface tension the standard deviation of the measurements (taken at each temperature as described above) were multiplied by 2. When a normal distribution is assumed, multiplying by a coverage factor of 2 produces a 95% confidence interval. The purity of a sample also impacts the precision of the measurements, and this was taken into account when determining the combined expanded uncertainty.[20]

4. RESULTS

4.1. Density. The density values of n-heptane and 2,2,4-trimethylpentane are given as a function temperature in Table 2 along with literature values. The densities of the pure

Table 2. Comparison of the Measured Density and Speed of Sound Values of n-Heptane and 2,2,4-Trimethylpentane with Literature Values[a]

T/K	density, kg·m⁻³		speed of sound, m·s⁻¹	
	this study	literature	this study	literature
		Heptane		
293.15	683.85	683.74 ± 0.09[b], 683.81[c]	1151.7	1149.4[c], 1152.6[d]
298.15	679.61	679.49 ± 0.09[b], 679.60[c]	1130.1	1128.5[c], 1130[m], 1131.0[l], 1133[k], 1137[j]
303.15	675.35	675.22 ± 0.09[b], 675.36[c]	1109.1	1107.8[c], 1108.55[e], 1109.6[d], 1117[j]
308.15	671.05	670.94 ± 0.09[b], 671.10[c]	1087.5	1087.2[c], 1090[j]
313.15	666.73	666.63 ± 0.09[b], 666.82[c]	1066.6	1066.5[f], 1066.7[c], 1067.1[d], 1073[j]
318.15	662.38	662.29 ± 0.10[b], 662.51[c]	1045.4	1046.4[c], 1059[j]
323.15	657.99	657.94 ± 0.10[b], 658.18[c]	1024.7	1022[m], 1026.1[c]
328.15	653.57	653.55 ± 0.11[b], 653.81[c]	1003.6	1006[c]
333.15	649.11	649.13 ± 0.12[b], 649.41[c]	983.0	985.9[c]
338.15	644.60	644.48 ± 0.13[b], 644.98[c]	962.3	965.9[c]
		2,2,4-Trimethylpentane		
293.15	691.84	691.89 ± 0.4[h] 691.95 ± 0.15[g]	1103.2	1104.3 ± 0.4[h], 1104.6[i]
298.15	687.70	687.77 ± 0.4[h] 687.83 ± 0.15[g]	1082.0	1080[k], 1083.1 ± 0.4[h], 1084[j]
303.15	683.59	683.64 ± 0.4[h] 683.70 ± 0.15[g]	1061.4	1059[j], 1061.7[i], 1062.4 ± 0.4[h]
308.15	679.40	679.48 ± 0.4[h] 679.54 ± 0.15[g]	1040.4	1041.6 ± 0.4[h], 1043[j]
313.15	675.23	675.28 ± 0.4[h] 675.37 ± 0.17[g]	1020.0	1019.1[i], 1020.9 ± 0.4[h], 1023[j]
318.15	670.98	671.07 ± 0.4[h] 671.17 ± 0.18[g]	999.3	1000.5 ± 0.4[h], 1002[j]
323.15	666.75	666.81 ± 0.4[h] 666.94 ± 0.19[g]	979.2	977.9[i], 980.0 ± 0.4[h]
328.15	662.44	662.52 ± 0.4[h] 662.68 ± 0.20[g]	958.7	959.7 ± 0.4[h]
333.15	658.16	658.19 ± 0.4[h] 658.39 ± 0.22[g]	938.6	935.8[i], 939.7 ± 0.4[h]
338.15	653.80	653.81 ± 0.4[h] 654.07 ± 0.23[g]	918.7	919.17 ± 0.4[h]
343.15	649.40	649.40 ± 0.06[h] 649.70 ± 0.15[g]	899.0	897.3[i], 900.0 ± 0.4[h]

[a]Standard uncertainties u are u(T) = 0.01 K, and combined expanded uncertainties U_c are $U_c(\rho)$ = 0.06 kg·m⁻³ and $U_c(c)$ = 0.5 m·s⁻¹, (level of confidence = 0.95, $k \approx 2$), except for the 343.15 K values that are $U_c(\rho)$ = 0.10 kg·m⁻³ for 2,2,4-trimethylpentane. [b]From equation fit by ref 21 to "reliable data" from over 15 sources. For heptane, the equation is ρ = 8.70405·10² −2.38753·10⁻⁵T − 4.65917·10⁻³T² + 1.20283·10⁻⁵T³ − 1.210791·10⁻⁸ T³. [c]From ref 22 "The uncertainties of the equation of state are approximately··· 2% in the speed of sound". [d]Reference 23. [e]Reference 24. [f]Reference 25. [g]From equation fit by ref 21 to "reliable data" from over 15 sources. For 2,2,4-trimethylpentane, the equation is ρ = 9.94553·10² − 1.53687T + 2.72542·10⁻³T² − 3.42509·10⁻⁶T³. [h]Reference 26. [i]Reference 27. [j]Reference 28. [k]Reference 29. [l]Reference 30. [m]Reference 31.

components match reported values within the error of the measurements. The measured density values of the NIST-

certified toluene standard and the NIST-certified isooctane standard match the certified values within the error of the measurements (Table 3), demonstrating the accuracy of the

Table 3. Comparison of the Measured Density of NIST-Certified Toluene and 2,2,4-Trimethylpentane with Certified Values

	density, kg·m⁻³	
T/K	this study	literature
NIST Certified Toluene Standard		
293.15	866.84	866.828 ± 0.031[a]
303.15	857.52	857.507 ± 0.032[a]
313.15	848.14	848.131 ± 0.033[a]
323.15	838.69	838.684 ± 0.034[a]
333.15	829.16	829.152 ± 0.035[a]
343.15	819.53	819.516 ± 0.037[a]
NIST Certified 2,2,4-Trimethylpentane Standard		
288.15	695.93	695.969 ± 0.035[b]
293.15	691.84	691.872 ± 0.035[b]
298.15	687.72	687.753 ± 0.035[b]

[a]Reference 32; values for liquid density of SRM 211d "as shipped". Error bars are the reported standard uncertainties. [b]Reference 33; error bars are the reported standard uncertainties.

instrument. The density values of the 2,2,4-trimethylpentane and *n*-heptane mixtures are given in Table 4 as a function of the mole fraction of 2,2,4-trimethylpentane (X_1). The values for the mixtures at 298.15 K fall between values reported by Awad and Allos[13] and Malhotra and Wolf[14] at the same temperature as shown in Figure 1.

For the mixtures, the density increased as mole fraction of the 2,2,4-trimethylpentane increased, but the increase was not linear as shown in Figure 2. A second order polynomial was used to fit the density and mole fraction data:

$$\rho/\text{kg·m}^{-3} = AX_1^2 + BX_1 + C \qquad (1)$$

In this equation X_1 is the mole fraction of the 2,2,4-trimethylpentane and A, B, and C are fitting parameters, which are given in Table 5. The standard error of the fit, as calculated by

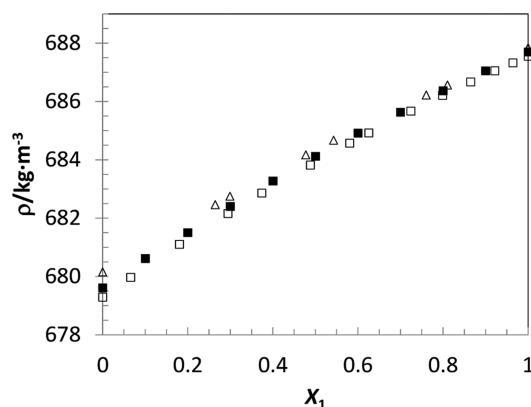$$\sigma = \sqrt{\frac{\sum (P_{\text{measured}} - P_{m,\text{cal}})^2}{N - n}} \qquad (2)$$

Figure 1. Comparison of the density of 2,2,4-trimethylpentane (X_1) and *n*-heptane mixtures at 298.15 K: ■, this study; □, ref 13; △, ref 14.
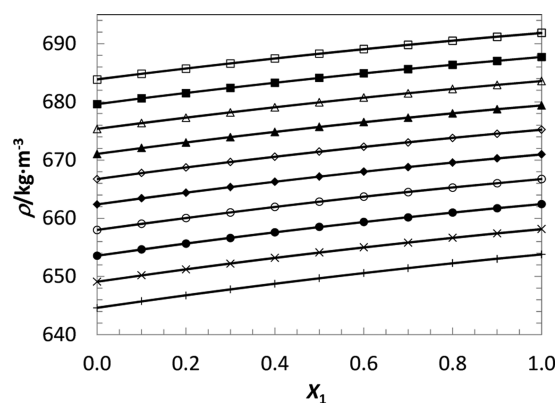

Figure 2. Density of 2,2,4-trimethylpentane (X_1) + *n*-heptane mixtures at □, 293.15 K; ■, 298.15 K; △, 303.15 K; ▲, 308.15 K; ◊, 313.15 K; ♦, 318.15 L; ○, 323.15 K; ●, 328.15 K; ×, 333.15 K; +, 338.15 K. Error bars, which are the combined expanded uncertainties with 0.95 level of confidence (k ≈ 2), are smaller than the symbols. Lines shown are second order fits using eq 1 with the coefficients in Table 5.

is also given in Table 5. In this equation P_{measured} is the measured density and $P_{m,\text{cal}}$ is the fitted density, N is the number of experimental data, and n is the number of parameters in the fitting equation. Microsoft Excel 2010 was used to conduct the fitting operation. The fits are good with

Table 4. Density (kg·m⁻³) of Mixtures of 2,2,4-Trimethylpentane (1) in *n*-Heptane from T = (293.15 to 338.15) K and 0.1 MPa[a]

T/K	$X_1 = 0.1000$	$X_1 = 0.2001$	$X_1 = 0.2999$	$X_1 = 0.4001$	$X_1 = 0.5001$	$X_1 = 0.6000$	$X_1 = 0.6999$	$X_1 = 0.8000$	$X_1 = 0.9000$
293.15	684.83	685.71	686.59	687.45	688.28	689.06	689.77	690.50	691.17
298.15	680.61	681.50	682.40	683.27	684.12	684.91	685.63	686.36	687.05
303.15	676.36	677.27	678.18	679.07	679.93	680.73	681.46	682.20	682.89
308.15	672.09	673.01	673.93	674.83	675.71	676.52	677.26	678.02	678.72
313.15	667.78	668.71	669.65	670.57	671.46	672.28	673.03	673.80	674.52
318.15	663.44	664.39	665.34	666.28	667.18	668.02	668.78	669.55	670.28
323.15	659.07	660.04	661.00	661.95	662.86	663.71	664.49	665.28	666.02
328.15	654.65	655.64	656.61	657.59	658.52	659.37	660.16	660.98	661.73
333.15	650.21	651.22	652.20	653.19	654.14	655.01	655.81	656.64	657.40
338.15	645.76	646.75	647.77	648.75	649.71	650.60	651.41	652.29	653.03

[a]X_1 is the mole fraction of 2,2,4-trimethylpentane in (2,2,4-trimethylpentane + *n*-heptane). Standard uncertainties *u* are $u(T)$ = 0.01 K, and combined expanded uncertainties U_c is $U_c(\rho)$ = 0.08 kg·m⁻³, (level of confidence = 0.95, k ≈ 2), except for the X_1 = 0.1000, which has a combined expanded uncertainty of 0.13 kg·m⁻³.

Table 5. Parameters^a for Equation 1, $\rho = AX_1{}^2 + BX_1 + C$, that Correlate Density (kg·m^{-3}) to Mole Fraction of 2,2,4-Trimethylpentane (X_1) in n-Heptane Mixtures, and the Excess Molar Volume^b (V_m^E) at $X_1 = 0.5001$, $T = (293$ to $338)$ K, and 0.1 MPa^a

T/K	A	B	C	R^2	σ	V_m^E/cm^3·mol^{-1}
293.15	-1.7 ± 0.2	9.7 ± 0.2	683.86 ± 0.03	0.9999	0.02	-0.04
298.15	-1.8 ± 0.1	9.9 ± 0.1	679.62 ± 0.03	0.9999	0.02	-0.05
303.15	-1.8 ± 0.2	10.0 ± 0.2	675.36 ± 0.03	0.9999	0.02	-0.05
308.15	-1.8 ± 0.1	10.2 ± 0.1	671.06 ± 0.03	0.9999	0.02	-0.05
313.15	-1.8 ± 0.2	10.3 ± 0.2	666.74 ± 0.03	0.9999	0.02	-0.05
318.15	-1.9 ± 0.1	10.5 ± 0.1	662.38 ± 0.03	0.9999	0.02	-0.06
323.15	-1.9 ± 0.2	10.6 ± 0.2	658.00 ± 0.04	0.9999	0.02	-0.06
328.15	-2.0 ± 0.2	10.8 ± 0.2	653.57 ± 0.04	0.9999	0.02	-0.06
333.15	-1.9 ± 0.2	11.0 ± 0.2	649.11 ± 0.04	0.9999	0.02	-0.06
338.15	-1.9 ± 0.2	11.1 ± 0.2	644.62 ± 0.05	0.9999	0.03	-0.06

^{a}X_1 is the mole fraction of 2,2,4-trimethylpentane in (2,2,4-trimethylpentane + n-heptane). The errors for the coefficients A, B, and C represent the 95% confidence interval. ^{b}The standard deviation in the excess volume was calculated to be 0.014 cm^3·mol^{-1}. The σ is the standard error of the fit as given by eq 2.

Table 6. Speed of Sound (m·s^{-1}) of Mixtures of 2,2,4-Trimethylpentane (1) in n-Heptane from $T = (293.15$ to $338.15)$ K and 0.1 MPa^a

T/K	$X_1 = 0.1000$	$X_1 = 0.2001$	$X_1 = 0.2999$	$X_1 = 0.4001$	$X_1 = 0.5001$	$X_1 = 0.6000$	$X_1 = 0.6999$	$X_1 = 0.8000$	$X_1 = 0.9000$
293.15	1146.5	1141.7	1136.6	1131.6	1127.0	1122.0	1117.2	1112.5	1107.7
298.15	1125.3	1120.5	1115.5	1110.5	1105.9	1101.0	1096.2	1091.6	1086.7
303.15	1103.9	1099.2	1094.2	1089.3	1084.7	1079.9	1075.1	1070.5	1065.8
308.15	1082.7	1078.0	1073.1	1068.2	1063.7	1058.9	1054.2	1049.7	1045.0
313.15	1061.7	1057.0	1052.2	1047.3	1042.8	1038.1	1033.5	1029.0	1024.3
318.15	1040.7	1036.1	1031.3	1026.5	1022.1	1017.4	1012.8	1008.4	1003.8
323.15	1019.8	1015.2	1010.5	1005.7	1001.4	996.8	992.3	987.9	983.3
328.15	999.0	994.4	989.8	985.1	980.8	976.3	971.8	967.4	963.0
333.15	978.3	973.9	969.2	964.6	960.4	955.8	951.6	947.3	942.9
338.15	957.8	953.3	948.7	944.3	940.1	935.8	931.3	927.2	922.9

^{a}X_1 is the mole fraction of 2,2,4-trimethylpentane in (2,2,4-trimethylpentane + n-heptane). Standard uncertainties u are $u(T) = 0.01$ K, and combined expanded uncertainty U_c is $U_c(c) = 0.5$ m·s^{-1}, (level of confidence = 0.95, $k \approx 2$).

$R^2 > 0.9999$ as shown in Figure 2. These fits can be used in numerical simulations of the transport and combustion of these primary reference fuels.

The excess molar volumes (V_m^E) of 2,2,4-trimethylpentane in n-heptane mixtures were calculated using the following equation:

$$V_m^E = \frac{M_1 X_1 + M_2 X_2}{\rho_m} - \frac{M_1 X_1}{\rho_1} - \frac{M_2 X_2}{\rho_2} \qquad (3)$$

where ρ_m is the density of the mixture, ρ_1 and ρ_2 are the pure component densities, M_1 and M_2 are the molar masses, and X_1 and X_2 are the mole fractions of the 2,2,4-trimethylpentane as component 1 and n-heptane as component 2. The calculated excess molar volumes for a mole fraction of 2,2,4-trimethylpentane of 0.5001 in n-heptane are given in Table 5. The excess molar volumes are small negative values that do not vary significantly over the temperature range studied, suggesting that the behavior of these mixtures is close to ideal. Additional excess molar volumes, their fitting using a Redlich−Kister type expression, and a comparison with literature values can be found in the Supporting Information.

4.2. Speed of Sound and Bulk Modulus. The speed of sound values of n-heptane and 2,2,4-trimethylpentane are given as a function temperature in Table 2 along with literature values. The values measured herein agree with or are slightly lower (within 1.4 m·s^{-1}) than the reported values. At temperatures of 328 K and higher, the only available numbers

with which to compare the n-heptane values were model values from NIST, which were reported to have a 2% error. The numbers reported herein are lower than the model values, but are within that 2% error. The speed of sound values of the 2,2,4-trimethylpentane and n-heptane mixtures are given in Table 6 as a function of the mole fraction of 2,2,4-trimethylpentane (X_1). As the mole fraction of the 2,2,4-trimethylpentane increased, the speed of sound decreased linearly as shown in Figure 3. The linearity was confirmed by calculating the speed of sound deviation (Δc) using

$$\Delta c = c_m - (X_1 c_1) - (X_2 c_2) \qquad (4)$$

c_m is the speed of sound of the binary mixture, c_1 and c_2 are the speeds of sound of the pure components, and X_1 and X_2 are the mole fractions of 2,2,4-trimethylpentane as component 1 and n-heptane as component 2. The calculated values of the speed of sound deviation are very close to zero and are smaller than their errors for more than 94 % of the mixtures, and the remaining values are very close to their errors. Such small deviations suggest that a linear model is appropriate. The speed of sound and mole fraction data were fit to

$$c/\text{m·s}^{-1} = AX_1 + B \qquad (5)$$

In this equation X_1 is the mole fraction of the 2,2,4-trimethylpentane, and A and B are fitting parameters, which are given in Table 7. The standard error for the fit (σ) was determined by eq 2, where $P_{measured}$ is the measured speed of
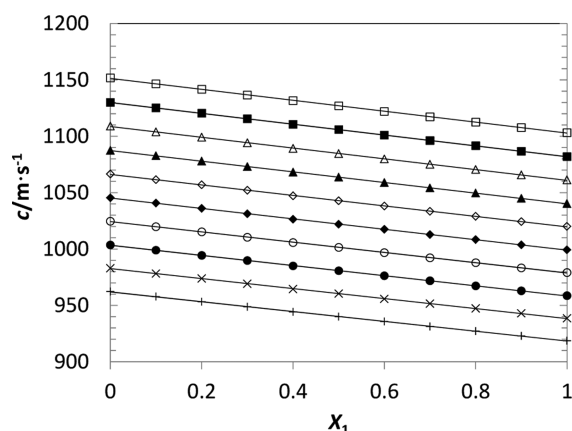
Figure 3. Speed of sound of 2,2,4-trimethylpentane (X_1) + n-heptane mixtures at □, 293.15 K; ■, 298.15 K; △, 303.15 K; ▲, 308.15 K; ◇, 313.15 K; ◆, 318.15 L; ○, 323.15 K; ●, 328.15 K; ×, 333.15 K; +, 338.15 K. Error bars, which are the combined expanded uncertainties with 0.95 level of confidence ($k \approx 2$), are smaller than the symbols. Lines shown are linear fits using eq 5 with the coefficients in Table 7.

Table 7. Parameters for Equation 8: $c = AX_1 + B$, that Correlates Speed of Sound c (m·s^{-1}), to the Mole Fraction of 2,2,4-Trimethylpentane (X_1) in n-Heptane and Associated Standard Error (Equation 2) over the Temperature Range T = (293 to 338) K[a]

T/K	A	B/m·s^{-1}	R^2	σ
293.15	−48.5 ± 0.5	1151.3 ± 0.3	0.999	0.25
298.15	−48.1 ± 0.3	1130.0 ± 0.2	0.999	0.13
303.15	−47.7 ± 0.5	1108.7 ± 0.3	0.999	0.24
308.15	−47.2 ± 0.3	1087.4 ± 0.2	0.999	0.16
313.15	−46.6 ± 0.5	1066.3 ± 0.3	0.999	0.22
318.15	−46.2 ± 0.3	1045.2 ± 0.2	0.999	0.16
323.15	−45.5 ± 0.5	1024.3 ± 0.3	0.999	0.24
328.15	−45.0 ± 0.4	1003.4 ± 0.2	0.999	0.17
333.15	−44.3 ± 0.5	982.7 ± 0.3	0.999	0.24
338.15	−43.5 ± 0.4	962.0 ± 0.3	0.999	0.20

[a]X_1 is the mole fraction of 2,2,4-trimethylpentane in (2,2,4-trimethylpentane + n-heptane). The errors for the coefficients A and B are the 95% confidence interval.

sound and $P_{m,cal}$ is the fitted speed of sound. The fits are good with R^2 > 0.999 as shown in Figure 3.

The isentropic bulk modulus of the 2,2,4-trimethylpentane and n-heptane mixtures, E_v, was calculated at each temperature and ambient pressure from the speed of sound (c) and density (ρ) by[16−19]

$$E_v/\text{Pa} = (c^2/\text{m}^2 \cdot \text{s}^{-2})(\rho/\text{kg} \cdot \text{m}^{-3}) \tag{6}$$

The calculated values are given in Table 8. The bulk modulus decreases with increasing temperature and increasing mole fraction of 2,2,4-trimethylpentane. Higher bulk modulus values lead to advanced injection timing in engines.[10,34]

4.3. Viscosity. The viscosity values of n-heptane and 2,2,4-trimethylpentane are given as a function temperature in Table 9 along with literature values. The viscosities of the pure components match reported values within the error of the measurements. The dynamic and kinematic viscosity values of n-heptane, 2,2,4-trimethylpentane, and their mixtures are given in Table 10 as a function of the mole fraction of 2,2,4-trimethylpentane (X_1). The mixture data agree fairly well with data reported by Awwad and Allos[13] at 298.15 K, as shown in Figure 4. While the pure component data reported herein and by Awwad and Allos[13] agree with other literature values, their pure component values of 0.3942 and 0.4788 mPa·s for pure n-heptane and 2,2,4-trimethylpentane, respectively, fall at the higher end of the reported viscosity values (Table 9), while the values reported herein are at the lower end of the reported viscosity values (Table 9). These small differences are then reflected in their mixtures values being slightly higher than those reported herein.

The kinematic viscosity data were fit using the McAllister three-body model:[51]

$$\ln \nu_m = X_1^3 \ln \nu_1 + 3X_1^2 X_2 \ln \nu_{1,2} + 3X_1 X_2^2 \ln \nu_{2,1} + X_2^3 \ln \nu_2$$
$$- \ln\left(X_1 + X_2 \frac{M_2}{M_1}\right) + 3X_1^2 X_2 \ln\left(\frac{1}{3}\left(2 + \frac{M_2}{M_1}\right)\right)$$
$$+ 3X_1 X_2^2 \ln\left(\frac{1}{3}\left(1 + 2\frac{M_2}{M_1}\right)\right) + X_2^3 \ln\left(\frac{M_2}{M_1}\right) \tag{7}$$

Here ν_m is the kinematic viscosity of the binary mixture, x_1 and x_2 are the mole fractions, ν_1 and ν_2 are the kinematic viscosities of the pure components, and M_1 and M_2 are the molar masses of 2,2,4-trimethylpentane as component 1 and n-heptane as component 2. The interaction parameters $\nu_{2,1}$ and $\nu_{1,2}$ were determined using the GRG nonlinear engine of the SOLVER function in Microsoft Excel 2010 to minimize the sum of the

Table 8. Bulk Modulus (MPa) of Mixtures of 2,2,4-Trimethylpentane (1) in n-Heptane from T = (293.15 to 338.15) K and 0.1 MPa[a]

T/K	X_1 = 0.00	X_1 = 0.1000	X_1 = 0.2001	X_1 = 0.2999	X_1 = 0.4001	X_1 = 0.5001	X_1 = 0.6000	X_1 = 0.6999	X_1 = 0.8000	X_1 = 0.9000	X_1 = 1.00
293.15	907.1	900.2	893.8	887.0	880.3	874.2	867.5	861.0	854.7	848.0	842.0
298.15	867.9	861.8	855.6	849.1	842.6	836.7	830.2	823.9	817.8	811.4	805.0
303.15	830.7	824.3	818.3	812.0	805.7	800.0	793.8	787.7	781.8	775.6	770.1
308.15	793.7	787.9	782.1	776.1	770.0	764.5	758.6	752.7	747.1	741.1	735.4
313.15	758.5	752.7	747.1	741.3	735.5	730.2	724.5	718.9	713.4	707.7	702.5
318.15	723.9	718.6	713.2	707.6	702.0	696.9	691.5	686.0	680.8	675.3	670.0
323.15	690.9	685.4	680.3	675.0	669.5	664.7	659.5	654.2	649.3	644.0	639.3
328.15	658.3	653.4	648.3	643.3	638.1	633.4	628.5	623.5	618.5	613.6	608.8
333.15	627.3	622.2	617.7	612.7	607.7	603.4	598.4	593.8	589.3	584.5	579.9
338.15	596.9	592.4	587.7	583.0	578.5	574.2	569.7	565.0	560.8	556.3	551.8

[a]X_1 is the mole fraction of 2,2,4-trimethylpentane in (2,2,4-trimethylpentane + n-heptane). Standard uncertainties u are $u(T)$ = 0.01 K, and combined expanded uncertainty U_c is U_c(bulk modulus) = 0.5 MPa, (level of confidence = 0.95, $k \approx 2$).

Table 9. Comparison of the Measured Viscosity Values^a (mPa·s) of n-Heptane and 2,2,4-Trimethylpentane with Literature Values

	heptane		2,2,4-trimethylpentane	
T/K	measured	literature values	measured	literature values
293.15	0.410 ± 0.002	0.409[h], 0.4107[c], 0.41136[b], 0.4181[j],	0.501 ± 0.002	0.497 to 0.530[j]
298.15	0.389 ± 0.002	0.3860[f], 0.3866[d], 0.388[h,l], 0.38848[b], 0.3889[c], 0.3890[e], 0.3903[q], 0.392[r], 0.3967[j]	0.473 ± 0.002	0.473[k], 0.4740[m], 0.478[l], 0.484[o], 0.4842[s], 0.492[r]
303.15	0.368 ± 0.002	0.365[g], 0.36751[b], 0.368[h,l], 0.372[r], 0.3772[j]	0.447 ± 0.002	0.444[n], 0.447[p], 0.4474[m], 0.451[l], 0.466[r]
308.15	0.349 ± 0.002	0.34823[b], 0.350[l], 0.3506[c], 0.354[r], 0.3592[j]	0.423 ± 0.002	0.418[j], 0.4243[m], 0.426[l], 0.441[r]
318.15	0.315 ± 0.002	0.31404[b], 0.317[l], 0.3272[j]	0.380 ± 0.002	0.380[p], 0.381[l]
323.15	0.300 ± 0.002	0.29883[b], 0.300[g], 0.3128[j]	0.361 ± 0.002	0.354[j], 0.365[k]
328.15	0.284 ± 0.005	0.2847[b], 0.2993[j]	0.343 ± 0.002	
333.15	0.271 ± 0.009	0.27155[b], 0.274[g], 0.280[i], 0.2867[j]	0.326 ± 0.002	0.327[p]

^{a}Standard uncertainties u are $u(T)$ = 0.01 K, and combined expanded uncertainties U_c are given as the error bars (level of confidence = 0.95, $k \approx 2$);. ^{b}Reference 22. ^{c}Reference 35. ^{d}Reference 36. ^{e}Reference 37. ^{f}Reference 38. ^{g}Reference 39. ^{h}Reference 40. ^{i}Reference 41. ^{j}Reference 42. ^{k}Reference 43. ^{l}Reference 28. ^{m}Reference 44. ^{n}Reference 45. ^{o}Reference 46. ^{p}Reference 47. ^{q}Reference 48. ^{r}Reference 49. ^{s}Reference 50.

Table 10. Viscosity of Mixtures of 2,2,4-Trimethylpentane (1) in n-Heptane from T = (293.15 to 333.15) K and 0.1 MPa^a

		T/K							
X_1	viscosity units	293.15	298.15	303.15	308.15	318.15	323.15	328.15	333.15
0.000	μ/mPa·s	0.410	0.389	0.368	0.349	0.315	0.300	0.284	0.271
	ν/mm^2·s^{-1}	0.600	0.572	0.545	0.521	0.476	0.457	0.435	0.417
0.1000	μ/mPa·s	0.416	0.394	0.373	0.355	0.320	0.305	0.291	0.276
	ν/mm^2·s^{-1}	0.607	0.579	0.552	0.528	0.482	0.463	0.444	0.425
0.2001	μ/mPa·s	0.423	0.400	0.379	0.360	0.325	0.309	0.295	0.280
	ν/mm^2·s^{-1}	0.616	0.588	0.560	0.535	0.489	0.469	0.450	0.431
0.2999	μ/mPa·s	0.430	0.407	0.386	0.366	0.330	0.314	0.300	0.286
	ν/mm^2·s^{-1}	0.626	0.597	0.569	0.543	0.497	0.476	0.457	0.438
0.4001	μ/mPa·s	0.438	0.415	0.393	0.373	0.336	0.320	0.305	0.290
	ν/mm^2·s^{-1}	0.637	0.607	0.578	0.553	0.505	0.483	0.463	0.444
0.5001	μ/mPa·s	0.447	0.423	0.400	0.380	0.343	0.326	0.311	0.294
	ν/mm^2·s^{-1}	0.649	0.619	0.589	0.562	0.514	0.491	0.472	0.449
0.6000	μ/mPa·s	0.456	0.432	0.408	0.387	0.349	0.332	0.316	0.300
	ν/mm^2·s^{-1}	0.662	0.630	0.600	0.572	0.523	0.500	0.480	0.458
0.6999	μ/mPa·s	0.466	0.441	0.417	0.396	0.356	0.338	0.323	0.306
	ν/mm^2·s^{-1}	0.675	0.644	0.612	0.584	0.533	0.509	0.489	0.466
0.8000	μ/mPa·s	0.477	0.451	0.426	0.404	0.363	0.345	0.329	0.313
	ν/mm^2·s^{-1}	0.690	0.656	0.625	0.596	0.543	0.518	0.497	0.476
0.9000	μ/mPa·s	0.488	0.462	0.436	0.413	0.372	0.353	0.335	0.319
	ν/mm^2·s^{-1}	0.706	0.672	0.639	0.609	0.554	0.530	0.506	0.485
1.00	μ/mPa·s	0.501	0.473	0.447	0.423	0.380	0.361	0.343	0.326
	ν/mm^2·s^{-1}	0.724	0.688	0.654	0.623	0.566	0.541	0.518	0.496

^{a}X_1 is the mole fraction of 2,2,4-trimethylpentane in (2,2,4-trimethylpentane + n-heptane). Standard uncertainties u are $u(T)$ = 0.01 K, and combined expanded uncertainty U_c is $U_c(\mu)$ = 0.002 mPa·s and $U_c(\nu)$ = 0.002 mm^2·s^{-1}, except for the mixtures at 333.15 K where the $U_c(\mu)$ = 0.004 mPa·s and $U_c(\nu)$ = 0.007 mm^2·s^{-1} (level of confidence = 0.95, $k \approx 2$).

square of the difference between the value calculated by the model in eq 7, $\nu_{m,calc}$, and the measured kinematic viscosity of the binary mixture, $\nu_{measured}$:[17,19]

$$\min \Sigma(\nu_{m,calc} - \nu_{measured})^2 \qquad (8)$$

The standard error for the fit (σ) was determined by eq 2, in which $P_{measured}$ is the measured viscosity and $P_{m,cal}$ is the fitted viscosity. The fitted values of $\nu_{2,1}$, and $\nu_{1,2}$, and the standard errors of the fits are given in Table 11 for each temperature. The model fits the data well as shown in Figure 5. These fits can be used in numerical simulations of the transport and combustion of these primary reference fuels.

The viscosity deviation ($\Delta\nu$) in these two component systems was calculated using

$$\Delta\nu = \nu_m - (X_1\nu_1) - (X_2\nu_2) \qquad (9)$$

where ν_m is the kinematic viscosity of the binary mixture, ν_1 and ν_2 are the kinematic viscosities of the pure components, and X_1 and X_2 are the mole fractions of 2,2,4-trimethylpentane as component 1 and n-heptane as component 2. The calculated values of the viscosity deviations for all 2-component mixtures are given in Table S3 of the Supporting Information. Figure 6 shows that the viscosity deviations for the mixtures are negative. As the temperature increases, the values deviate less from zero.

A Redlich−Kister type expression[19] was used to fit the viscosity deviations:

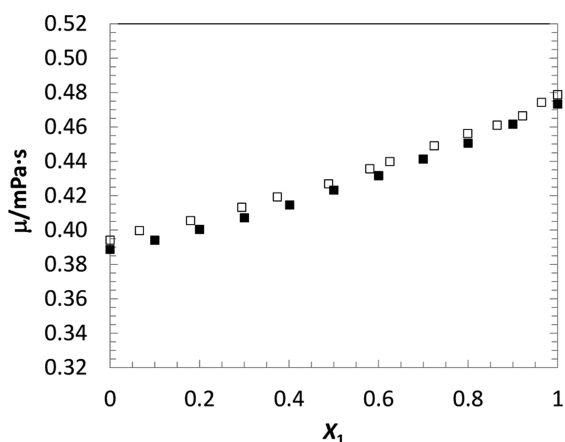$$\Delta\nu = X_1 X_2 \sum_{j=0}^{j-1} A_j(X_1 - X_2)^j \qquad (10)$$

Figure 4. Comparison of the viscosity of 2,2,4-trimethylpentane (X_1) and n-heptane mixtures at 298.15 K: ■, this study; □, ref 13.

Table 11. Values of the Coefficients for McAllister Equation (Equation 7) and Associated Standard Error (Equation 2) for Binary Mixtures of 2,2,4-Trimethylpentane and n-Heptane from T = (293 to 333) K

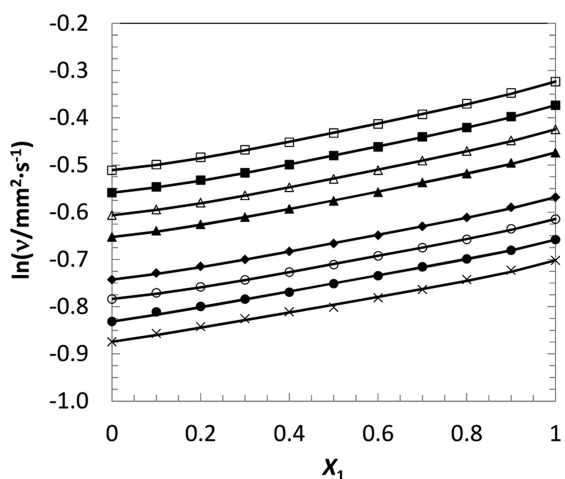| T/K	ν_{12}/mm$^2\cdot$s^{-1}	ν_{21}/mm$^2\cdot$s^{-1}	σ/10^4 mm$^2\cdot$s^{-1}
293.15	0.719	0.633	8.5
298.15	0.685	0.603	5.7
303.15	0.652	0.575	6.7
308.15	0.623	0.549	7.0
318.15	0.568	0.504	6.2
323.15	0.543	0.482	5.8
328.15	0.520	0.465	6.0
333.15	0.495	0.446	14.5

Figure 5. Viscosity of 2,2,4-trimethylpentane (X_1) + n-heptane mixtures at □, 293.15 K; ■, 298.15 K; △, 303.15 K; ▲, 308.15 K; ◆, 318.15 L; ○, 323.15 K; ●, 328.15 K; ×, 333.15 K. Error bars, which are the combined expanded uncertainties with 0.95 level of confidence ($k \approx 2$), are smaller than the symbols. Lines shown are fits using eq 7 with the coefficients in Table 11.

where A_j are adjustable parameters, j is the order of the polynomial, and X_1 and X_2 are the mole fraction of the 2,2,4-trimethylpentane and n-heptane, respectively. The standard error for the fit (σ) was determined by eq 2, where P_{measured} is the calculated viscosity deviation and P_{fit} is the fitted viscosity deviation. The fitted values of A_1, A_2, and A_3, and the standard
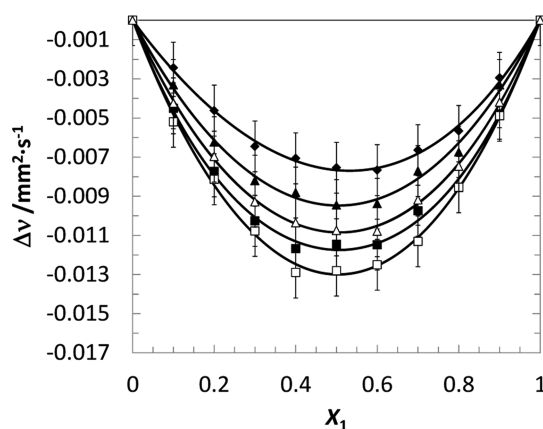

Figure 6. Viscosity deviation of 2,2,4-trimethylpentane (X_1) + n-heptane mixtures as calculated by eq 9 shown at selected temperatures: □, 293.15 K; ■, 298.15 K; △, 303.15 K; ▲, 308.15 K; ◆, 318.15 K. Lines shown are fits to eq 10 with the coefficients in Table 12. Data can be found in the Supporting Information.

Table 12. Parameters for Redlich–Kister Equation, Equation 10, for Excess Viscosity of Mixtures of 2,2,4-Trimethylpentane and n-Heptane and Associated Standard Error (Equation 2) at 0.1 MPa

T	$A_1\cdot10^2$	$A_2\cdot10^3$	$A_3\cdot10^3$	$\sigma\cdot10^4$
K	mm$^2\cdot$s^{-1}	mm$^2\cdot$s^{-1}	mm$^2\cdot$s^{-1}	mm$^2\cdot$s^{-1}
293.15	−5.2	−0.83	−3.3	2.8
298.15	−4.7	−0.98	−8.6	3.3
303.15	−4.3	−1.1	−4.9	1.7
308.15	−3.8	−0.72	−2.4	3.1
318.15	−3.1	−3.8	−1.7	2.1
323.15	−3.0	−2.0	−4.3	3.9
328.15[a]	−2.0	−7.2	−5.8	5.0

[a]Lowest mole fraction was not included because its value for excess viscosity does not differ from zero when including the error.

Table 13. Surface Tension of Mixtures of 2,2,4-Trimethylpentane (X_1) in n-Heptane[a]

X_1	surface tension (mN$\cdot$m^{-1})
0.0000	20.3(3) ± 0.16
0.1000	19.9(4) ± 0.14
0.2001	19.7(3) ± 0.20
0.2999	19.5(6) ± 0.23
0.4001	19.4(5) ± 0.13
0.5001	19.2(3) ± 0.22
0.6999	19.0(9) ± 0.27
0.8000	18.9(5) ± 0.16
1.00	18.7(2) ± 0.31

[a]X_1 is the mole fraction of 2,2,4-trimethylpentane in (2,2,4-trimethylpentane + n-heptane). Combined expanded uncertainties U_c are $U(x_1) = 0.0001$, and the values of U_c(surface tension) are given in the table (level of confidence = 0.95, $k \approx 2$). Surface tension measurements were taken at room temperature, 294.4 ± 1 K.

errors of the fits are given in Table 12 for each temperature. The model fits the data well as shown in Figure 6.

4.4. Surface Tension. The surface tension values are given in Table 13 for the mixtures studied herein as a function of the mole fraction of 2,2,4-trimethylpentane, X_1. A linear regression of surface tension versus temperature data found in the

literature[52−54] for 2,2,4-trimethylpentane yields the following relationship:

$$\text{surface tension } (mN \cdot m^{-1}) = -0.0893 \ T/K + 44.98 \quad (11)$$

that is shown in Figure 7. This equation predicts that the value of surface tension at 294.4 K should be 18.7 mN·m^{-2}, which
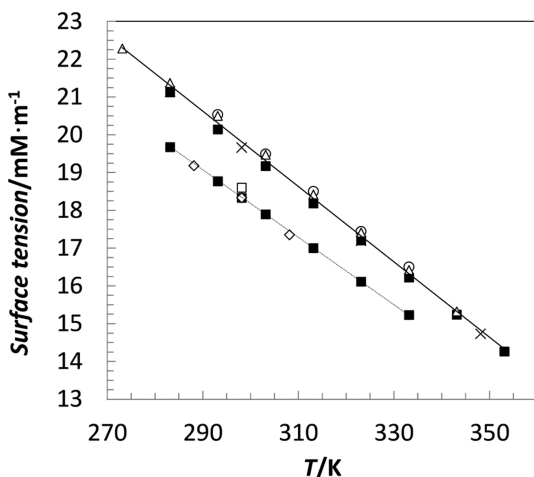

Figure 7. Surface tension data for *n*-heptane from ■, ref 53; △, ref 57; ○, ref 55; ✕, ref 56, and for 2,2,4-trimethylpentane: □, ref 52; ■, ref 53; ◇, ref 54. Lines shown are linear fits to data from these references.

agrees with the data reported herein of 18.7 ± 0.3 mN·m^{-2}. Similarly for *n*-heptane, a linear regression of surface tension versus temperature data found in the literature[53,55−57] yields

$$\text{surface tension } (mN \cdot m^{-1}) = -0.0997 \ T/K + 49.548 \quad (12)$$

that is also shown in Figure 7. This equation predicts that the value of surface tension at 294.4 K should be 20.2 mN·m^{-2}, which agrees with the data reported herein of 20.3 ± 0.2 mN·m^{-2}. As can be seen from the data in Table 13, the surface tension decreases as the mole fraction of the 2,2,4-trimethylpentane increases, but the trend is not linear. Similar nonlinear trends have been found for other mixtures of linear and branched alkanes.[16,17,19] Variation in the surface tension will affect the shape of droplets of the fuel formed in an engine and their combustion.

5. CONCLUSIONS

The physical properties of mixtures of the primary reference fuels of *n*-heptane and 2,2,4-trimethylpentane were measured. Most of the pure component measurements fell within values reported in the literature. The densities of the mixtures at each temperature were well modeled using a second-order polynomial function, and the viscosity values of the mixtures at each temperature were well modeled using the McAllister three-body model. A linear relationship was found between the speed of sound and mole fraction of 2,2,4-trimethylpentane. The surface tension values were not linearly related to mole fraction of the 2,2,4-trimethylpentane. These measurements may be useful for those who are modeling the transport and reaction of primary reference fuels.

■ ASSOCIATED CONTENT

⑤ Supporting Information

The values of the excess molar volume and viscosity deviation for the mixtures. This material is available free of charge via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

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