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U. Weidlich

HEATS OF MIXING DATA COLLECTION

Binary Systems

Chemistry Data Series

Vol. III, Part 1

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PREFACE OF AUTHORS

The heat which is absorbed or evolved during the mixing of liquids is called "heat of mixing" or "excess enthalpy". In this work we use the name "excess enthalpy", although the term "heats of mixing" appears in the title because it is more widely used in the engineering community.

The work consists of two parts. Part 1 deals with data for binary systems and Part 2 with data for binary and multicomponent systems.

This data compilation of molar excess enthalpies (h^E) for liquid mixtures is a natural continuation of the previous collections of data for low pressure vapor-liquid equilibria (VLE) and liquid-liquid equilibria (LLE) published as volumes I and V in DECHEMA Chemistry Data Series. The VLE data bank has been established at the University of Dortmund, FRG, while the LLE and h^E data banks are the results of a close collaboration between the universities in Dortmund and Lyngby, Denmark. We are most grateful to U. Onken (Dortmund) and Aa. Fredenslund (Lyngby) for their continued interest and help during the establishment of the h^E data bank.

The authors thank colleagues and students in Lyngby and Dortmund for many fruitful discussions and various kinds of assistance. Special thanks are dedicated to N. Hagemann who collected many data for us, to B. Hansen and L. Kunzner, who punched thousands of data cards, and to F. Vesely who most kindly allowed us to use his data collection. We acknowledge with thanks the financial support from the Danish National Council for Scientific and Technical Research (STVF) and from the DECHEMA and the Fachinformationszentrum Chemie, Berlin.

The h^E data collection contains almost all published data up to the end of 1981. It may be used as a convenient data source for the chemical engineer who needs information on heat effects due to mixing of liquids. Another important use is for the development of new liquid models. In order to test thoroughly such models for temperature dependency one needs data for h^E.

The authors hope that the data collection will be of use both in industry and at universities.

The authors

PREFACE OF EDITORS

The DECHEMA Chemistry Data Series is concerned with the physical and thermodynamic property data of chemical compounds and their mixtures in the fluid state, in particular PVT and phase equilibrium data, heat capacity, enthalpy and entropy data and transport and interfacial tension data.

Thermophysical property information is required by those engaged in process design and development. Computer based calculations demand accurate data and appropriate correlation methods which are often difficult to locate in the open literature. There is thus a pressing need for classified, critically evaluated and comprehensive experimental data, a need which this Series aims to meet.

DECHEMA gives authors, especially from universities, the opportunity to publish not only their theoretical results, but also their measured or compiled data, often a large amount, which would otherwise have never been published.

After a successful group contribution method for vapor-liquid equilibrium prediction (UNIFAC) had been presented to the scientific community several years ago, it was the need to develop a similar method for the prediction of excess enthalpies and the correct temperature dependence of fluid phase equilibria which gave the impetus to the present work. Co-operation between the University of Dortmund and the Instituttet for Kemiteknik in Lyngby, Denmark, led to the following compilation of excess enthalpy data which is now being published in two parts as Volume III of the DECHEMA Chemistry Data Series. The experimental data is reproduced together with correlation constants.

We hope this material will enable users to solve their problems considerably more easily and quickly than before.

Frankfurt/Main, August 1984

Dieter Behrens
Reiner Eckermann

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Vol. III, Part 2

(1) METHANE,DEUTERO TRICHLORO	CCL3D
(2) ACETIC ACID,NITRILE	C2H3N

HANDA Y.P.,JONES D.E.
CAN.J.CHEM. 55,2977(1977).

TEMPERATURE = 24.85 DEG C (298.00 K) 1

X(1)	HE(J/MOL)
0.113900	-200.40
0.271000	-507.70
0.390700	-697.00
0.482400	-810.90
0.559100	-868.50
0.656500	-865.30
0.759200	-745.50

(1) METHANE,DEUTERO TRICHLORO	CCL3D
(2) 2-PROPANONE,PERDEUTERO	C3D6O

HANDA Y.P.,FENBY D.V.
J.CHIM.PHYS.PHYS.-CHIM.BIOL. 72,1235(1975).

TEMPERATURE = 25.00 DEG C (298.15 K) 2

X(1)	HE(J/MOL)
0.178300	-823.00
0.323000	-1393.00
0.479000	-1772.00
0.598100	-1829.00
0.663100	-1750.00
0.799900	-1253.00
0.864900	-954.00

(1) 2-PROPANONE	C3H6O
(2) METHANE,DEUTERO TRICHLORO	CCL3D

HANDA Y.P.,FENBY D.V.
J.CHIM.PHYS.PHYS.-CHIM.BIOL. 72,1235(1975).

TEMPERATURE = 25.00 DEG C (298.15 K) 3

X(1)	HE(J/MOL)
0.144100	-1087.00
0.235100	-1600.00
0.305000	-1823.00
0.380400	-1929.00
0.514100	-1928.00
0.672400	-1493.00
0.830400	-844.00

CCl_3D

MORCOM K.W.,TRAVERS D.N.
TRANS.FARADAY SOC. 61,230(1965).

TEMPERATURE = 25.00 DEG C (298.15 K) 4

X(1)	HE(J/MOL)
0.307800	-1809.00
0.324100	-1884.00
0.364100	-1946.00
0.377300	-1984.00
0.403500	-1989.00
0.421600	-1991.00
0.462100	-2007.00
0.541200	-1918.00
0.555700	-1866.00
0.806100	-887.00

TEMPERATURE = 50.00 DEG C (323.15 K) 5

X(1)	HE(J/MOL)
0.329000	-1678.00
0.446300	-1782.00
0.498300	-1779.00
0.626300	-1644.00

(1) ETHER,DIETHYL	C4H10O
(2) METHANE,DEUTERO TRICHLORO	CCL3D

HANDA Y.P.,MATTINGLEY B.I.,FENBY D.V.
J.CHEM.SOC.FARADAY TRANS. I 72,1355(1976).

TEMPERATURE = 25.00 DEG C (298.15 K) 6

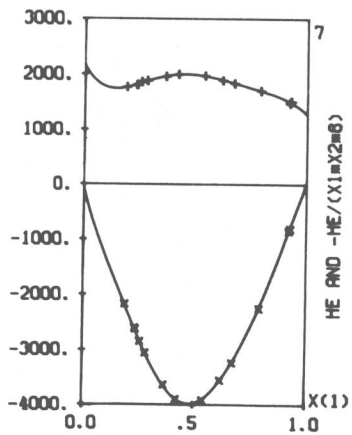
X(1)	HE(J/MOL)
0.121700	-990.00
0.275100	-2040.00
0.413000	-2560.00
0.516300	-2660.00
0.614400	-2480.00
0.770600	-1720.00
0.839600	-1270.00

(1) METHANE,DEUTERO TRICHLORO	CCL3D
(2) AMINE,TRIETHYL	C6H15N

HANDA Y.P.,MATTINGLEY B.I.,FENBY D.V.
J.CHEM.SOC.FARADAY TRANS. I 72,1355(1976).

TEMPERATURE = 25.00 DEG C (298.15 K) 7

X(1)	HE(J/MOL)
0.189100	-2170.00
0.235500	-2600.00
0.237400	-2620.00
0.257900	-2850.00
0.283500	-3060.00
0.366700	-3640.00
(CONT.) 0.422300	-3900.00



(CONT.) X(1)	HE(J/MOL)
0.541500	-3920.00
0.620700	-3560.00
0.673100	-3240.00
0.791900	-2250.00
0.922300	-850.00
0.927900	-810.00

R-K PARAMETERS (RMSD = 12.47 J/MOL)

A1 = -15924. A2 = 1614.9 A3 = 7711.8
A4 = -5749.6 A5 = -5601.2 A6 = 7752.6

(1) METHANE,TRICHLORO CHCL3

(2) METHANE,TETRACHLORO CCL4

CHEESMAN G.H.,WHITAKER A.M.B.
PROC.ROY.SOC.LONDON A212,406(1952).

TEMPERATURE = 24.70 DEG C (297.85 K) 8

X(1)	HE(J/MOL)	X(1)	HE(J/MOL)
0.293000	195.00	0.547000	230.00
0.296000	196.00	0.549000	228.00
0.300000	196.00	0.551000	228.00
0.322000	203.00	0.578000	228.00
0.324000	202.00	0.579000	228.00
0.327000	202.00	0.613000	223.00
0.332000	204.00	0.614000	222.00
0.434000	227.00	0.616000	221.00
0.438000	228.00	0.647000	213.00
0.441000	227.00	0.651000	213.00
0.468000	228.00	0.748000	170.00
0.470000	229.00	0.751000	171.00
0.471000	228.00	0.752000	170.00
0.495000	230.00	0.769000	158.00
0.510000	230.00	0.769000	157.00
0.513000	231.00	0.771000	158.00

HIROBE H.
J.FAC.SCI.,IMP.UNIV.TOKYO 1,155(1926).

TEMPERATURE = 25.00 DEG C (298.15 K) 9

X(1)	HE(J/MOL)
0.182200	146.54
0.270500	184.64
0.458900	226.51
0.566900	228.18
0.637700	219.39
0.757200	175.85
0.885000	103.41

(1) METHANE,DICHLORO	CH2CL2
(2) METHANE,TETRACHLORO	CCL4

CHEESMAN G.H.,WHITAKER A.M.B.
PROC.ROY.SOC.LONDON A212,406(1952).

TEMPERATURE = 24.70 DEG C (297.85 K) 10

X(1)	HE(J/MOL)	X(1)	HE(J/MOL)
0.252000	431.00	0.492000	590.00
0.257000	438.00	0.525000	591.00
0.277000	465.00	0.527000	591.00
0.344000	527.00	0.567000	581.00
0.344000	530.00	0.628000	556.00
0.350000	528.00	0.675000	523.00
0.376000	543.00	0.702000	500.00
0.376000	545.00	0.703000	503.00
0.491000	587.00	0.794000	403.00
0.491000	587.00	0.813000	375.00
0.491000	588.00	0.821000	372.00

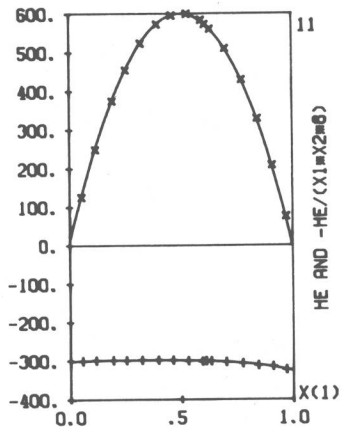
NAGATA I.,TAMURA K.,TOKURINI S.
FLUID PHASE EQUILIBRIA 8,75(1982).

TEMPERATURE = 25.00 DEG C (298.15 K) 11

X(1)	HE(J/MOL)	X(1)	HE(J/MOL)
0.055300	125.70	0.633400	560.00
0.117800	248.90	0.700500	509.70
0.194300	374.70	0.774400	429.40
0.254500	454.60	0.844200	328.80
0.323600	523.20	0.909200	208.00
0.397000	572.30	0.970100	75.10
0.462900	595.30		
0.530700	599.20		
0.594600	583.10		
0.610900	572.10		

R-K PARAMETERS (RMSD = 0.92 J/MOL)

A1 = 2399.3 A2 = 40.621 A3 = 68.477
A4 = 59.583 A5 = 47.422

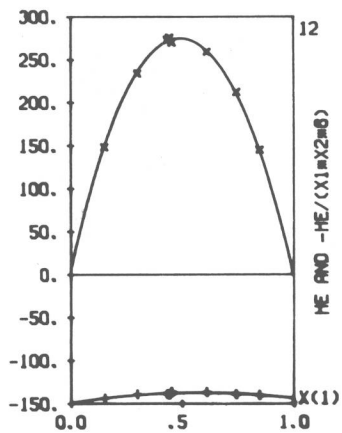


(1) METHANE,IODO	CH3I
(2) METHANE,TETRACHLORO	CCL4

MOELWYN-HUGHES E.A.,MISSEN R.W.
TRANS.FARADAY SOC. 53,607(1957).

TEMPERATURE = 25.00 DEG C (298.15 K) 12

X(1)	HE(J/MOL)
0.152000	148.21
0.301000	234.04
0.435000	272.98
0.445000	275.49
0.455000	270.05
0.612000	259.16
0.743000	212.27
(CONT.) 0.847000	144.86



R-K PARAMETERS (RMSD = 1.92 J/MOL)

A1 = 1099.2 A2 = -20.467 A3 = 71.876

(1) METHANE,TETRACHLORO	CCL4
(2) METHANE,NITRO	CH3NO2

BROWN I.,FOCK W.
AUST.J.CHEM. 9,180(1956).

TEMPERATURE = 45.00 DEG C (318.15 K) 13

X(1)	HE(J/MOL)
0.156000	773.00
0.313000	1204.00
0.403000	1346.00
0.405000	1376.00
0.417000	1377.00
0.564000	1407.00
0.629000	1367.00
0.789000	1095.00
0.819000	1017.00

R-K PARAMETERS (RMSD = 7.25 J/MOL)

A1 = 5702.2 A2 = 323.42 A3 = 289.22
A4 = 1300.8 A5 = 3018.6

(1) METHANOL	CH4O
(2) METHANE,TETRACHLORO	CCL4

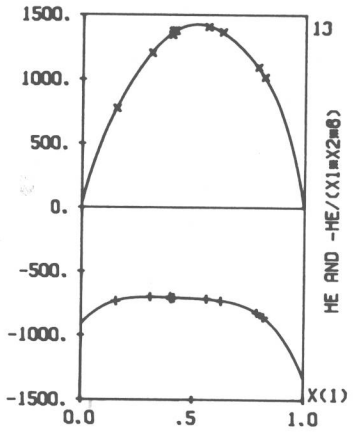
ABRAMOV E.V.,MIRZAYAIN A.S.,DEVINA O.A.
IZV.AKAD.NAUK.KAZ.SSR.,SER.KHIM. 23(3),29(1973).

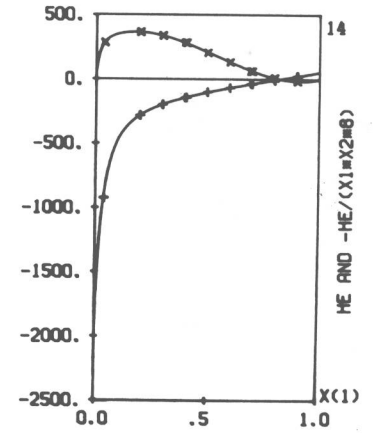
TEMPERATURE = 25.00 DEG C (298.15 K) 14

X(1)	HE(J/MOL)	X(1)	HE(J/MOL)
0.039000	278.00	0.693000	61.80
0.040000	283.00	0.700000	61.40
0.198000	361.00	0.799000	10.50
0.200000	363.00	0.800000	10.10
0.299000	336.00	0.900000	-17.10
0.300000	334.00	0.902000	-16.90
0.400000	281.00		
0.406000	278.00		
0.500000	202.00		
0.600000	131.00		

SSF PARAMETERS (RMSD = 2.20 J/MOL)

A1 = 806.53 A2 = 231.71 A3 = -900.27
A4 = 1249.7 A5 = 1657.0 A6 = 751.29





CCl_4

DACRE B.,BENSON G.C.
CAN.J.CHEM. 41,278(1963).

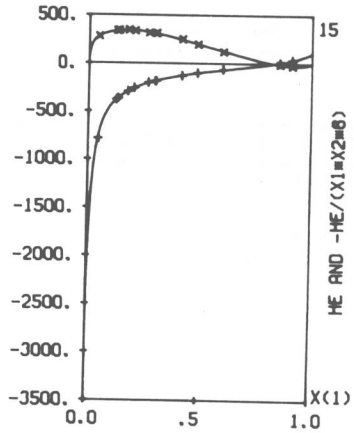
TEMPERATURE = 25.00 DEG C (298.15 K)

X(1)	HE(J/MOL)	X(1)	HE(J/MOL)
0.046500	279.07	0.603400	121.34
0.127400	337.23	0.857700	-9.20
0.134600	339.74	0.912700	-25.10
0.179600	344.76		
0.207200	336.81		
0.270500	315.89		
0.301000	310.87		
0.304000	312.96		
0.419500	250.20		
0.489200	198.32		

SSF PARAMETERS (RMSD = 3.65 J/MOL)

A1 = 602.76	A2 = 170.75	A3 = -294.56
A4 = 2075.2	A5 = 1217.3	A6 = 562.30

15



MOELWYN-HUGHES E.A.,MISSEN R.W.
J.PHYS.CHEM. 61,518(1957).

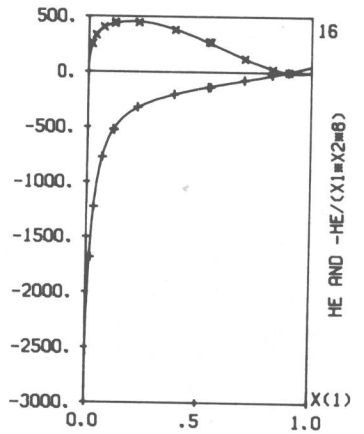
TEMPERATURE = 35.00 DEG C (308.15 K)

X(1)	HE(J/MOL)	X(1)	HE(J/MOL)
0.019000	251.21	0.827000	25.12
0.035000	330.76	0.900000	0.0
0.070000	401.93		
0.119000	435.43		
0.120000	443.80		
0.226000	443.80		
0.389000	381.00		
0.542000	272.14		
0.550000	267.96		
0.703000	121.42		

SSF PARAMETERS (RMSD = 5.19 J/MOL)

A1 = 955.04	A2 = 219.47	A3 = 1660.7
A4 = 705.74	A5 = -533.00	A6 = 1570.2

16



OTTERSTEDT J.-E.A.,MISSEN R.W.
TRANS.FARADAY SOC. 58,879(1962).

TEMPERATURE = 0.0 DEG C (273.15 K)

X(1)	HE(J/MOL)	X(1)	HE(J/MOL)
0.011000	100.48	0.475000	20.93
0.024000	125.60	0.634000	-79.55
0.051000	146.54	0.645000	-75.36
0.071000	159.10	0.734000	-104.67
0.109000	163.29	0.735000	-108.86
0.125000	159.10	0.861000	-96.30
0.165000	154.91	0.930000	-66.99
0.260000	117.23	0.934000	-62.80
0.273000	117.23		
0.470000	8.37		

SSF PARAMETERS (RMSD = 5.61 J/MOL)

A1 = 305.99	A2 = 126.97	A3 = -654.28
A4 = 1500.0	A5 = 753.70	A6 = 509.10

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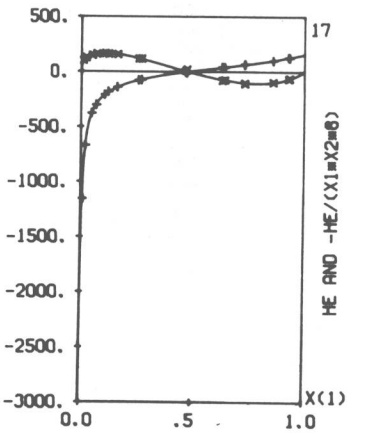


TEMPERATURE = 20.00 DEG C (293.15 K) 18

X(1)	HE(J/MOL)	X(1)	HE(J/MOL)
0.026000	221.90	0.730000	12.56
0.038000	234.46	0.859000	-37.68
0.073000	280.52	0.930000	-37.68
0.094000	297.26	0.931000	-33.49
0.118000	314.01		
0.144000	314.01		
0.169000	314.01		
0.279000	284.70		
0.463000	175.85		
0.638000	66.99		

TEMPERATURE = 35.00 DEG. C (308.15 K) 19

X(1)	HE(J/MOL)	X(1)	HE(J/MOL)
0.050000	376.81	0.728000	117.23
0.087000	427.05	0.729000	117.23
0.168000	456.36	0.865000	25.12
0.268000	460.55		
0.274000	447.99		
0.287000	460.55		
0.474000	314.01		
0.478000	322.38		
0.641000	180.03		
0.642000	192.59		

TEMPERATURE = 50.00 DEG C (323.15 K) 20

X(1)	HE(J/MOL)	X(1)	HE(J/MOL)
0.022000	301.45	0.258000	665.70
0.035000	376.81	0.468000	556.84
0.052000	477.30	0.468000	531.72
0.053000	468.92	0.631000	389.37
0.075000	548.47	0.632000	368.44
0.096000	586.15	0.637000	368.44
0.120000	623.83	0.732000	226.09
0.121000	628.02	0.736000	230.27
0.137000	628.02	0.739000	234.46
0.140000	648.95	0.867000	87.92
0.149000	669.89	0.870000	100.48
0.155000	648.95	0.943000	29.31
0.254000	695.01		

SSF PARAMETERS (RMSD = 11.59 J/MOL)

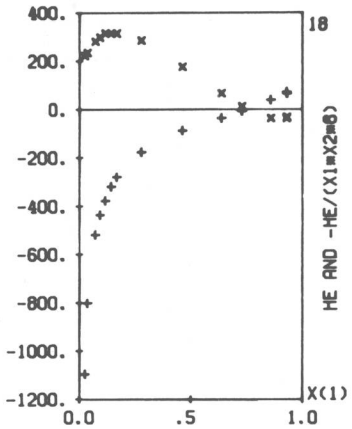
A1 = 857.82	A2 = 231.09	A3 = 2411.5
A4 = 634.49	A5 = -177.18	A6 = 2130.4

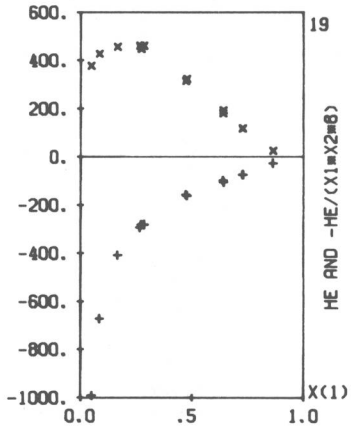
(1) CARBON DISULFIDE	CS2
(2) METHANE,TETRACHLORO	CCL4

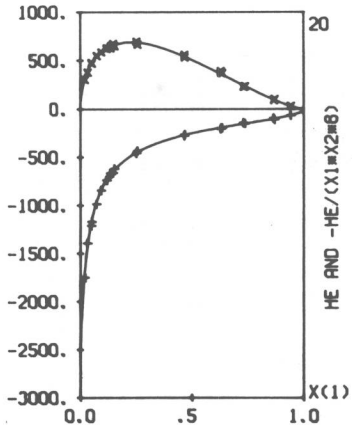
HARSTED B.S.,THOMSEN E.S.
J.CHEM.THERMODYN. 7,369(1975).

TEMPERATURE = 20.00 DEG C (293.15 K) 21

X(1)	HE(J/MOL)
0.069000	74.80
0.092200	96.80
(CONT.) 0.402600	295.60







CCl_4

(CONT.) X(1)	HE(J/MOL)
0.623900	306.60
0.803700	222.10

HIROBE H.
J.FAC.SCI.,IMP.UNIV.TOKYO 1,155(1926).

TEMPERATURE = 25.00 DEG C (298.15 K) 22

X(1)	HE(J/MOL)
0.184700	179.20
0.330730	263.77
0.460690	311.50
0.599930	306.89
0.716230	276.33
0.857500	180.03
0.906600	127.28

(1) METHANE,TETRACHLORO CCL4
(2) ETHENE,TETRACHLORO C2CL4

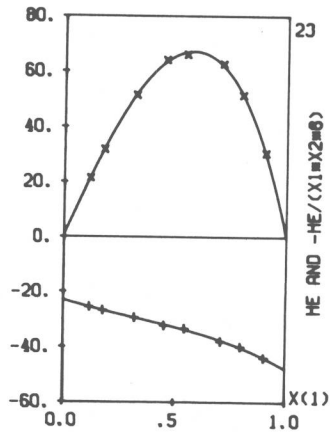
POON D.P.L.,LU B.C.Y.
J.CHEM.ENG.DATA 13,435(1968).

TEMPERATURE = 25.00 DEG C (298.15 K) 23

X(1)	HE(J/MOL)
0.118100	21.35
0.180300	31.69
0.322600	51.33
0.455600	64.06
0.547400	66.07
0.709100	62.63
0.798700	51.33
0.904000	30.48

R-K PARAMETERS (RMSD = 0.47 J/MOL)

A1 = 262.26 A2 = 79.670 A3 = 20.825
A4 = 19.806

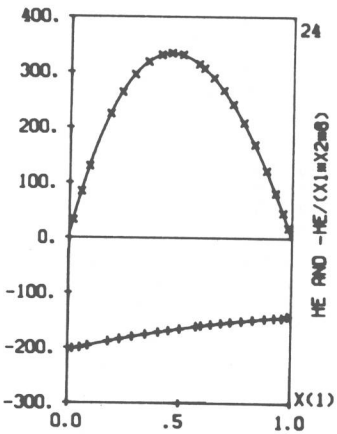


(1) ETHENE,1,2-DICHLORO (CIS) C2H2CL2
(2) METHANE,TETRACHLORO CCL4

TANAKA R.,MURAKAMI S.,FUJISHIRO R.
J.CHEM.THERMODYN. 5,777(1973).

TEMPERATURE = 25.00 DEG C (298.15 K) 24

X(1)	HE(J/MOL)
0.020500	32.30
0.055900	84.10
0.091000	129.60
0.182200	224.20
0.234200	263.40
0.289700	295.10
(CONT.) 0.348900	318.10



(CONT.) X(1)	HE(J/MOL)	X(1)	HE(J/MOL)
0.407000	330.60	0.882100	121.70
0.451800	333.80	0.924300	81.10
0.501900	330.90	0.959300	45.30
0.574500	314.20	0.983600	18.30
0.597900	306.40		
0.641000	289.10		
0.685900	266.80		
0.728900	241.60		
0.778400	208.20		
0.828600	168.90		

R-K PARAMETERS (RMSD = 0.31 J/MOL)

A1 = 1321.9 A2 = -244.92 A3 = 62.720

(1) ETHENE,1,2-DICHLORO (TRANS) C2H2CL2

(2) METHANE,TETRACHLORO CCL4

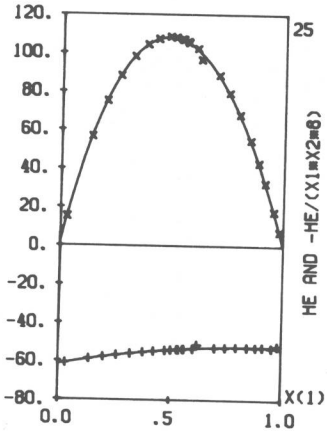
TANAKA R.,MURAKAMI S.,FUJISHIRO R.
J.CHEM.THERMODYN. 5,777(1973).

TEMPERATURE = 25.00 DEG C (298.15 K) 25

X(1)	HE(J/MOL)	X(1)	HE(J/MOL)
0.031700	15.00	0.562700	105.50
0.139500	56.50	0.603300	102.40
0.204000	75.10	0.621500	96.60
0.263400	88.20	0.701700	88.60
0.324300	98.20	0.749300	79.30
0.381600	104.40	0.797000	68.00
0.428700	107.30	0.846700	54.60
0.480000	108.50	0.884900	42.90
0.505600	108.10	0.915200	32.60
0.533400	107.20	0.956000	17.80
0.539000	107.10	0.982100	7.30
0.559600	106.00		

R-K PARAMETERS (RMSD = 0.73 J/MOL)

A1 = 432.20 A2 = -36.211 A3 = 25.166



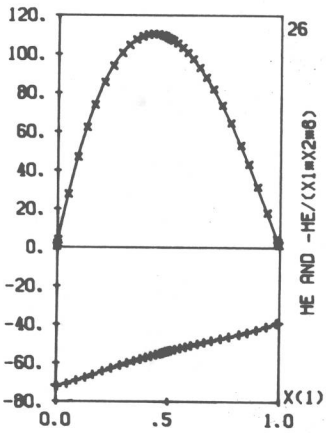
(1) ETHANE,1,1,1-TRICHLORO C2H3CL3

(2) METHANE,TETRACHLORO CCL4

VAN MILTENBURG J.C.,OBBINK J.H.,MEIJER E.L
J.CHEM.THERMODYN. 11,37(1979).

TEMPERATURE = 25.00 DEG C (298.15 K) 26

(CONT.) X(1)	HE(J/MOL)
0.000820	0.47
0.003420	1.96
0.006660	3.82
0.051320	27.61
0.093480	46.83
0.132480	62.15
0.167480	73.73



(CONT.) X(1')	HE(J/MOL)	X(1)	HE(J/MOL)
0.210440	85.38	0.557250	103.30
0.249190	93.85	0.579900	100.70
0.288520	100.55	0.604640	97.48
0.320970	104.64	0.634460	92.98
0.351270	107.46	0.663770	88.00
0.378830	109.17	0.696300	81.97
0.403740	110.05	0.736420	73.59
0.426350	110.41	0.775730	64.51
0.448890	110.23	0.821180	53.01
0.468380	109.74	0.856960	43.28
0.479590	109.31	0.897410	31.51
0.491270	108.39	0.941940	17.99
0.503400	107.71	0.985910	4.37
0.514610	107.03	0.990730	2.87
0.534130	105.51	0.995340	1.45

R-K PARAMETERS (RMSD = 0.13 J/MOL)

A1 = 431.88 A2 = -121.18 A3 = 38.216
A4 = -20.866 A5 = -26.518 A6 = 8.8315

(1) METHANE,TETRACHLORO CCL4

(2) ACETIC ACID,NITRILE C2H3N

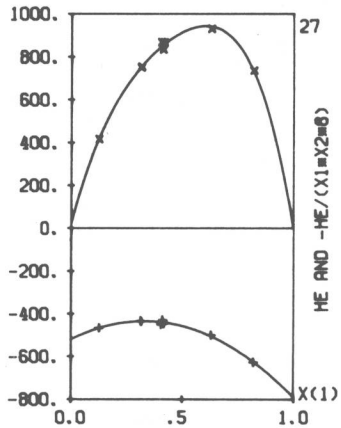
BROWN I.,FOCK W.
AUST.J.CHEM. 9,180(1956).

TEMPERATURE = 45.00 DEG C (318.15 K) 27

X(1)	HE(J/MOL)
0.128000	416.00
0.317000	750.00
0.318000	755.00
0.407000	868.00
0.415000	834.00
0.419000	867.00
0.631000	930.00
0.821000	737.00

R-K PARAMETERS (RMSD = 11.61 J/MOL)

A1 = 3653.6 A2 = 1070.2 A3 = 1589.6



LIEN T.R.,MISSEN R.W.
J.CHEM.ENG.DATA 19,84(1974).

TEMPERATURE = 45.00 DEG C (318.15 K) 28

(CONT.) X(1)	HE(J/MOL)	X(1)	HE(J/MOL)
0.155000	468.92	0.736000	820.61
0.165000	527.54	0.745000	820.61
0.303000	736.88	0.748000	808.05
0.550000	921.10	0.754000	799.68
0.554000	942.03	0.759000	812.24
0.601000	900.16	0.782000	766.18
0.615000	916.91	0.864000	586.15
0.620000	895.98		
0.639000	887.60		
0.647000	891.79