EXPRESIONES PARA LA ENERGÍA GIBBS DE EXCESO

ECUACIÓN SIMÉTRICA

Mezcla binaria: $g^E/RT = Ax_1x_2$

SCATCHARD-HILDEBRAND

Mezcla binaria: $g^E = \frac{x_1v_1x_2v_2}{x_1v_1 + x_2v_2}(\delta_1 - \delta_2)^2$

MARGULES

Mezcla binaria: $g^E/RT = x_1x_2(A_{21}x_1 + A_{12}x_2)$

VAN LAAR

Mezcla binaria: $g^E/RT = 1/[(1/A_{12}x_1) + (1/A_{21}x_2)]$

WILSON

Mezcla binaria: $g^E/RT = -x_1\ln(x_1 + \Lambda_{12}x_2) - x_2\ln(\Lambda_{21}x_1 + x_2)$

Mezcla multicomponente $g^E/RT = -\sum_i x_i \ln\left(\sum_j x_j\Lambda_{ij}\right)$

NRTL

Mezcla binaria: $g^E/RT = x_1x_2\left[\frac{\tau_{21}G_{21}}{x_1 + G_{21}x_2} + \frac{\tau_{12}G_{12}}{G_{12}x_1 + x_2}\right]$

Mezcla multicomponente $g^E/RT = \sum_i x_i\left[\frac{\sum_j \tau_{ji}G_{ji}x_j}{\sum_k G_{ki}x_k}\right]$

UNIQUAC

Mezcla binaria:

$$g^E/RT = x_1\left[\ln\frac{\phi_1}{x_1} + \frac{z}{2}q_1\ln\frac{\theta_1}{\phi_1} - q_1\ln(\theta_1 + \theta_2\tau_{21})\right] + x_2\left[\ln\frac{\phi_2}{x_2} + \frac{z}{2}q_2\ln\frac{\theta_2}{\phi_2} - q_2\ln(\theta_1\tau_{12} + \theta_2)\right]$$

Mezcla multicomponente:

$$g^E/RT = \sum_i x_i\ln\frac{\phi_i}{x_i} + \frac{z}{2}\sum_i q_i x_i\ln\frac{\theta_i}{\phi_i} - \sum_i q_i x_i\ln\left(\sum_j \theta_j\tau_{ji}\right)$$

COEFICIENTES DE ACTIVIDAD DE MEZCLAS BINARIAS

ECUACIÓN SIMÉTRICA

Parámetro: A

$$\boxed{\begin{aligned}\ln\gamma_1 &= Ax_2^2\\ \ln\gamma_2 &= Ax_1^2\end{aligned}}$$

SCATCHARD-HILDEBRAND

Parámetros: $\delta_1,\ \delta_2,\ \phi_i = \dfrac{v_i^L x_i}{\sum v_i^L x_j}$

$$\boxed{\begin{aligned}RT\ln\gamma_1 &= v_1^L\phi_2^2(\delta_1-\delta_2)^2\\ RT\ln\gamma_2 &= v_2^L\phi_1^2(\delta_1-\delta_2)^2\end{aligned}}$$

MARGULES

Parámetros: $A_{12},\ A_{21}$

$$\boxed{\begin{aligned}\ln\gamma_1 &= [A_{12}+2(A_{21}-A_{12})x_1]x_2^2\\ \ln\gamma_2 &= [A_{21}+2(A_{12}-A_{21})x_2]x_1^2\end{aligned}}$$

VAN LAAR

Parámetros: $A_{12},\ A_{21}$

$$\boxed{\begin{aligned}\ln\gamma_1 &= A_{12}\left(\frac{x_2A_{21}}{x_1A_{12}+x_2A_{21}}\right)^2\\ \ln\gamma_2 &= A_{21}\left(\frac{x_1A_{12}}{x_1A_{12}+x_2A_{21}}\right)^2\end{aligned}} \Rightarrow \boxed{\begin{aligned}A_{12} &= \ln\gamma_1\left(1+\frac{x_2\ln\gamma_2}{x_1\ln\gamma_1}\right)^2\\ A_{21} &= \ln\gamma_2\left(1+\frac{x_1\ln\gamma_1}{x_2\ln\gamma_2}\right)^2\end{aligned}}$$

WILSON

Parámetros: $\Lambda_{12} = \dfrac{v_2^L}{v_1^L}\exp\left(-\dfrac{\lambda_{12}-\lambda_{22}}{RT}\right),\quad \Lambda_{21} = \dfrac{v_1^L}{v_2^L}\exp\left(-\dfrac{\lambda_{21}-\lambda_{11}}{RT}\right)$

$$\boxed{\begin{aligned}\ln\gamma_1 &= -\ln(x_1+\Lambda_{12}x_2)+x_2\left(\frac{\Lambda_{12}}{x_1+\Lambda_{12}x_2}-\frac{\Lambda_{21}}{\Lambda_{21}x_1+x_2}\right)\\ \ln\gamma_2 &= -\ln(\Lambda_{21}x_1+x_2)-x_1\left(\frac{\Lambda_{12}}{x_1+\Lambda_{12}x_2}-\frac{\Lambda_{21}}{\Lambda_{21}x_1+x_2}\right)\end{aligned}}$$

NRTL

Parámetros: α_{12}

$\tau_{12} = (g_{12}-g_{22})/RT \qquad G_{12} = \exp(-\alpha_{12}\tau_{12})$

$\tau_{21} = (g_{21}-g_{11})/RT \qquad G_{21} = \exp(-\alpha_{12}\tau_{21})$

$$\boxed{\begin{aligned}\ln\gamma_1 &= x_2^2\left[\tau_{21}\left(\frac{G_{21}}{x_1+x_2G_{21}}\right)^2+\left(\frac{\tau_{12}G_{12}}{(x_1G_{12}+x_2)^2}\right)\right]\\ \ln\gamma_2 &= x_1^2\left[\tau_{12}\left(\frac{G_{12}}{\quad}\right)^2+\left(\frac{\tau_{21}G_{21}}{\quad}\right)\right]\end{aligned}}$$

UNIQUAC

Parámetros:

$$\theta_i = \frac{q_i x_i}{\sum_j q_j x_j} \qquad \phi_i = \frac{r_i x_i}{\sum_j r_j x_j} \qquad l_i = \frac{z}{2}(r_i - q_i) - (r_i - 1)$$

$$\tau_{12} = \exp\left(-\frac{u_{12} - u_{22}}{RT}\right) = \exp\left(-\frac{a_{12}}{T}\right)$$

$$\tau_{21} = \exp\left(-\frac{u_{21} - u_{11}}{RT}\right) = \exp\left(-\frac{a_{21}}{T}\right)$$

$$\ln\gamma_1 = \ln\frac{\phi_1}{x_1} + \frac{z}{2}q_1\ln\frac{\theta_1}{\phi_1} + \phi_2\left(l_1 - \frac{r_1}{r_2}l_2\right) - q_1\ln(\theta_1 + \theta_2\tau_{21}) + \theta_2 q_1\left(\frac{\tau_{21}}{\theta_1 + \theta_2\tau_{21}} - \frac{\tau_{12}}{\theta_1\tau_{12} + \theta_2}\right)$$

$$\ln\gamma_2 = \ln\frac{\phi_2}{x_2} + \frac{z}{2}q_2\ln\frac{\theta_2}{\phi_2} + \phi_1\left(l_2 - \frac{r_2}{r_1}l_1\right) - q_2\ln(\theta_1\tau_{12} + \theta_2) + \theta_1 q_2\left(\frac{\tau_{12}}{\theta_1\tau_{12} + \theta_2} - \frac{\tau_{21}}{\theta_1 + \theta_2\tau_{21}}\right)$$

COEFICIENTES DE ACTIVIDAD A DILUCIÓN INFINITA EN MEZCLAS BINARIAS

VAN LAAR Y MARGULES

$$A_{12} = \ln\gamma_1^\infty$$
$$A_{21} = \ln\gamma_2^\infty$$

WILSON

$$\ln\Lambda_{12} + \Lambda_{21} = 1 - \ln\gamma_1^\infty = k_1$$
$$\Lambda_{12} + \ln\Lambda_{21} = 1 - \ln\gamma_2^\infty = k_2$$

$$\Lambda_{12} = \exp[k_1 - \exp(k_2 - \Lambda_{12})]$$
$$\Lambda_{21} = \exp(k_2 - \Lambda_{12})$$

NRTL

$$\tau_{12}\exp(-\alpha_{12}\tau_{12}) + \tau_{21} = \ln\gamma_1^\infty = k_3$$
$$\tau_{12} + \tau_{21}\exp(-\alpha_{12}\tau_{21}) = \ln\gamma_2^\infty = k_4$$

$$\tau_{21} = k_3 - \tau_{12}\exp(-\alpha_{12}\tau_{12})$$
$$\tau_{12} = k_4 - \tau_{21}\exp(-\alpha_{12}\tau_{21})$$

UNIQUAC

$$k_5 = \frac{1}{q_1}\left[\ln\frac{r_1}{r_2} - \ln\gamma_1^\infty + 5q_1\ln\frac{q_1 r_2}{q_2 r_1} - \frac{r_1 l_2}{r_2} + q_1 + l_1\right]$$

$$k_6 = \frac{1}{q_2}\left[\ln\frac{r_2}{r_1} - \ln\gamma_2^\infty + 5q_2\ln\frac{q_2 r_1}{q_1 r_2} - \frac{r_2 l_1}{r_1} + q_2 + l_2\right]$$

$$\tau_{12} = \exp[k_6 - \exp(k_5 - \tau_{12})]$$
$$\tau_{21} = \exp(k_5 - \tau_{12})$$

COEFICIENTES DE ACTIVIDAD: MEZCLAS MULTICOMPONENTES

SCATCHARD-HILDEBRAND: $$RT\ln\gamma_i = v_i^L\left(\delta_i - \sum_i \phi_i\delta_i\right)$$

WILSON: $$\ln\gamma_i = 1 - \ln\left(\sum_{j=1}^{c} x_j\Lambda_{ij}\right) - \sum_{k=1}^{c}\frac{x_k\Lambda_{ki}}{\sum_{j=1}^{c} x_j\Lambda_{kj}}$$

NRTL: $$\ln\gamma_i = \frac{\sum_{j=1}^{c}\tau_{ji}G_{ji}x_j}{\sum_{k=1}^{c}G_{ki}x_k} + \sum_{j=1}^{c}\frac{x_jG_{ij}}{\sum_{k=1}^{c}G_{kj}x_k}\left(\tau_{ij} - \frac{\sum_{n=1}^{c}\tau_{nj}G_{nj}x_n}{\sum_{k=1}^{c}G_{kj}x_k}\right)$$

UNIQUAC: $$\ln\gamma_i = \ln\frac{\phi_i}{x_i} + \frac{z}{2}q_i\ln\frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i}\sum_{j=1}^{c}x_jl_j + q_i\left[1 - \ln\left(\sum_{j=1}^{c}\theta_j\tau_{ji}\right) - \sum_{j=1}^{c}\frac{\theta_j\tau_{ij}}{\sum_{k=1}^{c}\theta_k\tau_{kj}}\right]$$

COEFICIENTES DE ACTIVIDAD: CONTRIB. GRUPOS (UNIFAC)

$$\ln\gamma_i = \ln\frac{\phi_i}{x_i} + \frac{z}{2}q_i\ln\frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i}\sum_{j=1}^{c}x_jl_j + \sum_{k=1}^{s}v_k^{(i)}\left[\ln\Gamma_k - \ln\Gamma_k^{(i)}\right]$$

$$\theta_i = \frac{q_ix_i}{\sum_{j=1}^{c}q_jx_j} \qquad r_i = \sum_{k=1}^{s}v_k^{(i)}R_k$$

$$q_i = \sum_{k=1}^{s}v_k^{(i)}Q_k$$

$$\phi_i = \frac{r_ix_i}{\sum_{j=1}^{c}r_jx_j} \qquad l_i = \frac{z}{2}(r_i - q_i) - (r_i - 1)$$

$$\ln\Gamma_k = Q_k\left[1 - \ln\left(\sum_{m=1}^{s}\Theta_m\Psi_{mk}\right) - \sum_{m=1}^{s}\frac{\Theta_m\Psi_{km}}{\sum_{n=1}^{s}\Theta_n\Psi_{nm}}\right]$$

$$\Theta_m = \frac{Q_mX_m}{\sum_{n}^{s}Q_nX_n}$$

PARÁMETROS ESTRUCTURALES DEL MODELO UNIFAC

Grupo	Subgrupo	Nº	R_k	Q_k	Ejemplo	
1	CH_3	1	0.9011	0.848	Hexano	2 CH_3, 4 CH_2
"CH_2"	CH_2	2	0.6744	0.540		
	CH	3	0.4469	0.228	2-Metilpropano	3 CH_3, 1 CH
	C	4	0.2195	0.000	Neopentano	4 CH_3, 1 C
2	CH_2=CH	5	1.3454	1.176	1-Hexeno	1 CH_3, 3 CH_2, 1 CH_2=CH
"C=C"	CH=CH	6	1.1167	0.867	2-Hexeno	2 CH_3, 2 CH_2, 1 CH=CH
	CH_2=C	7	1.1173	0.988	2-Metil-1-buteno	2 CH_3, 1 CH_2, 1 CH_2=C
	CH=C	8	0.8886	0.676	2-Metil-2-buteno	2 CH_3, 1 CH=C
	C=C	9	0.6605	0.485	2,3-Dimetilbuteno	4 CH_3, 1 C=C
3	ACH	10	0.5313	0.400	Naftaleno	8 ACH, 2 AC
"ACH"	AC	11	0.3652	0.120	Estireno	1 CH_2=CH, 5 ACH, 1 AC
4	$ACCH_3$	12	1.2663	0.968	Tolueno	5 ACH, 1 $ACCH_3$
"$ACCH_2$"	$ACCH_2$	13	1.0396	0.660	Etilbenceno	1 CH_3, 5 ACH, 1 $ACCH_2$
	ACCH	14	0.8121	0.348	Cumeno	2 CH_3, 5 ACH, 1 ACCH
5 "OH"	OH	15	1.0000	1.200	2-Propanol	2 CH_3, 1 CH, 1 OH
6 "CH_3OH"	CH_3OH	16	1.4311	1.432	Metanol	1 CH_3OH
7 "H_2O"	H_2O	17	0.9200	1.400	Agua	1 H_2O
8 "ACOH"	ACOH	18	0.8952	0.680	Fenol	5 ACH, 1 ACOH
9	CH_3CO	19	1.6724	1.488	2-Butanona	1 CH_3, 1 CH_2, 1 CH_3CO
"CH_2CO"	CH_2CO	20	1.4457	1.180	3-Pentanona	2 CH_3, 1 CH_2, 1 CH_2CO
10 "CHO"	CHO	21	0.9980	0.948	Acetaldehído	1 CH_3, 1 CH_2, 1 CHO
11	CH_3COO	22	1.9031	1.728	Acetato de butilo	1 CH_3, 3 CH_2, 1
"CCOO"	CH_2COO	23	1.6764	1.420	Propionato de metilo	CH_3COO
						2 CH_3, 1 CH_2COO
12 "HCOO"	HCOO	24	1.2420	1.188	Formiato de etilo	1 CH_3, 1 CH_2, 1 HCOO
13	CH_3O	25	1.1450	1.088	Dimetiléter	1 CH_3, 1 CH_3CO
"CH_2O"	CH_2O	26	0.9183	0.780	Dietiléter	2 CH_3, 1 CH_2, 1 CH_2O
	CHO	27	0.6908	0.468	Diisopropiléter	4 CH_3, 1 CH, 1 CHO
	THF	28	0.9183	1.100	Tetrahidrofurano	3 CH_2, 1 THF
14	CH_3NH_2	29	1.5959	1.544	Metilamina	1 CH_3NH_2
"CNH_2"	CH_2NH_2	30	1.3692	1.236	Etilamina	1 CH_3, 1 CH_2NH_2
	$CHNH_2$	31	1.1417	0.924	Isopropilamina	2 CH_3, 1 $CHNH_2$
15	CH_3NH	32	1.4337	1.244	Dimetilamina	1 CH_3, 1 CH_3NH
"CNH"	CH_2NH	33	1.2070	0.936	Dietilamina	2 CH_3, 1 CH_2, 1 CH_2NH
	CHNH	34	0.9795	0.624	Diisopropilamina	4 CH_2, 1 CH, 1 CHNH
16	CH_3N	35	1.1865	0.940	Trimetilamina	2 CH_3, 1 CH_3N
"$(C)_3N$"	CH_2N	36	0.9597	0.632	Trietilamina	3 CH_3, 2 CH_2, 1 CH_2N
17 "$ACNH_2$"	$ACNH_2$	37	1.0600	0.816	Anilina	5 ACH, 1 $ACNH_2$
18	C_5H_5N	38	2.9993	2.113	Piridina	1 C_5H_5N
"Piridina"	C_5H_4N	39	2.8332	1.833	2-Metilpiridina	1 CH_3, 1 C_5H_4N
	C_5H_3N	40	2.6670	1.553	2,3-Dimetilpiridina	2 CH_3, 1 C_5H_3N
19	CH_3CN	41	1.8701	1.724	Acetonitrilo	1 CH_3CN
"CCN"	CH_2CN	42	1.6434	1.416	Propionitrilo	1 CH_3, 1 CH_2CN
20	COOH	43	1.3013	1.224	Ácido acético	1 CH_3, 1 COOH
"COOH"	HCOOH	44	1.5280	1.532	Ácido fórmico	1 HCOOH
21	CH_2Cl	45	1.4654	1.264	1-Clorobutano	1 CH_3, 2 CH_2, 1 CH_2Cl
"CCl"	CHCl	46	1.2380	0.952	2-Cloropropano	2 CH_3, 1 CHCl
	CCl	47	1.0106	0.724	2-Cloro-2-metilpropano	3 CH_3, 1 CCl
22	CH_2Cl_2	48	2.2564	1.998	Diclorometano	1 CH_2Cl_2
"CCl_2"	$CHCl_2$	49	2.0606	1.684	1,1-Dicloroetano	1 CH_3, 1 $CHCl_2$
	CCl_2	50	1.8016	1.448	2,2-Dicloropropano	2 CH_3, 1 CCl_2
23	$CHCl_3$	51	2.8700	2.410	Cloroformo	1 $CHCl_3$
"CCl_3"	CCl_3	52	2.6401	2.184	1,1,1-Tricloroetano	1 CH_3, 1 CCl_3
24 "CCl_4"	CCl_4	53	3.3900	2.910	Tetraclorometano	1 CCl_4
25 "ACCl"	ACCl	54	1.1562	0.844	Clorobenceno	5 ACH, 1 ACCl
26	CH_3NO_2	55	2.0086	1.868	Nitrometano	1 CH_3NO_2

Grupo	Subgrupo	Nº	R_k	Q_k	Ejemplo	
30 “Furfural”	Furfural	62	3.1680	2.484	Furfural	1 Furfural
31 “DOH”	DOH	63	2.4088	2.248	1,2-Etanodiol	1 DOH
32 “I”	I	64	1.2640	0.992	1-Iodoetano	1 CH_3, 1 CH_2, 1 I
33 “Br”	Br	65	0.9492	0.832	Bromoetano	1 CH_3, 1 CH_2, 1 Br
34	CH≡C	66	1.2920	1.088	1-Hexino	1 CH_3, 3 CH_2, 1 CH≡C
“C ≡ C”	C≡C	67	1.0613	0.784	2-Hexino	2 CH_3, 2 CH_2, 1 C≡C
35 “DMSO”	DMSO	68	2.8266	2.472	Dimetilsulfóxido	1 DMSO
36 “ACRY”	ACRY	69	2.3144	2.052	Acrilonitrilo	1 ACRY
37 “ClCC”	Cl-(C=C)	70	0.7910	0.724	Tricloroetileno	1 CH=C, 3 Cl-(C=C)
38 “ACF”	ACF	71	0.6948	0.524	Hexafluorobenceno	6 ACF
39	DMF	72	3.0856	2.736	N,N-Dimetilformamida	1 DMF
“DMF”	$HCON(CH_2)_2$	73	2.6322	2.120	N,N,-Dietilformamida	2 CH_3, 1 $HCON(CH_2)_2$
40	CF_3	74	1.4060	1.380	Perfluorohexano	2 CF_3, 4 CF_2
“CF_2”	CF_2	75	1.0105	0..920		
	CF	76	0.6150	0.460	Perfluorometilciclohenano	1 CF_3, 5 CF_2, 1 CF
41 “COO”	COO	77	1.3800	1.200	Acrilato de metilo	1 CH_3, 3 CH_2=CH, 1 COO
42	SiH_3	78	1.6035	1.263	Metilsilano	1 CH_3, 1SiH_3
“SiH_2”	SiH_2	79	1.4443	1.006	Dietilsilano	2 CH_3, 2 CH_2, 1 SiH_2
	SiH	80	12853	0.749	Heptametiltrisiloxano	7 CH_3, 2 SiO, 1 SiH
	Si	81	1.0470	0.410	Heptametildisiloxano	6 CH_3, 1 SiO, 1 Si
43	SiH_2O	82	1.4838	1.062	1,3-Dimetildisiloxano	3 CH_3, 1 SiH_2O, 1 SiH_2
“SiO”	SiHO	83	1.3030	0.764	1,1,3,3-Tetrametildisiloxano	4 CH_3, 1SiHO, 1 SiH
	SiO	84	1.1044	0.466	Octametilciclotetrasiloxano	8 CH_3, 4 SiO
44 “NMP”	NMP	85	3.9810	3.200	N-Metilpirrolidona	1 NMP
45	CCl_3F	86	3.0356	2.644	Triclorofluorometano	1 CCl_3F
“CClF”	CCl_2F	87	2.2287	1.916	Tetracloro-1,2-difluoroetano	2 CCl_2F
	$HCCl_2F$	88	2.4060	2.116	Diclorofluorometano	1 $HCCl_2F$
	HCClF	89	1.6493	1.416	1-Cloro-1,2,2,2-	1 CF_3, 1 HCClF
	$CClF_2$	90	1.8174	1.648	tetrafluoroetano	2 $CClF_2$
	$HCClF_2$	91	1.9670	1.828	1,2-Diclorotetrafluoroetano	1 $HCClF_2$
	$CClF_3$	92	2.1721	2.100	Clorodifluorometano	1 $CClF_3$
	CCl_2F_2	93	2.6243	2.376	Clorotrifluorometano	1CCl_2F_2
					Diclorodifluorometano	
46	$CONH_2$	94	1.4515	1.248	Acetamida	1 CH_3, 1 $CONH_2$
“CON”	$CONHCH_3$	95	2.1905	1.796	N-Metilacetamida	1 CH_3, 1 $CONHCH_3$
	$CONHCH_2$	96	1.9637	1.488	N-Etilacetamida	2 CH_3, 1$CONHCH_2$
	$CON(CH_3)_2$	97	2.8589	2.428	N,N-Dimetilacetamida	1 CH_3, 1 $CON(CH_3)_2$
	$CONCH_3CH_2$	98	2.6322	2.120	N,N-Metiletilacetamida	2 CH_3, 1 $CONCH_3CH_2$
	$CON(CH_2)_2$	99	2.4054	1.812	N,N-Dietilacetamida	3 CH_3, 1 $CON(CH_2)_2$
47	$C_2H_5O_2$	100	2.1226	1.904	2-Etoxietanol	1 CH_3, 1 CH_2, 1 $C_2H_5O_2$
“OCCOH”	$C_2H_4O_2$	101	1.8952	1.592	2-Etoxi-1-propanol	2 CH_3, 1 CH_2, 1 $C_2H_4O_2$
48	CH_3S	102	1.6130	1.368	Dimetilsulfuro	1 CH_3, 1 CH_3S
“CH_2S”	CH_2S	103	1.3863	1.060	Dietilsulfuro	2 CH_3, 1 CH_2, 1 CH_2S
	CHS	104	1.1589	0.748	Diisopropilsulfuro	4 CH_3, 1 CH, 1CHS
49“Morfolina”	MORPH	105	3.4740	2.796	Morfolina	1 MORPH
50	C_4H_4S	106	2.8569	2.140	Tiofeno	1 C_4H_4S
“Tiofeno”	C_4H_3S	107	2.6908	1.860	2-Metiltiofeno	1 CH_3, 1 C_4H_3S
	C_4H_2S	108	2.5247	1.580	2,3-Dimetiltiofeno	2 CH_3, 1 C_4H_2S

PARÁMETROS DE INTERACCIÓN DE GRUPOS FUNCIONALES DEL MODELO UNIFAC

	1 CH_2	2 C=C	3 ACH	4 $ACCH_2$	5 OH	6 CH_3OH	7 H_20	8 ACOH
1 CH_2	0.0	86.02	61.13	76.50	986.5	697.2	1318.	1333.
2 C=C	-35.36	0.0	38.81	74.15	524.1	787.6	270.6	526.1
3 ACH	-11.12	3.446	0.0	167.0	636.1	637.4	903.8	1329.
4 $ACCH_2$	-69.70	-113.6	-146.8	0.0	803.2	603.3	5695.	884.9
5 OH	156.4	457.0	89.60	25.82	0.0	-137.1	353.5	-259.7
6 CH_3OH	16.51	-12.52	-50.00	-44.50	249.1	0.0	-181.0	-101.7
7 H_2O	300.0	496.1	362.3	377.6	-229..1	289.6	0.0	324.5
8 ACOH	275.8	217.5	25.34	244.2	-451.6	-265.2	-601.8	0.0
9 CH_2CO	26.76	42.92	140.1	365.8	164.5	108.7	472.5	-133.1
10 CHO	505.7	56.30	23.39	106.0	529.0	-340.2	480.8	-155.6
11 CCOO	114.8	132.1	85.84	-170.0	245.4	249.6	200.8	-36.72
12 HCOO	329.3	110.4	18.12	428.0	139.4	227.8	---	---
13 CH_2O	83.36	26.51	52.13	65.69	237.7	238.4	-314.7	-178.5
14 CNH_2	-30.48	1.163	-44.85	296.4	-242.8	-481.7	-330.4	---
15 CNH	65.33	-28.70	-22.31	223.0	-150.0	-370.3	-448.2	---
16 $(C)_3N$	-83.98	-25.38	-223.9	109.9	28.60	-406.8	-598.8	---
17 $ACNH_2$	1139.	2000.	247.5	762.8	-17.40	-118.1	-341.6	-253.1
18 Piridina	-101.6	-47.63	31.87	49.80	-132.3	-378.2	-332.9	-341.6
19 CCN	24.82	-40.62	-22.97	-138.4	185.4	162.6	242.8	---
20 COOH	315.3	1264.	62.32	89.86	-151.0	339.8	-66.17	-11.00
21 CCl	91.46	40.25	4.680	122.9	562.2	529.0	698.2	---
22 CCl_2	34.01	-23.50	121.3	140.8	527.6	669.9	708.7	---
23 CCl_3	36.70	51.06	288.5	69.90	742.1	649.1	826.8	---
24 CCl_4	-78.45	160.9	-4.700	134.7	856.3	709.6	1201.	10000.
25 ACCl	106.8	70.32	-97.27	402.5	325.7	612.8	-274.5	622.3
26 CNO_2	-32.69	-1.996	10.38	-97.05	261.6	252.6	417.9	---
27 $ACNO_2$	5541.	---	1824.	-127.8	561.6	---	360.7	---
28 CS_2	-52.65	16.62	21.50	40.68	609.8	914.2	1081.	1421.
29 CH_3SH	-7.481	---	28.41	19.56	461.6	448.6	---	---
30 Furfural	-25.31	82.64	157.3	128.8	521.6	---	23.48	---
31 DOH	139.9	---	221.4	150.6	267.6	240.8	-137.4	838.4
32 I	128.0	---	58.68	26.41	501.3	431.3	---	---
33 Br	-31.52	174.6	-154.2	1112.	524.9	494.7	---	---
34 C≡C	-72.88	41.38	---	---	68.95	---	---	---
35 DMSO	50.49	64.07	-2.504	-143.2	-25.87	695.0	-240.0	---
36 ACRY	-165.9	573.0	-123.6	397.4	389.3	218.8	386.6	---
37 CICC	47.41	124.2	395.8	419.1	738.9	528.0	---	---
38 ACF	-5.132	-131.7	-237.2	-157.3	649.7	645.9	---	---
39 DMF	-31.95	249.0	-133.9	-240.2	64.16	172.2	-287.1	---
40 CF_2	147.3	62.40	140.6	---	---	---	---	---
41 COO	529.0	1397.	317.6	615.8	88.63	171.0	284.4	-167.3
42 SiH_2	-34.36	---	787.9	---	1913.	---	180.2	---
43 SiO	110.2	---	234.4	---	---	---	---	---
44 NMP	13.89	-16.11	-23.88	6.214	796.9	---	832.2	-234.7
45 CCIF	30.74	---	167.9	---	794.4	762.7	---	---
46 CON	27.97	9.755	---	---	394.8	---	-509.3	---
47 OCCOH	-11.92	132.4	-86.88	-19.45	517.5	---	-205.7	---
48 CH_2S	39.93	543.6	---	---	---	420.0	---	---
49 Morfolina	-23.61	161.1	142.9	274.1	-61.20	-89.24	-384.3	---
50 Tiofeno	-8.479	---	23.93	2.845	682.5	597.8	---	810.5

	9 CH_2CO	10 CHO	11 CCOO	12 HCOO	13 CH_2O	14 CNH_2	15 CNH	16 $(C)_3N$
1 CH_2	476.4	677.0	232.1	507.0	251.5	391.5	255.7	**206.6**
2 C=C	182.6	448.8	37.85	333.5	214.5	240.9	163.9	61.11
3 ACH	25.77	347.3	5.994	287.1	32.14	161.7	122.8	90.49
4 $ACCH_2$	-52.10	586.8	5688.	197.8	213.1	19.02	-49.29	23.50
5 OH	84.00	-203.6	101.1	267.8	28.06	8.642	42.70	-323.0
6 CH_3OH	23.39	306.4	-10.72	179.7	-128.6	359.3	-20.98	53.90
7 H_2O	-195.4	-116.0	72.87	---	540.5	48.89	168.0	304.0
8 ACOH	-356.1	-271.1	-449.4	---	-162.9	---	---	---
9 CH_2CO	0.0	-37.36	-213.7	-190.4	-103.6	---	-174.2	-169.0
10 CHO	128.0	0.0	-110.3	766.0	304.1	---	---	---
11 CCOO	372.2	185.1	0.0	-241.8	-235.7	---	-73.50	-196.7
12 HCOO	385.4	-236.5	1167.	0.0	-234.0	---	---	---
13 CH_2O	191.1	-7.838	461.3	457.3	0.0	-78.36	251.5	5422.
14 CNH_2	---	---	---	---	222.1	0.0	-107.2	-41.11
15 CNH	394.6	---	136.0	---	-56.08	127.4	0.0	-189.2
16 $(C)_3N$	225.3	---	2889.	---	-194.1	38.89	865.9	0.0
17 $ACNH_2$	-450.3	---	-294.8	---	---	-15.07	---	---
18 Piridina	29.10	---	---	554.4	-156.1	---	---	---
19 CCN	-287.5	---	-266.6	99.37	38.81	-157.3	-108.5	---
20 COOH	-297.8	-165.5	-256.3	193.9	-338.5	---	---	---
21 CCl	286.3	-47.51	35.38	---	225.4	131.2	---	---
22 CCl_2	82.86	190.6	-133.0	---	-197.7	---	---	-141.4
23 CCl_3	552.1	242.8	176.5	235.6	-20.93	---	---	-293.7
24 CCl_4	372.0	---	129.5	351.9	113.9	261.1	91.13	316.9
25 ACCl	518.4	---	-171.1	383.3	-25.15	108.5	102.2	2951.
26 CNO_2	-142.6	---	129.3	---	-94.49	---	---	---
27 $ACNO_2$	-101.5	---	---	---	---	---	---	---
28 CS_2	303.7	---	243.8	---	112.4	---	---	---
29 CH_3SH	160.6	---	---	201.5	63.71	106.7	---	---
30 Furfural	317.5	---	-146.3	---	-87.31	---	---	---
31 DOH	135.4	---	152.0	---	9.207	---	---	---
32 I	138.0	245.9	21.92	---	476.6	---	---	---
33 Br	142.6	---	24.37	---	736.4	---	---	---
34 C≡C	443.6	---	---	---	---	---	---	---
35 DMSO	110.4	---	41.57	---	-93.51	---	---	-257.2
36 ACRY	---	354.0	175.5	---	---	---	---	---
37 ClCC	-40.90	183.8	611.3	134.5	-217.9	---	---	---
38 ACF	---	---	---	---	167.3	---	-198.8	116.5
39 DMF	97.04	13.89	-82.12	-116.7	-158.2	49.70	---	-185.2
40 CF_2	---	---	---	---	---	---	---	---
41 COO	123.4	577.5	-234.9	145.4	-247.8	---	284.5	---
42 SiH_2	992.4	---	---	---	448.5	961.8	1464.	---
43 SiO	---	---	---	---	---	-125.2	1604.	---
44 NMP	---	---	---	---	---	---	---	---
45 CClF	---	---	---	---	---	---	---	---
46 CON	---	---	---	---	---	---	---	---
47 OCCOH	156.4	---	-3.444	---	---	---	---	---
48 CH_2S	---	---	---	---	---	---	---	---
49 Morfolina	---	---	---	---	---	---	---	**---**
50 Tiofeno	278.8	---	---	---	---	---	---	---