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Parameters of the Original UNIFAC Model

This page shows the **published** parameters for original UNIFAC. Many new, updated, and revised parameters can be obtained from [UNIFAC Consortium](#).

[\[List of References\]](#)[\[List of Interaction Parameters\]](#)[\[List of Sub Groups and their Group Surfaces and Volumes\]](#)[\[List of Main Groups\]](#)[\[Interaction Parameters Matrix\]](#)

List of References

The parameters shown here have been published in the articles

1. Skjold-Joergensen S., Kolbe B., Gmehling J., Rasmussen P., "Vapor-Liquid Equilibria by UNIFAC Group Contribution. Revision and Extension", Ind.Eng.Chem. Process Des.Dev., 18(4), 714-722, 1979
2. Gmehling J., Rasmussen P., Fredenslund A., "Vapor-Liquid Equilibria by UNIFAC Group Contribution. Revision and Extension. 2", Ind.Eng.Chem. Process Des.Dev., 21(1), 118-127, 1982
3. Macedo E.A., Weidlich U., Gmehling J., Rasmussen P., "Vapor-Liquid Equilibria by UNIFAC Group-Contribution. Revision and Extension. 3", Ind.Eng.Chem. Process Des.Dev., 22(4), 676-678, 1983
4. Tieg D., Gmehling J., Rasmussen P., Fredenslund A., "Vapor-Liquid Equilibria by UNIFAC Group Contribution. 4. Revision and Extension", Ind.Eng.Chem.Res., 26(1), 159-161, 1987
5. Hansen H.K., Rasmussen P., Fredenslund A., Schiller M., Gmehling J., "Vapor-Liquid Equilibria by UNIFAC Group-Contribution. 5. Revision and Extension", Ind.Eng.Chem.Res., 30(10), 2352-2355, 1991
6. Wittig R., Lohmann J., Gmehling J., "Vapor-Liquid Equilibria by UNIFAC Group Contribution. 6. Revision and Extension", Ind.Eng.Chem.Res., 42(1), 183-188, 2003

List of Interaction Parameters

i	j	A _{ij}	A _{ji}
1	2	86.0200	-35.3600
1	3	61.1300	-11.1200
1	4	76.5000	-69.7000
1	5	986.5000	156.4000
1	6	697.2000	16.5100
1	7	1318.0000	300.0000
1	8	1333.0000	275.8000
1	9	476.4000	26.7600
1	10	677.0000	505.7000
1	11	232.1000	114.8000
1	12	507.0000	329.3000
1	13	251.5000	83.3600
1	14	391.5000	-30.4800
1	15	255.7000	65.3300
1	16	206.6000	-83.9800
1	17	920.7000	1139.0000
1	18	287.7700	-101.5600
1	19	597.0000	24.8200
1	20	663.5000	315.3000
1	21	35.9300	91.4600
1	22	53.7600	34.0100
1	23	24.9000	36.7000
1	24	104.3000	-78.4500
1	25	11.4400	106.8000
1	26	661.5000	-32.6900
1	27	543.0000	5541.0000

Latest News

2022-09-14 17:00 [19th Joint DDBST User and UNIFAC Consortium Member Meeting Closed](#)

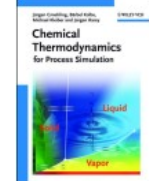
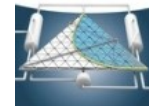
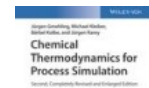
2022-05-13 11:41 [DDB Version 2022 released](#)

2022-05-06 12:43 [DDB version 2022 waits in the wings](#)

2022-01-27 13:51 [19th joint DDBST user and UNIFAC consortium member meeting announced](#)

2021-05-04 09:20 [Prof. Dr. Onken passed away](#)

2021-04-27 08:57 [DDB Version 2021 available](#)

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1	33	479.5000	-31.5200
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1	35	526.5000	50.4900
1	36	689.0000	-165.9000
1	37	-4.1890	47.4100
1	38	125.8000	-5.1320
1	39	485.3000	-31.9500
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1	42	-450.4000	-34.3600
1	43	252.7000	110.2000
1	44	220.3000	13.8900
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1	46	390.9000	27.9700
1	47	553.3000	-11.9200
1	48	187.0000	39.9300
1	49	216.1000	-23.6100
1	50	92.9900	-8.4790
1	51	699.1300	456.1900
1	55	808.5900	245.2100
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1	85	637.6500	221.5600
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2	5	524.1000	457.0000
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2	10	448.7500	56.3000
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2	12	333.5000	110.4000
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2	22	58.5500	-23.5000
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2	25	100.1000	70.3200
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2	37	-66.4600	124.2000
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3	29	-10.4300	28.4100
3	30	-64.6900	157.2900
3	31	210.3660	221.4000
3	32	113.3000	58.6800
3	33	261.3000	-154.2000
3	34	154.2600	-101.1200
3	35	169.9000	-2.5040
3	36	383.9000	-123.6000
3	37	-259.1000	395.8000
3	38	389.3000	-237.2000
3	39	245.6000	-133.9000
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4	11	5688.0000	-170.0000
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4	41	69.2600	615.8000
4	44	46.3800	6.2140
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5	10	-203.6000	529.0000
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6	23	-139.3500	649.1000
6	24	-44.7600	709.6000
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6	26	75.1400	252.5600
6	27	457.8800	511.2900
6	28	-31.0900	914.2000
6	29	17.5000	448.6000
6	30	-61.7600	287.0000
6	31	-119.2000	240.8000
6	32	212.1000	431.3000
6	33	106.3000	494.7000
6	34	-119.1000	967.7100
6	35	-399.3000	695.0000
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6	37	33.4700	528.0000
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7	17	243.2000	-341.6000
7	18	459.0000	-332.9000
7	19	112.6000	242.8000
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7	55	-255.6300	627.3900
8	9	-356.1000	-133.1000
8	10	-271.1000	-155.6000
8	11	-449.4000	-36.7200
8	12	-32.5200	-234.2500
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8	14	-832.9700	-870.8000
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9	17	6201.0000	-450.3000
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9	23	-354.5500	552.1000
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9	25	-119.8000	518.4000
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9	27	548.5000	-101.5000
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9	29	-46.2800	160.6000
9	30	-163.7000	317.5000
9	31	71.4600	135.4000
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9	34	-246.6000	443.6150
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9	36	-63.5000	114.5500
9	37	-34.5700	-40.9000
9	39	-61.7000	97.0400
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10	13	304.1000	-7.8380

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1021	751.9000	-47.5100
1022	67.5200	190.6000
1023	-483.7000	242.8000
1032	117.0000	245.9000
1034	2.2100	-55.8700
1036	-339.2000	354.0000
1037	172.4000	183.8000
1039	-268.8000	13.8900
1041	-275.5000	577.5000
1112	-241.8000	1167.0000
1113	-235.7000	461.3000
1115	-73.5000	136.0000
1116	-196.7000	2888.6001
1117	475.5000	-294.8000
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1122	108.8500	-132.9500
1123	-209.6600	176.4500
1124	54.5700	129.4900
1125	442.4000	-171.1000
1126	-81.1300	129.3000
1128	183.0460	243.7750
1130	202.2500	-146.3100
1131	-101.7000	152.0000
1132	148.3000	21.9200
1133	18.8800	24.3700
1134	71.4800	-111.4500
1135	52.0800	41.5700
1136	-28.6100	175.5300
1137	-275.2000	611.3000
1139	85.3300	-82.1200
1141	560.2000	-234.9000
1147	151.8000	-3.4440
1213	-234.0000	457.3000
1218	-233.4000	554.4000
1219	-47.2500	99.3700
1220	-268.1000	193.9000
1222	31.0000	80.9900
1223	-126.2000	235.6000
1224	179.7000	351.9000
1225	24.2800	383.3000
1229	103.9000	201.5000
1233	298.1300	-92.2600
1237	-11.4000	134.5000
1239	308.9000	-116.7000
1241	-122.3000	145.4000
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1315	251.5000	-56.0800
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1317	-46.3900	285.3600
1318	213.2000	-156.1000
1319	-18.5100	38.8100
1320	664.6000	-338.5000
1321	301.1400	225.3900
1322	137.7700	-197.7100
1323	-154.3000	-20.9300
1324	47.6700	113.9000
1325	134.8000	-25.1500
1326	95.1800	-94.4900
1327	155.1100	220.6600
1328	140.8960	112.3820
1329	-8.5380	63.7100

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1335	128.8000	-93.5100
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1338	-273.9500	167.3000
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1340	-172.5100	278.1500
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1416	-41.1100	38.8900
1417	-200.7000	-15.0700
1419	358.9000	-157.3000
1421	-82.9200	131.2000
1424	-99.8100	261.1000
1425	30.0500	108.5000
1429	-70.1400	106.7000
1435	874.1900	-366.5100
1439	-164.0000	49.7000
1442	-664.4000	961.8000
1443	275.9000	-125.2000
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1517	138.5400	64.3000
1518	431.4900	-207.6600
1519	147.1000	-108.5000
1524	71.2300	91.1300
1525	-18.9300	102.2000
1531	939.0700	-213.7400
1538	570.9000	-198.8000
1539	-255.2200	10.0300
1541	-38.7700	284.5000
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1543	-1327.0000	1603.8000
1617	287.4300	-24.4600
1619	1255.1000	-446.8600
1621	-182.9100	151.3800
1622	-73.8500	-141.4000
1623	-352.9000	-293.7000
1624	-262.0000	316.9000
1625	-181.9000	2951.0000
1635	243.1000	-257.2000
1638	-196.3120	116.4780
1639	22.0500	-185.2000
1718	89.7000	117.4000
1719	-281.6000	777.4000
1720	-396.0000	493.8000
1721	287.0000	429.7000
1722	-111.0000	140.8000
1724	882.0000	898.2000
1725	617.5000	334.9000
1727	-139.3000	134.9000
1731	0.1004	192.3000
1739	-334.4000	343.7000
1741	-89.4200	-22.1000
1819	-169.6700	134.2800
1820	-153.7000	-313.5000
1822	-351.6000	587.3000
1823	-114.7300	18.9800
1824	-205.3000	368.5000
1825	-2.1700	20.1800
1827	2845.0000	2475.0000
1833	-60.7800	-42.7100
1837	160.7000	281.6000

1838	-158.8000	159.8000
1850	-136.6000	221.4000
1920	205.2700	92.0700
1921	4.9330	54.3200
1922	-152.7000	258.6000
1923	-15.6200	74.0400
1924	-54.8600	491.9500
1925	-4.6240	363.5000
1926	-0.5150	0.2830
1928	230.8520	335.7430
1929	0.4604	161.0000
1931	177.5000	169.6000
1933	-62.1700	136.9000
1934	-203.0200	329.1200
1936	81.5700	-42.3100
1937	-55.7700	335.2000
1939	-151.5000	150.6000
1941	120.3000	-61.6000
1947	16.2300	119.2000
2021	13.4100	519.1000
2022	-44.7000	543.3000
2023	39.6300	504.2000
2024	183.4000	631.0000
2025	-79.0800	993.4000
2030	-208.9000	570.6000
2032	228.4000	616.6000
2033	-95.0000	5256.0000
2035	-463.6000	-180.2000
2037	-11.1600	898.2000
2039	-228.0000	-97.7700
2041	-337.0000	1179.0000
2046	-322.3000	-70.2500
2122	108.3100	-84.5300
2123	249.1500	-157.1000
2124	62.4200	11.8000
2125	153.0000	-129.7000
2126	32.7300	113.0000
2127	86.2000	1971.0000
2128	450.0880	-73.0920
2129	59.0200	-27.9400
2130	65.5600	-39.4600
2132	2.2200	179.2500
2133	344.4000	-262.3000
2137	-168.2000	383.2000
2139	6.5700	-55.2100
2141	63.6700	182.2000
2223	0.0000	0.0000
2224	56.3300	17.9700
2225	223.1000	-8.3090
2226	108.9000	-9.6390
2230	149.5600	-116.2100
2232	177.6000	-40.8200
2233	315.9000	-174.5000
2235	215.0000	-215.0000
2237	-91.8000	301.9000
2239	-160.2800	397.2400
2241	-96.8700	305.4000
2247	361.1000	-194.7000
2324	-30.1000	51.9000
2325	192.1000	-0.2266
2328	116.6120	-26.0580
2330	-64.3800	48.4840
2332	86.4000	21.7600
2333	168.8000	-46.8000
2335	363.7000	-343.6000
2337	111.2000	-149.8000

2341	255.8000	-193.0000
2344	-35.6800	-196.2000
2348	565.9000	-363.1000
2425	-75.9700	248.4000
2426	490.8800	-34.6800
2427	534.7000	514.6000
2428	132.2000	-60.7100
2430	546.6800	-133.1600
2432	247.8000	48.4900
2433	146.6000	77.5500
2435	337.7000	-58.4300
2436	369.4900	-85.1480
2437	187.1000	-134.2000
2438	215.2000	-124.6000
2439	498.6000	-186.7000
2441	256.5000	335.7000
2443	233.1000	70.8100
2447	423.1000	3.1630
2448	63.9500	-11.3000
2450	108.5000	-79.3400
2455	585.1900	75.0400
2526	132.7000	132.9000
2527	2213.0000	-123.1000
2533	593.4000	-185.3000
2535	1337.3700	-334.1200
2539	5143.1401	-374.1600
2540	309.5800	33.9500
2541	-71.1800	956.1000
2544	-209.7000	161.5000
2547	434.1000	7.0820
2627	533.2000	-85.1200
2628	320.2000	277.8000
2631	139.8220	481.3480
2632	304.3000	64.2800
2633	10.1700	125.3000
2634	-27.7010	174.4330
2637	10.7600	379.4000
2639	-223.1000	223.6000
2641	248.4000	-124.7000
2645	-218.9000	844.0000
2650	-4.5650	176.3000
2732	2990.0000	2448.0000
2733	-124.0000	4288.0000
2832	292.7000	-27.4500
2837	-47.3700	167.9000
2841	469.8000	885.5000
2935	31.6600	85.7000
2939	78.9200	-71.0000
2944	1004.2000	-274.1000
2948	-18.2700	6.9710
3041	43.3700	-64.2800
3135	-417.2000	535.8000
3139	302.2000	-191.7000
3141	347.8000	-264.3000
3144	-262.0000	262.0000
3147	-353.5000	515.8000
3233	6.3700	37.1000
3241	68.5500	288.1000
3335	32.9000	-111.2000
3337	-48.3300	322.4200
3339	336.2500	-176.2600
3341	-195.1000	627.7000
3437	2073.2000	631.5000
3439	-119.8000	6.6990
3539	-97.7100	136.6000
3541	153.7000	-29.3400

36	37	-208.8000	837.2000
36	39	-8.8040	5.1500
36	41	423.4000	-53.9100
37	39	255.0000	-137.7000
37	41	1730.8000	-198.0000
37	44	26.3500	-66.3100
37	48	2429.0000	148.9000
38	39	-110.6500	50.0600
38	40	-117.1700	185.6000
39	40	-5.5790	55.8000
39	41	72.3100	-28.6500
40	45	111.8000	-32.1700
41	47	122.4000	101.2000
42	43	-2166.0000	745.3000
84	85	1517.5000	-1869.9000

List of Sub Groups and their Group Surfaces and Volumes

This table also shows the assignment of sub groups to the coresponding main groups.

No.	Subgroup Name	Maingroup	R	Q
1	CH3	[1]CH2	0.9011	0.8480
2	CH2	[1]CH2	0.6744	0.5400
3	CH	[1]CH2	0.4469	0.2280
4	C	[1]CH2	0.2195	0.0000
5	CH2=CH	[2]C=C	1.3454	1.1760
6	CH=CH	[2]C=C	1.1167	0.8670
7	CH2=C	[2]C=C	1.1173	0.9880
8	CH=C	[2]C=C	0.8886	0.6760
9	ACH	[3]ACH	0.5313	0.4000
10	AC	[3]ACH	0.3652	0.1200
11	ACCH3	[4]ACCH2	1.2663	0.9680
12	ACCH2	[4]ACCH2	1.0396	0.6600
13	ACCH	[4]ACCH2	0.8121	0.3480
14	OH	[5]OH	1.0000	1.2000
15	CH3OH	[6]CH3OH	1.4311	1.4320
16	H2O	[7]H2O	0.9200	1.4000
17	ACOH	[8]ACOH	0.8952	0.6800
18	CH3CO	[9]CH2CO	1.6724	1.4880
19	CH2CO	[9]CH2CO	1.4457	1.1800
20	CHO	[10]CHO	0.9980	0.9480
21	CH3COO	[11]CCOO	1.9031	1.7280
22	CH2COO	[11]CCOO	1.6764	1.4200
23	HCOO	[12]HCOO	1.2420	1.1880
24	CH3O	[13]CH2O	1.1450	1.0880
25	CH2O	[13]CH2O	0.9183	0.7800
26	CHO	[13]CH2O	0.6908	0.4680
27	THF	[13]CH2O	0.9183	1.1000
28	CH3NH2	[14]CNH2	1.5959	1.5440
29	CH2NH2	[14]CNH2	1.3692	1.2360
30	CHNH2	[14]CNH2	1.1417	0.9240
31	CH3NH	[15]CNH	1.4337	1.2440
32	CH2NH	[15]CNH	1.2070	0.9360
33	CHNH	[15]CNH	0.9795	0.6240
34	CH3N	[16](C)3N	1.1865	0.9400
35	CH2N	[16](C)3N	0.9597	0.6320
36	ACNH2	[17]ACNH2	1.0600	0.8160
37	C5H5N	[18]PYRIDINE	2.9993	2.1130
38	C5H4N	[18]PYRIDINE	2.8332	1.8330
39	C5H3N	[18]PYRIDINE	2.6670	1.5530
40	CH3CN	[19]CCN	1.8701	1.7240
41	CH2CN	[19]CCN	1.6434	1.4160
42	COOH	[20]COOH	1.3013	1.2240
43	HCOOH	[20]COOH	1.5280	1.5320
44	CH2CL	[21]CCL	1.4654	1.2640

45	CHCL	[21]CCL	1.2380	0.9520
46	CCL	[21]CCL	1.0106	0.7240
47	CH2CL2	[22]CCL2	2.2564	1.9880
48	CHCL2	[22]CCL2	2.0606	1.6840
49	CCL2	[22]CCL2	1.8016	1.4480
50	CHCL3	[23]CCL3	2.8700	2.4100
51	CCL3	[23]CCL3	2.6401	2.1840
52	CCL4	[24]CCL4	3.3900	2.9100
53	ACCL	[25]ACCL	1.1562	0.8440
54	CH3NO2	[26]CNO2	2.0086	1.8680
55	CH2NO2	[26]CNO2	1.7818	1.5600
56	CHNO2	[26]CNO2	1.5544	1.2480
57	ACNO2	[27]ACNO2	1.4199	1.1040
58	CS2	[28]CS2	2.0570	1.6500
59	CH3SH	[29]CH3SH	1.8770	1.6760
60	CH2SH	[29]CH3SH	1.6510	1.3680
61	FURFURAL	[30]FURFURAL	3.1680	2.4840
62	DOH	[31]DOH	2.4088	2.2480
63	I	[32]I	1.2640	0.9920
64	BR	[33]BR	0.9492	0.8320
65	CH=-C	[34]C=-C	1.2920	1.0880
66	C=-C	[34]C=-C	1.0613	0.7840
67	DMSO	[35]DMSO	2.8266	2.4720
68	ACRY	[36]ACRY	2.3144	2.0520
69	CL-(C=C)	[37]CLCC	0.7910	0.7240
70	C=C	[2]C=C	0.6605	0.4850
71	ACF	[38]ACF	0.6948	0.5240
72	DMF	[39]DMF	3.0856	2.7360
73	HCON(..	[39]DMF	2.6322	2.1200
74	CF3	[40]CF2	1.4060	1.3800
75	CF2	[40]CF2	1.0105	0.9200
76	CF	[40]CF2	0.6150	0.4600
77	COO	[41]COO	1.3800	1.2000
78	SIH3	[42]SIH2	1.6035	1.2632
79	SIH2	[42]SIH2	1.4443	1.0063
80	SIH	[42]SIH2	1.2853	0.7494
81	SI	[42]SIH2	1.0470	0.4099
82	SIH2O	[43]SIO	1.4838	1.0621
83	SIHO	[43]SIO	1.3030	0.7639
84	SIO	[43]SIO	1.1044	0.4657
85	NMP	[44]NMP	3.9810	3.2000
86	CCL3F	[45]CCLF	3.0356	2.6440
87	CCL2F	[45]CCLF	2.2287	1.9160
88	HCCL2F	[45]CCLF	2.4060	2.1160
89	HCCLF	[45]CCLF	1.6493	1.4160
90	CCLF2	[45]CCLF	1.8174	1.6480
91	HCCLF2	[45]CCLF	1.9670	1.8280
92	CCLF3	[45]CCLF	2.1721	2.1000
93	CCL2F2	[45]CCLF	2.6243	2.3760
94	AMH2	[46]CON(AM)	1.4515	1.2480
95	AMHCH3	[46]CON(AM)	2.1905	1.7960
96	AMHCH2	[46]CON(AM)	1.9637	1.4880
97	AM(CH3)2	[46]CON(AM)	2.8589	2.4280
98	AMCH3CH2	[46]CON(AM)	2.6322	2.1200
99	AM(CH2)2	[46]CON(AM)	2.4054	1.8120
100	C2H5O2	[47]OCCOH	2.1226	1.9040
101	C2H4O2	[47]OCCOH	1.8952	1.5920
102	CH3S	[48]CH2S	1.6130	1.3680
103	CH2S	[48]CH2S	1.3863	1.0600
104	CHS	[48]CH2S	1.1589	0.7480
105	MORPH	[49]MORPH	3.4740	2.7960
106	C4H4S	[50]THIOPHEN	2.8569	2.1400

107 C4H3S	[50]THIOPHEN 2.6908 1.8600
108 C4H2S	[50]THIOPHEN 2.5247 1.5800
109 NCO	[51]NCO 1.0567 0.7320
118 (CH2)2SU	[55]SULFONES 2.6869 2.1200
119 CH2CHSU	[55]SULFONES 2.4595 1.8080
178 IMIDAZOL	[84]IMIDAZOL 2.0260 0.8680
179 BTI	[85]BTI 5.7740 4.9320

List of Main Groups

This table shows the list of main groups and the sub group belonging to every main group.

No.	Maingroup Name	Subgroups
1	CH2	[1]CH3 [2]CH2 [3]CH [4]C
2	C=C	[5]CH2=CH [6]CH=CH [7]CH2=C [8]CH=C [70]C=C
3	ACH	[9]ACH [10]AC
4	ACCH2	[11]ACCH3 [12]ACCH2 [13]ACCH
5	OH	[14]OH
6	CH3OH	[15]CH3OH
7	H2O	[16]H2O
8	ACOH	[17]ACOH
9	CH2CO	[18]CH3CO [19]CH2CO
10	CHO	[20]CHO
11	CCOO	[21]CH3COO [22]CH2COO
12	HCOO	[23]HCOO
13	CH2O	[24]CH3O [25]CH2O [26]CHO [27]THF
14	CNH2	[28]CH3NH2 [29]CH2NH2 [30]CHNH2
15	CNH	[31]CH3NH [32]CH2NH [33]CHNH
16	(C)3N	[34]CH3N [35]CH2N
17	ACNH2	[36]ACNH2
18	PYRIDINE	[37]C5H5N [38]C5H4N [39]C5H3N
19	CCN	[40]CH3CN [41]CH2CN
20	COOH	[42]COOH [43]HCOOH
21	CCL	[44]CH2CL [45]CHCL [46]CCL
22	CCL2	[47]CH2CL2 [48]CHCL2 [49]CCL2
23	CCL3	[50]CHCL3 [51]CCL3
24	CCL4	[52]CCL4
25	ACCL	[53]ACCL
26	CNO2	[54]CH3NO2 [55]CH2NO2 [56]CHNO2
27	ACNO2	[57]ACNO2
28	CS2	[58]CS2
29	CH3SH	[59]CH3SH [60]CH2SH
30	FURFURAL	[61]FURFURAL
31	DOH	[62]DOH
32	I	[63]I
33	BR	[64]BR
34	C=-C	[65]CH=-C [66]C=-C
35	DMSO	[67]DMSO
36	ACRY	[68]ACRY
37	CLCC	[69]CL-(C=C)
38	ACF	[71]ACF
39	DMF	[72]DMF [73]HCON(..
40	CF2	[74]CF3 [75]CF2 [76]CF
41	COO	[77]COO
42	SIH2	[78]SIH3 [79]SIH2 [80]SIH [81]SI
43	SIO	[82]SIH2O [83]SIHO [84]SIO
44	NMP	[85]NMP
45	CCLF	[86]CCL3F [87]CCL2F [88]HCCL2F [89]HCCLF [90]CCLF2 [91]HCCLF2 [92]CCLF3 [93]CCL2F2
46	CON(AM)	[94]AMH2 [95]AMHCH3 [96]AMHCH2 [97]AM(CH3)2 [98]AMCH3CH2 [99]AM(CH2)2
47	OCCOH	[100]C2H5O2 [101]C2H4O2
48	CH2S	[102]CH3S [103]CH2S [104]CHS

49 MORPH	[105]MORPH
50 THIOPHEN	[106]C4H4S [107]C4H3S [108]C4H2S
51 NCO	[109]NCO
55 SULFONES	[118](CH2)2SU [119]CH2CHSU
84 IMIDAZOL	[178]IMIDAZOL
85 BTI	[179]BTI

Interaction Parameters Matrix

