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Parameters of the Modified UNIFAC (Dortmund) Model

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

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[[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

- Weidlich, Gmehling, Ind.Eng.Chem.Res., 26, 1372 (1987)
- Gmehling, Li, Schiller, Ind.Eng.Chem.Res., 32, 178 (1993)
- Gmehling, Lohmann, Jakob, Li, Joh, Ind.Eng.Chem.Res., 37, 4876-4882 (1998)
- Gmehling, Wittig, Lohmann, Joh, Ind.Eng.Chem.Res., 41, 1678-1688 (2002)
- Wittig, Lohmann, Joh, Horstmann, Gmehling, Ind.Eng.Chem.Res., 40, 5831-5838 (2001)
- Lohmann, Joh, Gmehling, Ind.Eng.Chem.Res., 40, 957-964 (2001)
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- Wittig, Lohmann Gmehling, AIChE Journal 49, 2, 530-537 (2003)
- Jakob, Grensemann, Lohmann, Gmehling, Ind.Eng.Chem.Res. 45, 7924-7933 (2006)
- Hector, Gmehling, Fluid Phase Equilib. 371, 82-92 (2014)
- Constantinescu, Gmehling, J.Chem.Eng.Data, 61(8), 2738-2748 (2016)

List of Interaction Parameters

i	j	Aij	Bij	Cij	Aji	Bji	Cji
1	2	189.66	-0.27232		-95.41801	0.061708	
1	3	114.2	0.0933		16.07	-0.2998	
1	4	7.339	-0.4538		47.2	0.3575	
1	5	2777	-4.674	0.001551	1606	-4.746	0.0009181
1	6	2409.4	-3.0099		82.593	-0.48575	
1	7	1391.3	-3.6156	0.001144	-17.253	0.8389	0.0009021
1	8	1381	-0.9977		1987	-4.615	
1	9	433.6	0.1473		199	-0.8709	
1	10	875.85			256.21		
1	11	98.65601	1.9294	-0.0031331	632.22	-3.3912	0.0039282
1	12	508.4	-0.6215		238.5	-0.5358	
1	13	233.1	-0.3155		-9.654	-0.03242	
1	14	-164.04	4.9683	-0.010252	326.04	-2.6348	0.0033576
1	15	350.58	0.066729		207.26	-1.0916	
1	16	-175.7	1.857		205.65	-1.4436	
1	17	958.74	-0.14836		2257.3	-5.6676	
1	18	1802.3	-17.171	0.036	-436.15	3.4225	-0.0087
1	19	593.07	0.7335		293.81	-1.3979	
1	20	1182.2	-3.2647	0.009198	2017.7	-9.0933	0.010238
1	21	401	-0.72772		-65.68501	0.074091	
1	22	-233.66	1.2561		311.55	-1.1856	
1	23	-653.74	4.5311	-0.008735	1302.6	-8.427	0.014417
1	24	267.51	-1.7109	0.003388	-148.07	1.0927	-0.002416
1	25	-1385	15.89	-0.04831	3264	-20.84	0.03317
1	26	2345	-13.2	0.02156	-396.5	3.092	-0.006266
1	27	2383	-2.693		1744	-4.082	
1	28	24.33	1.521		72.12	-1.126	
1	29	465.9	-0.8557		-59.9	-0.008313	
1	30	577.7	0.9384		210.5	-1.081	
1	31	897.7			28.17		

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](#)

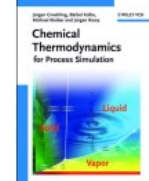
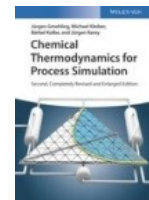
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2021-04-27 08:57 [DDB Version 2021 available](#)

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1	32	559.9	-0.3564		166	-0.7116	
1	33	527.7	-0.499		-62.08	-0.3658	
1	34	477.5	-0.6581		-22.04	-0.1018	
1	35	-547.5	3.457		477.1	-2.175	
1	36	1662			-291.9		
1	37	334.5	0.009102		3.202	-0.6894	
1	38	468.5	-1.042		-160.3	-0.0108	
1	39	406.2	0.6525		151	-0.9023	
1	40	342	-1.679		-484.3	2.467	
1	41	1312	-3.643		-314.6	1.287	
1	42	-117.1	0.5481	-0.00098	170.9	-0.8062	0.001291
1	43	79.507	0.70892	-0.0020983	186.71	-1.3546	0.0024016
1	44	1935.7			-21.23		
1	45	164.25	-0.26834		-44.069	0.027778	
1	46	677.32	-2.0066		-249.85	1.7054	
1	47	3150.86	-3.1003		189.911	-0.9413	
1	48	1529.52	-6.2025	0.00975	82.6	-0.615	-0.000623
1	49	-923.282	7.80959	-0.008808	183.02	-1.22588	0.000583
1	52	24.432	0.2915		-16.034	-0.5337	
1	53	269.67			-41		
1	55	407.47	-0.2037	-0.00016	-0.067	-0.3935	4e-05
1	56	1058.31	-1.1856		438.76	-1.2256	
1	61	860.51	-1.96009		-309.943	0.64856	
1	84	70.38	0.24511		77.7793	0.83298	
1	85	1260.02	-4.55446	0.0067607	996.5333	-5.48462	0.0095873
1	87	283.8202	-3.9547	0.0103753	907.3842	0.46568	-0.0055872
1	89	360.8016	2.05302	-0.0166992	454.5569	-1.47382	0.0010454
1	90	656.528	-4.2237	0.0074475	-307.8627	3.60996	-0.0081757
1	91	1094.303	-1.11888		243.462	-1.03559	
1	93	468.398	-2.55668		2660.16	-6.86512	
1	98	1859.374	4.06308		1131.305	-0.93175	
1	99	4041.479	-3.90698	-0.0254482	3504.325	2.66288	-0.0330202
2	3	174.1	-0.5886		-157.2	0.6166	
2	4	117.3	-0.8552		-113.1	1.172	
2	5	2649	-6.508	0.004822	1566	-5.809	0.005197
2	6	-628.07	10	-0.014972	-96.297	0.6304	-0.0018
2	7	778.3	0.1482		-1301	4.072	
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2	9	179.8	0.69911		91.811	-0.71715	
2	10	476.25			202.49		
2	11	980.74	-2.4224		-582.82	1.6732	
2	12	309.8			-28.63		
2	13	733.3	-2.509		-844.3	2.945	
2	14	1857	-8.653001	0.01088	498.8	-5.148	0.01039
2	15	224.8			-124.32		
2	16	165.3			-131.5		
2	17	2800	-10.72	0.01339	3982	-19.72	0.02783
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2	19	634.85			-181.93		
2	20	-2026.1	8.1549		-347.5	1.216	
2	21	498.9	-1.487		-359.6	1.238	
2	22	-44.958			55.881		
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2	24	616.62	-2.1164		-663.45	2.3281	
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2	28	46.06	1.545		70.88	-1.09	
2	30	470.4			-146.1		
2	33	-19.82	0.5941		160.4	-0.5148	
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2	37	967.9	-0.03862		-300.6	-0.09576	
2	38	141.1	-0.3025		-139.5	0.9076	
2	39	388.4			-152.2		
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2	45	389.28			-174.41		
2	46	491.23	-1.8285		-734.87	3.3463	
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2	48	249.18			-81.79		
2	49	1171.32	3.92127		90.0134	-0.920017	
2	52	-86.231			-39.373		
2	53	9.389999			57.86		
2	55	-456.08	2.4334		298.55	-1.4153	
2	56	775.56			-65.66		
2	61	324.316			-156.458		
2	84	-44.3408	-0.65212		1753.135	-3.112	
2	85	566.2915	-0.14057		-1213.93	5.14012	
2	87	-92.7302	-0.25088		-1151.296	4.7125	
2	89	1230.781	0.17033	0.0141503	4896.219	-1.86077	-0.0254894
2	90	1625.909	-2.40107		159.8103	1.85317	
2	91	2979.973	4.82369	-0.0272505	724.9113	-4.79411	0.0056279
2	93	-740.2421			232.905		
2	98	2487.632	-3.28182		1804.025	-5.18107	
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3	4	139.2	-0.65		-45.33	0.4223	
3	5	3972	-13.16	0.01208	3049	-12.77	0.01435
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3	7	792	-1.726		332.3	1.158	
3	8	1356	-2.118		2340	-5.043	
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3	10	-365.5	1.874		1011	-2.167	
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3	12	170.5	-0.02393		108.3	-0.262	
3	13	-87.08	-0.1859		179	0.05615	
3	14	2036	-8.729	0.008138	-121	-1.901	0.006999
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3	17	1044.7	-1.7112		154.39	1.2458	
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3	19	-17.44	0.9437		111.8	-0.5959	
3	20	69.561	1.8881		613.32	-1.595	
3	21	73.04601	-0.21322		-58.972	0.1046	
3	22	133.66	-0.46141		-142.2	0.39662	
3	23	66.214	-0.63629		-78.116	0.69975	
3	24	269	-1.776	0.002645	-305.5	2.12	-0.003239
3	25	595.2	3.309	-0.02844	1885	-10.98	0.01661
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3	27	936.3391	-4.4141	0.012232	1866.23	-9.28137	0.008299
3	28	3736	-25	0.04593	574.6	-3.702	0.003682
3	29	77.083	-0.3094		-2.1662	0.1196	
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3	31	-148.14	2.2658	-0.00353	-93.18999	1.5036	-0.00141
3	32	-82.28	0.5677		298.9	-0.8374	
3	33	-248.2	1.214		187.5	-0.9020001	
3	35	347.6	-1.43		-345.6	1.545	
3	37	602.1	-7.798	0.01966	1887	-8.707001	0.007813
3	38	808	-5.331	0.006077	-1367	7.883	-0.007754
3	39	-81.68999	1.1229	-0.00105	58.76	-0.6263	0.000668
3	40	123.26	-0.6133		419.04	-0.1703	
3	41	-126.2	0.386		670.8	-1.807	
3	42	134.6	-1.231	0.001488	-2.619	1.094	-0.001557
3	43	-26.852	-0.44215		47.23	0.64039	
3	44	-1172	10.106	-0.01428	-1141.6	8.656199	-0.015439
3	45	380.02	-0.23326		-201.52	-0.068774	
3	46	313.79	-1.1552		-258.12	1.4084	
3	47	1083.63	0.9144	-0.002141	160.13	-1.3578	0.001331
3	48	92.5	1.4186	1.8e-05	-14.89	-0.8126	2e-06
3	49	-103.146	2.6565	-0.002819	45.4296	-0.570848	0.000281
3	52	1412	-3.9917		-660.25	1.4602	

3	53	392.56			-260.22		
3	55	849.08	-6.5044	0.01219	-358.06	3.6831	-0.00782
3	56	-522.32	3.8856	-0.004212	562.72	-2.4316	0.00242
3	61	454.316	-1.21943		-388.19	1.04305	
3	84	277.4415	-0.1843		-223.7499	0.2781	
3	85	825.9189	-4.35541	0.0085572	20.2719	-0.33187	0.0025793
3	87	-1304.107	3.87435	0.0039496	26.3894	0.38631	-0.0027586
3	89	626.9603	-4.30606		2116.398	-2.11062	
3	90	161.7745	-0.56713		785.4488	-3.09114	
3	91	1690.065	-3.38808	0.0202432	-15.3556	-0.15571	-0.0001404
3	93	-630.416			-72.2694		
3	98	1014.686	-1.73087		877.6001	-1.96581	
3	99	4899.846	-3.53433	-0.0358313	-969.6266	3.81305	0.0028389
4	5	3989	-14.09	0.0153	2673	-5.765	-0.000332
4	6	436.21	1.9094		145.54	-0.48799	
4	7	1050.2	-1.9939		24.144	1.6504	
4	8	1375	-1.702		1825	-3.743	
4	9	1001	-1.871	0.000239	-146.6	0.2419	0.0001133
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4	11	-242.5	2.72	-0.003449	1624	-9.409	0.01338
4	12	136.98			377.26		
4	13	-595.1	2.978		375	-1.57	
4	14	2977	-19.16	0.03333	-45.44	5.141	-0.0142
4	15	1250			-316.22		
4	16	-2631	13.56	-0.007036	978.3	-6.481	0.007088
4	17	4000	-16.68	0.02112	3969	8.497001	-0.005945
4	18	135.3	-2.369	0.0039	1698.1	-9.8887	0.0153
4	19	208.1	1.333		170.1	-0.8218	
4	20	1352.5			29.747		
4	21	-46.994	0.30443		113.07	-0.59569	
4	22	213.85	0.19998		-75.01	-0.42684	
4	23	192.52	-0.25363		-38.939	-0.19378	
4	24	-106.2	0.6081		107.8	-0.6785	
4	25	-113.6	19.72		-69.23	-0.7359	
4	26	1358	-9.968	0.02093	1014	-4.702	0.004381
4	27	391.044	0.196357	2.24992e-05	1931.39	-5.15065	4.51638e-07
4	28	2586	-9.5	0.008819	-1494	7.679	-0.01225
4	30	157.9	1.408		181.2	-1.081	
4	31	1856.45	5.9959	-0.01862	1041.33	-5.2068	0.00717
4	32	69	0.4317		448.8	-0.9919	
4	33	277	-0.5955		-156.7	0.1221	
4	35	88.93	0.2236		178.6	-0.7113	
4	37	234.2	-0.2311		-115.9	-0.02925	
4	38	-172.2	0.2257		-13.15	0.001763	
4	39	444.29	0.1947		64.28	-0.5839	
4	40	29.57			153.32		
4	41	2303	-6.346		-736.8	3.332	
4	42	-107.1	0.2564		191.5	-0.5561	
4	43	-26.486	-0.29519		199.48	0.033695	
4	44	-514.79	4.9372		291.65	-1.2039	
4	45	297.73	-0.24204		-248.3	0.25471	
4	46	72.26	-0.1919		763.57	-1.3961	
4	47	1696.96	-0.7064		340.91	-1.008	
4	48	76.73	0.9394	-0.00045	246.08	-0.8198	-0.000137
4	49	-182.325	3.36729	-0.004625	119.767	-0.608934	0.000607
4	52	1000.8	-2.5194		-139.78	0.1146	
4	53	164.05			102.04		
4	55	558.08	0.565	-0.00331	562.34	-3.4373	0.00633
4	56	-307.42	4.1819	-0.007723	1661.26	-8.697001	0.01424
4	61	629.463	-1.39039		-305.273	0.669085	
4	84	930.7075	-4.30401	0.007841	365.3965	-1.20387	-0.0007792
4	85	-313.9384	2.06128		-134.6708	1.38462	
4	87	-935.3928	1.26386	0.0041351	4101.374	-1.19824	-0.0186009
4	89	524.3056	-4.26859		1259.47	-1.91791	
4	90	453.4621	-2.03845		3997.18	-2.994	
4	91	1077.47	-2.43883		-998.0735	4.48792	

4	93	-478.068			15.0501		
4	98	1113.436	-0.428312		-281.4692	1.00738	
4	99	335.1104	2.26653	0.0239277	3792.062	-2.55407	-0.0217293
5	6	346.31	-2.4583	0.0029287	-1218.2	9.7928	-0.016158
5	7	-801.9	3.824	-0.007514	1460	-8.673	0.01641
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5	10	-281.4	2.379	-0.006668	1590	-24.57	0.06212
5	11	973.8	-5.633	0.00769	310.4	1.538	-0.004885
5	12	235.9	-0.5874		839.6	-1.215	
5	13	816.7	-5.092	0.006065	650.9	-0.7132	0.000815
5	14	-923.7	2.468		-75.63	-0.1511	
5	15	-355.1	0.58		-660.2	1.743	
5	16	104.6	-5.014	0.008854	1876	11.5	0.09
5	17	-1114	5.916	-0.007126	1325	-6.263	0.007584
5	18	-3061.2	9.5413	0.1842	-643.09	2.9346	-0.0055
5	19	123.5	0.8503	-0.002478	-46	4.415	-0.00878
5	20	-1295	4.3634		1525.8	-4.9155	
5	21	238.1	-0.7077		2177	-4.363	
5	22	-126	0.1322		2389	-4.509	
5	23	1314.8			963.37		
5	24	925.6	-2.027		3139	-5.964	
5	25	1862	32.07	-0.009397	3664	34.13	0.002987
5	26	741.8	-2.098		1091	-1.274	
5	27	2100			316.6		
5	30	738.4	-1.771		616.5	-0.1457	
5	31	499.8	-2.41		-468.8	2.421	
5	32	838.8			774.7		
5	33	699.7	-1.767		1439	-1.673	
5	34	-148.9	1.034		1255	-2.538	
5	35	190.4	-1.2		-452.3	1.956	
5	36	1117	-2.196		1072	-1.248	
5	37	439.4			959.3		
5	38	848.6			1253		
5	39	1036	-2.995		-366.4	1.129	
5	41	403.8	-0.9346		703.4	-1.383	
5	42	3121	-13.69	0.01446	2601	-1.25	-0.006309
5	43	401.89	-0.43627	-0.002004	-238.36	5	-0.008186501
5	45	-32.643	-0.010434		2985.8	-6.227	
5	46	1201.3	-4.6803		-516.99	2.1888	
5	47	186.24	-3.1349	0.007737	1460.82	-5.962	0.004691
5	48	1627.81	-5.8598	0.005497	-808.4	3.8321	-0.005877
5	49	-150.961	0.527951		868.681	-2.20103	
5	52	-3745	4.5137	0.0636	7712.2	-7.6896	-0.035
5	53	495.28	-2.6496	0.00159	700.05	0.2237	-0.00244
5	56	34.94	1.0075	-0.002547	942.22	-2.3183	0.001188
5	61	1105.94	-1.68763		1343.95	-2.16488	
5	84	292.6468	-1.59145		147.0663	2.08434	
5	85	1026.29	-3.17777		-792.988	3.87681	
5	87	-348.7564	1.92474		1003.498	-2.48421	
5	89	-2448.212	-2.13997	0.0332832	-234.3916	4.01945	-0.0134709
5	90	1178.048	5.33766		1044.876	-3.71273	
5	91	-159.8631	2.41804		662.1286	-3.28127	
5	93	-367.321			34.7132		
5	98	225.0235	-4.3271	0.0030855	448.381	-1.61662	0.000518
5	99	-352.184	-1.58363	0.0090199	1751.43	-1.09998	-0.0148923
6	7	-328.5	1.0823	-0.0022	-524.3	4.6065	-0.004
6	8	-867	-1.258	0.02998	265.5	-2.905	0.002283
6	9	86.439	-0.46505		394.78	-0.36048	
6	10	-392.5	2.256		-158.4	-0.6469	
6	11	299.23	-1.2702		294.76	0.3745	
6	12	220.7	-0.6402		444.7	-0.06819	
6	13	-87.48	-0.5522		475.2	0.1198	
6	14	-495.25	1.0807		-467.95	0.65743	
6	15	-1508.5	4.4917		-278.09	-0.39888	
6	16	-1039	5.603	-0.006551	39.33	-3.354	0.006714

6	17	-2012	13.46	-0.02004	251.2	-1.274	0.002214
6	18	-341.34	-5.8042	0.0141	-230.38	-0.3825	0.0023
6	19	97.97301	-0.28666		615.01	-0.9444399	
6	20	-733.07	2.3351		1075.5	-3.4339	
6	21	-16.521	-0.28137		1831.2	-2.9694	
6	22	-85.926	-0.26371		1904.4	-2.7981	
6	23	-139.58			893.38		
6	24	-40.13	-0.06709		2150	-2.813	
6	25	3000	-11.81		2955	-6.383	
6	26	374.2	-2.212	0.002688	1079	-1.766	0.001238
6	28	-332.4	4.419	-0.007797	2645	-9.172001	0.01177
6	29	75.71	-0.3753		1334	-1.863	
6	30	-369.8	2.203		662	-1.903	
6	31	33.19	-0.2074		-3.428	0.483	
6	32	180.5	0.3161		1965	-3.858	
6	33	28.95	-0.3303		648.8	0.8050001	
6	35	-185.9	0.03906		145	-0.6343	
6	36	164			135.9		
6	37	-43.88			2421		
6	38	-99.57999			1235		
6	39	101.2	-1.078		-269.7	1.732	
6	41	308.7	-1.175		678.1	-1.335	
6	42	68.972	-0.41997		2540.7	-3.5236	
6	43	-308.7	1.7454	-0.00335	952.24	-3.3287	0.0053598
6	45	-242.6	0.29562	-9.0055e-05	4519.3	-19.456	0.025981
6	47	-119.08	0.9938		-52.69	-0.7465	
6	48	210.91	-2.4953	0.0048	-132.93	0.6584	-0.00208
6	49	197.395	-0.985958		-195.127	1.17652	
6	52	673.72	-2.3567		2676.7	-5.4899	
6	53	137.95	-1.4112	0.00172	524.52	0.4314	-0.00166
6	56	166.42	0.994	-0.003346	1683.48	-8.003099	0.01159
6	61	34.7884			641.041		
6	84	-704.2285	-1.26236	0.0149627	152.7192	2.17856	-0.0098745
6	85	-348.9494	1.41462		2127.895	-4.14737	
6	87	-1230.497	3.91001		1142.897	-2.92427	
6	89	-671.2604	1.58636	-0.0048637	985.4429	-2.42145	-0.0062036
6	90	53.7776	-0.9791		94.629	0.30192	
6	91	1741.061	-4.73718		-558.6751	1.11398	
6	93	1216.71	-5.44835		-386.355	3.77874	
6	98	1037.56	-5.46099		1421.557	0.34143	
7	8	-2686	19.44	-0.02702	148.4	-2.757	0.002329
7	9	190.5	-3.669	0.008838	770.6	-0.5873	-0.003252
7	10	-1545	6.512		512.6	-2.145	
7	11	-433.288	3.0862	-0.002012	311.974	-1.3412	0.001074
7	12	140.71			53.28		
7	13	177.665	-3.72906	0.010763	433.207	-0.605276	-0.000914
7	14	798.5	-5.869	0.01032	-980.6	3.671	-0.005908
7	15	1524	-2.531		-851	1.034	
7	16	274.5	-0.5905	0.002205	-446	-0.7738	0.002634
7	17	158.4	0.5246		-131	-0.7957	
7	18	-3178.5	9.8213	-0.0034	-393.18	0.5546	-0.0029
7	19	-634.1	3.59		509.6	-1.916	
7	20	-1795.2	12.708	-0.015455	624.97	-4.6878	0.0052371
7	21	86.68999	1.592		313.3	-0.5041	
7	22	134.1	0.9495		748.2	-1.319	
7	24	1008	-1.795		1282	-2.815	
7	25	-1895	9.303		591.6	-3.08	
7	26	-595.7	2.634		882.6	-2.606	
7	30	-123.8	3.847		501.4	-1.939	
7	31	372.5	-0.9091		-368.8	0.7775	
7	33	822.2			-17.99		
7	35	117	-0.611		-370.8	0.1043	
7	36	419.8	2.436		276.9	-0.9948	
7	39	-494.2	2.826		-121.8	-0.6029	
7	41	676	-0.9909		808.4	-2.929	
7	42	274.37	-0.5861	-0.00030011	1632.9	-2.8719	0.003455

7	43	-75.7467	-0.98514	0.0033318	717.485	-1.48515	-7.437899e-14
7	44	-804.28	2.828		594.45	-2.2535	
7	45	509.3	-0.29		-523.8	3.158	
7	46	659.22	-1.8841		-588.21	0.9707	
7	47	934.67	-4.4232	0.006054	-649.31	1.3487	-0.001586
7	48	64.43999	-0.0094		-439.58	0.3142	
7	49	-1119.8	7.95909	-0.008555	-128.903	-0.468519	-0.000916
7	53	499.44	-6.6553	0.01656	952.57	-0.8437	-0.0048
7	56	-302.93	0.5975		652.86	-1.8013	
7	61	1038.3			-270.53		
7	84	659.2109	-0.59252	0.0451602	151.31	-3.00895	0.0019814
7	85	2770.851	-2.00944		1996.724	-5.47448	
7	89	2707.161	-2.51124	-0.0022558	-399.1902	0.16195	-0.0067585
7	90	-1616.174	5.32305		275.7479	-1.97057	
7	91	318.2128	-1.42376		385.0068	-2.49001	
7	93	4878.28	-6.38758		-444.615	-0.776483	
7	98	206.2641	-2.57259	0.0032526	-371.2031	0.99046	-0.000807
8	9	-145.2	-0.738		-666.8	1.918	
8	10	5.604			-410.21		
8	11	-212.9			-224.4		
8	13	-329.3			-80.58		
8	17	542	-6.792	0.01655	-131.1	-0.9399	0.000469
8	18	-4080.9	12.859	-0.0101	-41.594	-3.5887	0.004
8	20	401.88			281.08		
8	24	2356	-3.347		2157	-3.718	
8	25	555.5			1554		
8	31	-309			191.7		
8	42	391.2	-0.8799		3630	-6.23	
8	52	4911.4	9.8501		2332.5	-4.0832	
9	10	197.6			-93.07999		
9	11	-16.486	-0.27924		33.415	0.21913	
9	12	-83.57			101.3		
9	13	3645	-26.91	0.04757	695.8	-0.9619	-0.002462
9	15	-47.97			119.5		
9	16	-389.6	0.1944	0.001863	2831	-13.01	0.01558
9	17	1732	-9.896001	0.0141	1460	-13.73	0.02917
9	18	-1908.7	4.1057		307.16	-0.8161	
9	19	-191	0.6835		79.08	-0.3808	
9	20	-109.51	0.96888		178.22	-0.91676	
9	21	-99.97601			55.27		
9	22	-18.695	-0.52606		-218.94	1.0749	
9	23	810.17	-3.2209	0.0021443	-48.641	-0.79498	0.0037129
9	24	-208.71	0.8293	-0.0014	155.73	1.4412	-0.0025
9	25	1297	-1.365	-0.02253	1375	2.499	0.006309
9	26	-35.89	-0.1009		-32.6	0.0847	
9	27	-169.6	2.986		-328.1	0.3045	
9	28	419.9	0.09772		315.3	-0.5617	
9	29	2.714			64.41		
9	30	-986	3.847		277	-1.357	
9	31	478.5	-1.148		-72.58	0.4909	
9	32	346.6	-0.7017		-182	0.7905	
9	33	-717.76	2.9431		319.69	-1.4362	
9	34	-62.43	-0.8977		-481.2	9.604	
9	35	-76.87	0.5372		38.06	-0.5189	
9	37	64.01	-1.077		-153.4	3.143	
9	39	80.79201	-3.702	0.011586	1955.5	-10	0.011386
9	41	64.21			-148.3		
9	42	437.739	-2.7983	0.00364	364.423	2.1022	-0.004653
9	43	-62.857	0.2898		80.038	-0.10124	
9	45	-497.98	0.79715	0.00029817	945.14	-3.8168	0.0045351
9	47	502.1	0.3401		141.01	-0.9829	
9	48	37.37			-116.4		
9	49	410.655	-1.1056		-201.105	0.7123	
9	52	-153.7	0.242		2311.5	-6.6054	
9	84	173.4451	-5.52695	0.0160979	958.3726	-4.73012	0.0047161
9	85	824.1235	-2.88368	0.0041569	670.0023	-5.05233	0.0074865

9	87	99.5504	0.45575		-1504.191	4.63058	
9	89	147.2528	-2.74448		177.8232	-2.24998	
9	90	331.1518	-1.11421		-30.955	-0.71244	
9	91	571.6566	-4.43975		-1449.573	4.44554	
9	98	519.4855	-5.4673	0.0068391	3306.365	0.15196	-0.0082641
10	11	-208.4			389.7		
10	12	-160.7			226.6		
10	13	209	-0.6241		235.7	0.1314	
10	20	435.64			-188		
10	21	985.7	-2.986		-888.3	3.426	
10	22	-41.537			354.71		
10	29	-373.7			-397.5		
10	30	-742.7			-214.8		
10	32	114.3			293.5		
10	34	236.6			-93.066		
10	37	-43.56			945.6		
10	39	2371			-225.3		
10	42	716.7	-1.516		1161	-0.5724	
11	12	342.4			-251.7		
11	13	195.3	-9.75	0.04051	824.2	-6.009	0.008271
11	15	3168	-24.07	0.04303	3329	-13.78	0.01193
11	16	152.8	-1.099		160.8	0.8719	
11	17	-1355	7.683001	-0.01012	3499	-22.96	0.03543
11	18	87.6	1.4109		45.309	-1.4281	
11	19	-193.23	0.43006		139.55	-0.43665	
11	20	62.031	1.0567		59.594	-0.71198	
11	21	-49.339			48.852		
11	22	168.17	-1.0536		-461.35	1.8569	
11	24	-5.71	-0.2724		223.4	0.1237	
11	25	3351	-14.54		-788.6	1.693	
11	26	9.222	-0.3292		-50.36	0.02448	
11	28	861.1	-1.693		280	-0.9491	
11	30	80.68999			-136.3		
11	31	-72.07			69.25		
11	32	82.96			11.62		
11	33	-386.3	1.892		248.3	-1.198	
11	35	296.8	-1.264		-337.1	0.8843	
11	36	-92.12	0.9031		503.5	-1.792	
11	37	-201.4	0.5487		-320	1.052	
11	39	96.77	0.4827		16.69	-0.5966	
11	41	-338.8	1.837		3.924	-1.174	
11	42	374.1	-1.976	0.001682	460.8	-0.06206	4.1e-05
11	43	-28.231			36.948		
11	44	745.4			-447.04		
11	45	-579.11	0.9455		966.35	-2.1861	
11	47	758.13	-0.2593		32.71	-0.8641	
11	48	611.47	-2.4783		-1031.78	3.9906	
11	49	2973.58	-5.45555		81.6384	-1.3111	
11	56	-1336.2	6.7742	-0.0082	1915.2	-9.9994	0.0126
11	61	-1366.59	5.90673	-0.007325	2622.04	-11.7013	0.013472
12	18	-9.2978			-123.73		
12	19	92.21			-33.64		
12	24	-142.2	0.572		465.8	-0.7730001	
12	25	1894			18.79		
12	29	161.8			13.97		
12	37	745.4	-0.622		-479.1	0.8031	
12	39	580.3			-285.5		
12	42	227.6	-0.7762		509	-0.2248	
12	44	489.15			-441.01		
12	45	260.64	-1.2868		-597.09	2.5295	
13	18	-199.94	-6.9867	0.0193	-430.49	-0.728	0.004
13	19	1987	-8.022	0.01065	-588.8	1.481	-0.002636
13	20	521.48			-310.82		
13	21	-208.6	-0.2571	0.002418	872	-2.939	0.001269
13	22	492.9	-6.475	0.01806	215.3	-2.482	0.002745
13	23	-607.35	2.3467		97.12801	-0.64386	

1324	-425.4	0.9514		641.2	-1.486	
1325	974	-1.368	-0.01983	381.1	-5.682	0.01675
1326	-305.1	0.7063		319.6	-1.368	
1328	35.02	1.702		198.5	-1.434	
1329	102.6			-210.1		
1330	513.7			-299.6		
1332	-104.8			464		
1334	-137.87			169.27		
1337	-422.7	2.23		-326.4	0.24	
1338	155.7	-1.578		-528.8	2.822	
1342	397	-1.379		-214.1	1.134	
1343	-124.33	-0.29398		561.14	-0.7058	
1344	-454.92			310.75		
1345	-515.93	0.3835		1368	-2.6254	
1348	1321.52			-361.25		
1349	3858.07	-9.278001	7e-06	-224.782	-0.410609	-4e-06
1356	-209.209	-0.470423	0.006918	1163.91	-7.1332	0.00839
1393	-584.728			178.501		
1415	1517	-12.72	0.02557	-1074	9	-0.01795
1416	-472.4	-0.2051	0.01058	836.6	-5.208	0.004801
1419	-412.38	-0.49092	0.0062553	2412.2	-10.495	0.0097411
1424	-65.76	-0.3148		333.9	-0.1415	
1425	2553	-11.9		3873	-9.315001	
1429	-205.1			244.4		
1439	162.14			-112.76		
1442	124.3	-1.147		621.9	0.258	
1443	-143.07			182.58		
1447	413.11			-293.93		
1456	190.882			14.9127		
1516	402.6	-1.614		-639.9	2.561	
1519	242.2			-131.9		
1524	-3.28			43.83		
1525	3888	-16.26		-868.8	2.948	
1538	-330.2			904.1		
1539	-88.49			-230.55		
1542	-131.9	-0.007369		1248	-2.79	
1543	-186.98			295.07		
1547	444.67	0.8351		-196.23	-0.0511	
1556	1178.79	-9.99911	0.020758	1667.89	-7.58704	0.008006
1622	-473	0.8883		406.8	-1.524	
1624	215.9	-1.399		-825.9	3.15	
1625	1622	-4.812	-0.01856	-94.87	-9.612	0.03722
1638	-7.532001	-0.8077		35.16	0.09722999	
1639	965			-311.9		
1642	324.15	-1.4264		-198.32	1.452	
1645	-420.24	0.26315		-1035.8	3.078	
1647	-729.5	6.2811		-66.61	-0.696	
1648	2111.24			-235.61		
1656	2662.02	-13.9855	0.017738	-1780.41	5.71975	-0.00165
1718	74.285	14.613	-0.0283	-558.39	1.2436	-0.0007
1719	393.9	-4.703	0.009003	2987	-9.336	0.007147
1721	582.1	-2.33	0.000377	-338	3.372	-0.003676
1724	3986	-16.15	0.01635	2626	-10.59	0.01466
1725	3709.2			1583.8		
1727	3770	1.686		1.655	-1.164	
1731	1268	-3.042		-818.8	3.229	
1739	-391.9			650.7		
1742	1371	-3.323		1091	-0.2657	
1747	1271.42	-6.4373	0.006451	-2476.18	10.9894	-0.009617
1819	746.12	-2.1937		-2307.8	5.8186	
1820	-451.49	-0.4031		-2617.7	4.614	
1821	-67.106	-0.4933		-1592.8	2.8397	
1822	-978.25	2.1884		946.79	-4.9886	
1824	229.66	-1.5005		-2111	6.3625	
1833	-713.65	1.9191		-763.19	0.603	
1838	197.95	-0.3316	-0.0004	-1052.5	1.6854	0.0027

1842	268.23	-1.4137		-5894.1	13.088	
1843	-250.25	0.3811		-1269.7	2.6335	
1845	-516.31	1.6943		-1646.8	2.7237	
1847	489.93	-0.5591	-0.00102	-2250.64	5.4638	-0.00015
1852	-674	1.8854		4998.6	1.1962	
1921	176.5	-1.237		-368.7	1.992	
1922	-78.96			14.76		
1924	65.82	-0.6265		357.6	0.7676	
1925	1283	3.361	-0.02978	2331	-9.238001	0.01158
1926	117.53	-0.44692		-128.21	0.50349	
1928	468.8			434.8		
1929	-18.8	-0.3652		41.54	0.646	
1931	506.6	-1.263		11.72	0.7004	
1933	-211.2			362.6		
1934	11.65	-1.229		-1428	7.698	
1936	267.1			-144.7		
1937	61.96	-0.4161		-19.1	1.195	
1939	57.08	-0.7417		-160.48	1.0644	
1941	-75.67			26.8		
1942	256.2	-1.526	0.001118	1336	-3.395	0.004586
1943	-28.653	-0.48152		56.754	0.89781	
1945	237.42	-1.2928		-642.44	2.8574	
1949	297.646	-0.66206		-116.794	0.54754	
1956	-50.8443	-0.025287		180.813	-0.0641231	
2021	27.618			702.4		
2022	94.606			425.97		
2024	701.95	-1.7576		213.34	2.1861	
2025	-1398.7			1000		
2032	146.06			780.71		
2033	-18.328			753.21		
2037	-447.95	1.5141		283.64	1.5491	
2039	-421.21			93.773		
2041	-271.176	1.4107		218.974	-0.8061	
2042	1060	-2.822		578.3	1.493	
2043	720.45	-1.5187		-140.77	0.309	
2044	-65.631			-14.016		
2045	508.72	-1.4005		-386.93	2.3961	
2047	-369.31			-0.29		
2048	-400.86			-244.69		
2122	70.79			-66.21		
2123	592.4	-4.2459	0.0069046	603.29	-3.977	0.0062484
2124	16.34	0.07287		95.05	-0.2348	
2125	3985	-15.7		15.62	-1.099	
2126	24.44	-0.4713		142.1	-0.153	
2127	1248	-2.04		1295	-4.224	
2128	295.9			-137.7		
2130	666			-390.6		
2133	128.8	-0.2077		-92.68	-0.01307	
2137	280			-207.3		
2139	-70.45			-59.29		
2142	-31.42	-0.248		370.6	-0.322	
2143	-325.77	2.0412		70.075	-1.149	
2144	530.3			17.052		
2145	207.12	-0.43964		-175.29	0.32745	
2149	955.8281	-1.00012		-151.036	-0.458824	
2156	842.486	-1.8434		-313.202	0.4139	
2223	187.43	-3.446	0.0067179	1468.9	-5	0.003701
2224	46.29	-0.2115		46.03	0.05388	
2225	3353	-14.2		368.6	-1.748	
2226	822.4	-2.05		-423.1	0.8154	
2230	-174.6			106.3		
2232	132.7	-0.1183		-23.81	-0.09203999	
2233	-139.6	1.022		96.4	-0.776	
2235	-178.3	0.7426		-39.45	-0.8556	
2237	160.7			-135.9		
2239	-147.64			75.45		

2242	10.7	-0.2702		224.4	-0.1399	
2243	108.83	-0.86059		-358.57	1.3307	
2245	7.3664	0.40456		-1.6641	-0.37825	
2248	102.8	-0.0879		-446.86	0.4276	
2249	-1017.26	3.0909		894.509	-2.93164	
2256	262.138			-229.081		
2324	-323.17	1.1973		350.92	-1.3456	
2333	599.82			-364.76		
2337	325.81			-199.87		
2342	289.08	-0.5852		-69.60101	-0.4274	
2356	401.698			157.634		
2425	-131.8	9.802	-0.03582	972.1	-6.82	0.009219
2426	441.5	-0.5353		-65.74	0.0967	
2427	3286			167.5		
2428	9.362	1.033		52.01	-0.9095	
2430	750.2	0.8165		100.5	-0.8269	
2432	49.51	0.6829		186.4	-0.7294	
2433	203.2	-1.328		-1360	7.402	
2435	325.2	0.4405		-60.89	-0.6321	
2436	902			-194.9		
2437	220.6	0.3756		-134.4	-0.3226	
2438	197.4	-0.4858		-98.98	-0.02128	
2439	512.7	0.02702		-168.4	-0.123	
2442	-37.183	-0.047827		60.78	0.024262	
2443	190.45	0.012716		-131.87	-0.014204	
2445	22.779	0.042145		14.947	-0.11086	
2449	516.966	0.19471	0.001855	-198.677	0.435084	-0.001271
2452	1366.3	-3.8385		-580.46	1.1653	
2456	120.59	1.2816		261.15	-0.8815	
2526	3986	25		3638	-14.25	
2527	-184.5	2.2806		2926.02	-1.8141	
2533	-69.88			981.5		
2539	-12.71	-0.4758		472.49	-0.5503	
2542	207.16	-1.2206		223.782	-0.5826	
2543	96.855	-1.2993		2991.9	-9.3959	
2545	-27.161	0.611		4235.3	-16.954	
2549	593.203	-0.7904		88.32201	0.1605	
2627	85.6			986		
2628	68.87	3.217		655.7	-2.203	
2632	643.8	-0.7376		17.81	-0.2245	
2633	9.258	-0.1079		121.4	0.05397	
2634	-70.24			132.2		
2637	159			108.4		
2639	606.9			-340.9		
2642	119.3	-0.5691		522.9	-0.2485	
2643	53.75			-47.089		
2652	324.62	-1.1828		11.442	0.7866	
2733	505.4			81.44501		
2742	2004	-4.5		2600	-4.8	
2832	212.4	-0.3692		200.6	-0.228	
2837	-93.31	-0.1286		319.4	0.03419	
2842	29.45	-0.9194		92.4	1.191	
2843	166.56	-1.0407		1.0902	1.5927	
2845	89.744	-1.0122		40.987	1.1526	
2935	467.1			-360		
2939	356.6			-247.6		
2942	-7.465	-0.4151		439.73	-0.2619	
3037	-277.6			1168		
3042	96.59	-0.7691		846.7	0.2545	
3044	778.78			-384.29		
3135	-228.4			-47.81		
3139	373.8			-231.6		
3147	-210.34	0.9103		106.79	-0.9536999	
3233	-536.2	1.995		558	-1.924	
3245	-47.772	-0.009201		92.429	0.17437	
3335	-83.7	0.1436		-116.7	-0.06775	

3341	-378.1	2.56		13.78	-0.936	
3342	-122.5	0.0913		476.9	-0.61	
3343	-186.4			265.42		
3356	2459.01			-271.226		
3439	1025			-416.5		
3539	-133.35	0.1022		221.74	-0.5021	
3545	-322.46	-0.020828		67.069	0.23965	
3549	-3.44708			-72.16901		
3637	-74.88			1004		
3639	-110.34			97.36		
3739	967.74			-306.22		
3741	-211.1			516.5		
3742	-24.82	-0.5324		81.56	0.7293	
3743	321.62	-4.9963	0.013871	713.9	-2.7759	0.00091722
3745	185.82			-139		
3839	190.06			-229.97		
3840	-57.38			110.4		
3842	112.7	-0.4103		21.04	-0.1288	
3843	-22.572			-7.56		
3942	141.2	-0.8783		666.5	-0.1555	
3943	53.871	-0.67747		-54.26	1.0612	
3944	-310.13			-367.48		
3949	-18.3768	-0.450261		-2.27584	0.601128	
4042	165.6			-109		
4142	683.3	6.321		865	-2.89	
4243	242.49	-0.038323		20.834	-0.34718	
4245	183.79	-0.15182		-61.922	-0.059442	
4246	298.46	-0.6823		499.59	-0.8158	
4247	2187.67	-1.057		165.66	-0.9151	
4248	499.19	0.5131		148.66	-1.0328	
4249	-49.6851	3.86633		159.179	-1.11479	
4252	313.43	0.0911		-30.564	-0.2455	
4255	373.49	0.0647		75.45	-0.6572	
4256	-581.16	4.1194		660.47	-2.0132	
4261	509.274	-0.533745		-108.172	-0.132539	
4284	-883.9302	4.0287		360.0808	-1.37211	
4285	493.7747	-4.10779	0.0119213	986.9591	-2.85003	0.0018563
4287	-501.6695	1.6261		-935.6061	4.67403	
4289	-381.9636	-3.00577	0.0076136	2358.513	-1.30922	0.0137839
4290	-1078.495	3.65154		1039.753	-3.51543	
4291	1654.642	-4.24837		-171.2349	0.62135	
4293	246.348	-1.9006		1120.89	-3.1028	
4298	449.5142	2.1727	0.0360498	4258.272	0.34026	-0.029654
4345	-523.96	0.4945		1414	-2.8776	
4356	19.221	0.4413		117.208	-0.3946	
4384	-617.0431	2.40181		-323.6833	-0.13058	
4385	826.0889	-0.93908		-450.7675	0.94786	
4389	580.1045	-2.24427	-0.0080098	4927.307	-0.63511	-0.0351738
4390	277.9974	0.25973		122.9861	-1.96464	
4391	-312.4461	1.126		186.7351	-0.9786	
4556	184.792			-76.1382		
4652	-1423.7	3.9162		1738.5	-3.9729	
4748	-91.65	-0.3411		117.57	0.7114	
4749	-188.913			308.235		
5356	912.2161	-2.02314		-604.897	1.04748	
5556	-9.63211	0.555403	-6.5e-05	125.526	0.289226	-0.000969
5661	200.04	0.1979	-0.0016	742.31	-4.1234	0.0078
8485	-103.0519	-1.42845	0.0094424	283.1673	-5.14586	0.0208006
8489	-107.3735	-3.90856	0.0005537	1094.895	-4.10982	2.63e-05
8491	133.3952	-2.64806	-0.0025991	-591.0368	0.45605	-0.0035024
8498	-113.0145	-1.48378		-35.932	-1.52136	
8499	4542.127	0.85207	-0.0518203	-4116.333	-1.71395	-0.0073933
8587	-1403.31	-4.02583	0.0382461	-516.843	-3.5941	0.0160959
8590	855.7144	-1.14021		-254.6989	-0.46519	
8791	-1138.034	0.70013		1824.841	-4.26948	
8990	-1679.977	4.40837	-0.0092342	4209.48	-0.75036	-0.0356672

List of Sub Groups and their Group Surfaces and Volumes

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

No.	Subgroup Name	Main Group No.	Main Group Name	R	Q
1	CH3	1	CH2	0.6325	1.0608
2	CH2	1	CH2	0.6325	0.7081
3	CH	1	CH2	0.6325	0.3554
4	C	1	CH2	0.6325	0.0000
5	CH2=CH	2	C=C	1.2832	1.6016
6	CH=CH	2	C=C	1.2832	1.2489
7	CH2=C	2	C=C	1.2832	1.2489
8	CH=C	2	C=C	1.2832	0.8962
9	ACH	3	ACH	0.3763	0.4321
10	AC	3	ACH	0.3763	0.2113
11	ACCH3	4	ACCH2	0.9100	0.9490
12	ACCH2	4	ACCH2	0.9100	0.7962
13	ACCH	4	ACCH2	0.9100	0.3769
14	OH (P)	5	OH	1.2302	0.8927
15	CH3OH	6	CH3OH	0.8585	0.9938
16	H2O	7	H2O	1.7334	2.4561
17	ACOH	8	ACOH	1.0800	0.9750
18	CH3CO	9	CH2CO	1.7048	1.6700
19	CH2CO	9	CH2CO	1.7048	1.5542
20	CHO	10	CHO	0.7173	0.7710
21	CH3COO	11	CCOO	1.2700	1.6286
22	CH2COO	11	CCOO	1.2700	1.4228
23	HCOO	12	HCOO	1.9000	1.8000
24	CH3O	13	CH2O	1.1434	1.6022
25	CH2O	13	CH2O	1.1434	1.2495
26	CHO	13	CH2O	1.1434	0.8968
27	THF	43	CY-CH2O	1.7023	1.8784
28	CH3NH2	14	CH2NH2	1.6607	1.6904
29	CH2NH2	14	CH2NH2	1.6607	1.3377
30	CHNH2	14	CH2NH2	1.6607	0.9850
31	CH3NH	15	CH2NH	1.3680	1.4332
32	CH2NH	15	CH2NH	1.3680	1.0805
33	CHNH	15	CH2NH	1.3680	0.7278
34	CH3N	16	(C)3N	1.0746	1.1760
35	CH2N	16	(C)3N	1.0746	0.8240
36	ACNH2	17	ACNH2	1.1849	0.8067
37	AC2H2N	18	PYRIDINE	1.4578	0.9022
38	AC2HN	18	PYRIDINE	1.2393	0.6330
39	AC2N	18	PYRIDINE	1.0731	0.3530
40	CH3CN	19	CH2CN	1.5575	1.5193
41	CH2CN	19	CH2CN	1.5575	1.1666
42	COOH	20	COOH	0.8000	0.9215
43	HCOOH	44	HCOOH	0.8000	1.2742
44	CH2CL	21	CCL	0.9919	1.3654
45	CHCL	21	CCL	0.9919	1.0127
46	CCL	21	CCL	0.9919	0.6600
47	CH2CL2	22	CCL2	1.8000	2.5000
48	CHCL2	22	CCL2	1.8000	2.1473
49	CCL2	22	CCL2	1.8000	1.7946
50	CHCL3	45	CHCL3	2.4500	2.8912
51	CCL3	23	CCL3	2.6500	2.3778
52	CCL4	24	CCL4	2.6180	3.1836
53	ACCL	25	ACCL	0.5365	0.3177
54	CH3NO2	26	CNO2	2.6440	2.5000
55	CH2NO2	26	CNO2	2.5000	2.3040
56	CHNO2	26	CNO2	2.8870	2.2410
57	ACNO2	27	ACNO2	0.4656	0.3589
58	CS2	28	CS2	1.2400	1.0680
59	CH3SH	29	CH3SH	1.2890	1.7620
60	CH2SH	29	CH3SH	1.5350	1.3160
61	FURFURAL	30	FURFURAL	1.2990	1.2890
62	DOH	31	DOH	2.0880	2.4000

63	I	32	I	1.0760	0.9169
64	BR	33	BR	1.2090	1.4000
65	CH=-C	34	C=-C	0.9214	1.3000
66	C=-C	34	C=-C	1.3030	1.1320
67	DMSO	35	DMSO	3.6000	2.6920
68	ACRY	36	ACRY	1.0000	0.9200
69	CL-(C=C)	37	CLCC	0.5229	0.7391
70	C=C	2	C=C	1.2832	0.4582
71	ACF	38	ACF	0.8814	0.7269
72	DMF	39	DMF	2.0000	2.0930
73	HCON(...	39	DMF	2.3810	1.5220
74	CF3	40	CF2	1.2840	1.2660
75	CF2	40	CF2	1.2840	1.0980
76	CF	40	CF2	0.8215	0.5135
77	COO	41	COO	1.6000	0.9000
78	CY-CH2	42	CY-CH2	0.7136	0.8635
79	CY-CH	42	CY-CH2	0.3479	0.1071
80	CY-C	42	CY-CH2	0.3470	0.0000
81	OH (S)	5	OH	1.0630	0.8663
82	OH (T)	5	OH	0.6895	0.8345
83	CY-CH2O	43	CY-CH2O	1.4046	1.4000
84	TRIOXAN	43	CY-CH2O	1.0413	1.0116
85	CNH2	14	CH2NH2	1.6607	0.9850
86	NMP	46	CY-CONC	3.9810	3.2000
87	NEP	46	CY-CONC	3.7543	2.8920
88	NIPP	46	CY-CONC	3.5268	2.5800
89	NTBP	46	CY-CONC	3.2994	2.3520
91	CONH2	47	CONR	1.4515	1.2480
92	CONHCH3	47	CONR	1.5000	1.0800
93	HCONHCH3	49	HCONR	2.4617	2.1920
94	HCONHCH2	49	HCONR	2.4617	1.8420
100	CONHCH2	47	CONR	1.5000	1.0800
101	AM(CH3)2	48	CONR2	2.4748	1.9643
102	AMCH3CH2	48	CONR2	2.2739	1.5754
103	AM(CH2)2	48	CONR2	2.0767	1.1866
104	AC2H2S	52	ACS	1.7943	1.3400
105	AC2HS	52	ACS	1.6282	1.0600
106	AC2S	52	ACS	1.4621	0.7800
107	H2COCH	53	EPOXIDES	1.3601	1.8031
108	COCH	53	EPOXIDES	0.6830	0.3418
109	HCOCH	53	EPOXIDES	0.9104	0.6538
110	(CH2)2SU	56	SULFONE	2.6870	2.1200
111	CH2SUCH	56	SULFONE	2.4600	1.8080
112	(CH3)2CB	55	CARBONAT	2.4200	2.4976
113	(CH2)2CB	55	CARBONAT	2.4200	2.0018
114	CH2CH3CB	55	CARBONAT	2.4200	2.2497
119	H2COCH2	53	EPOXIDES	1.0630	1.1230
122	CH3S	61	CH2S	1.6130	1.3680
123	CH2S	61	CH2S	1.3863	1.0600
124	CHS	61	CH2S	1.1589	0.7480
153	H2COC	53	EPOXIDES	0.9104	0.6538
178	C3H2N2+	84	IMIDAZOL	1.3662	0.6797
179	BTI-	85	BTI	5.6210	5.9463
184	C3H3N2+	84	IMIDAZOL	1.8430	1.6997
189	C4H8N+	87	PYRROL	2.7867	2.7723
195	BF4-	89	BF4	3.9628	0.6214
196	C5H5N+	90	PYRIDIN	2.1094	2.5106
197	OTF-	91	OTF	3.3710	2.0001
201	-S-S-	93	-S-S-	1.0678	2.2440
209	SO4	98	SO4	0.9903	3.5249
210	HSO4	98	SO4	1.5654	3.8076
211	PF6	99	PF6	3.8183	3.6018
220	C5H4N+	90	PYRIDIN	2.4873	2.4457

List of Main Groups

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

No.	Main Group Name	List of 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 (P) [81]OH (S) [82]OH (T)
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
14	CH2NH2	[28]CH3NH2 [29]CH2NH2 [30]CHNH2 [85]CNH2
15	CH2NH	[31]CH3NH [32]CH2NH [33]CHNH
16	(C)3N	[34]CH3N [35]CH2N
17	ACNH2	[36]ACNH2
18	PYRIDINE	[37]AC2H2N [38]AC2HN [39]AC2N
19	CH2CN	[40]CH3CN [41]CH2CN
20	COOH	[42]COOH
21	CCL	[44]CH2CL [45]CHCL [46]CCL
22	CCL2	[47]CH2CL2 [48]CHCL2 [49]CCL2
23	CCL3	[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	CY-CH2	[78]CY-CH2 [79]CY-CH [80]CY-C
43	CY-CH2O	[27]THF [83]CY-CH2O [84]TRIOXAN
44	HCOOH	[43]HCOOH
45	CHCL3	[50]CHCL3
46	CY-CONC	[86]NMP [87]NEP [88]NIPP [89]NTBP
47	CONR	[91]CONH2 [92]CONHCH3 [100]CONHCH2
48	CONR2	[101]AM(CH3)2 [102]AMCH3CH2 [103]AM(CH2)2
49	HCONR	[93]HCONHCH3 [94]HCONHCH2
52	ACS	[104]AC2H2S [105]AC2HS [106]AC2S
53	EPOXIDES	[107]H2COCH [108]COCH [109]HCOCH [119]H2COCH2 [153]H2COC
55	CARBONAT	[112](CH3)2CB [113](CH2)2CB [114]CH2CH3CB
56	SULFONE	[110](CH2)2SU [111]CH2SUCH
61	CH2S	[122]CH3S [123]CH2S [124]CHS
84	IMIDAZOL	[178]C3H2N2+ [184]C3H3N2+
85	BTI	[179]BTI-
87	PYRROL	[189]C4H8N+
89	BF4	[195]BF4-
90	PYRIDIN	[196]C5H5N+ [220]C5H4N+
91	OTF	[197]OTF-
93	-S-S-	[201]-S-S-
98	SO4	[209]SO4 [210]HSO4
99	PF6	[211]PF6

Interaction Parameters Matrix

