Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

The treatment of dispersion terms for solution systems

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Scheme S1 The numbereing system for the ligand exchange reactions

$(CO)_3Fe(BDA) + 2PMe_3 \longrightarrow (CO)_3Fe(PMe_3)_2 + BDA$ **(1a)**

$(CO)_3Fe(BDA) + 2PPh_3 \longrightarrow (CO)_3Fe(PPh_3)_2 + BDA$ **(1b)**

$(CO)_3Fe(BDA) + 2PCy_3 \longrightarrow (CO)_3Fe(PCy_3)_2 + BDA$ **(1c)**

$CpRu(Cl)(BDA) + 2PMe_3 \longrightarrow CpRu(Cl)(PMe_3)_2 + BDA$ **(2a)**

$CpRu(Cl)(BDA) + 2PPh_3 \longrightarrow CpRu(Cl)(PPh_3)_2 + BDA$ **(2b)**

$Cp^*Ru(Cl)(BDA) + 2PMe_3 \longrightarrow Cp^*Ru(Cl)(PMe_3)_2 + BDA$ **(3a)**

$Cp^*Ru(Cl)(BDA) + 2PPh_3 \longrightarrow Cp^*Ru(Cl)(PPh_3)_2 + BDA$ **(3b)**

$(CO)_3Fe(PMe_3)_2 + 2PPh_3 \longrightarrow (CO)_3Fe(PPh_3)_2 + 2PMe_3$ **(1ab)**

$(CO)_3Fe(PMe_3)_2 + 2PCy_3 \longrightarrow (CO)_3Fe(PCy_3)_2 + 2PMe_3$ **(1ac)**

$(CO)_3Fe(PPh_3)_2 + 2PCy_3 \longrightarrow (CO)_3Fe(PCy_3)_2 + 2PPh_3$ **(1bc)**

$CpRu(Cl)(PMe_3)_2 + 2PPh_3 \longrightarrow CpRu(Cl)(PPh_3)_2 + 2PMe_3$ **(2ab)**

$Cp^*Ru(Cl)(PMe_3)_2 + 2PPh_3 \longrightarrow Cp^*Ru(Cl)(PPh_3)_2 + 2PMe_3$ **(3ab)**

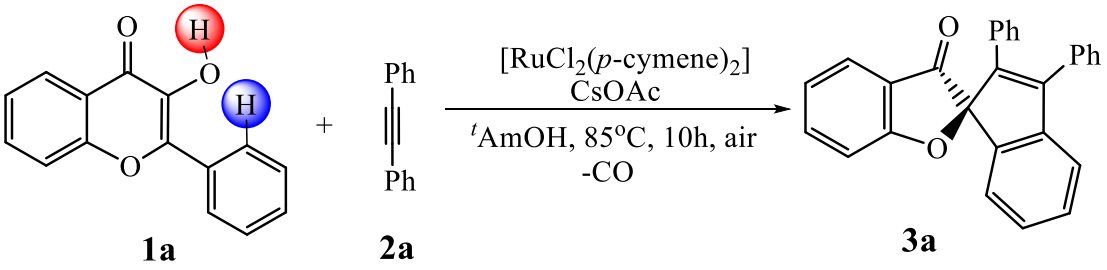
Table S1 The calculated total electronic energies, enthalpies, entropies and free energies in a.u.

Species	E_{elec}/a.u.[a]	H/a.u.[a]	E_{elec}/a.u.[b]	E_{elec}/a.u.[c]
$(CO)_3Fe(BDA)$	-2064.54367	-2064.32643	-2064.60774	-2064.58814
$CpRu(Cl)(BDA)$	-5366.92589	-5366.64224	-5367.01017	-5366.98021
$Cp^*Ru(Cl)(BDA)$	-5563.57757	-5563.14729	-5563.70234	-5563.65325
$(CO)_3Fe(PMe_3)_2$	-2524.27815	-2523.99943	-2524.36337	-2524.33181
$(CO)_3Fe(PPh_3)_2$	-3675.00903	-3674.38992	-3675.25202	-3675.15593
$(CO)_3Fe(Pcy_3)_2$	-3696.75957	-3695.71415	-3697.05928	-3696.93635
$CpRu(Cl)(PMe_3)_2$	-5976.98282	-5976.64453	-5977.08453	-5977.04579
$CpRu(Cl)(PPh_3)_2$	-7324.34510	-7323.51875	-7324.66570	-7324.53119
$Cp^*Ru(Cl)(PMe_3)_2$	-6173.62630	-6173.14109	-6173.76960	-6173.71135
$Cp^*Ru(Cl)(PPh_3)_2$	-7324.34510	-7323.51875	-7324.66570	-7324.53119
PMe_3	-461.07269	-460.95273	-461.09033	-461.08702
PPh_3	-1036.44972	-1036.15946	-1036.53456	-1036.50709
Pcy_3	-1047.32360	-1046.82093	-1047.43388	-1047.39503
BDA	-462.45949	-462.27770	-462.50610	-462.48806

(a)B3LYP+IDSCRF/TZP-DKH(-dfg) optimization and frequency calculations;
(b)B3LYP-D3-D3+IDSCRF/TZP-DKH(-dfg) single-point energy calculations;
(c) B3LYP-D3a+IDSCRF/TZP-DKH(-dfg) single-point energy calculations

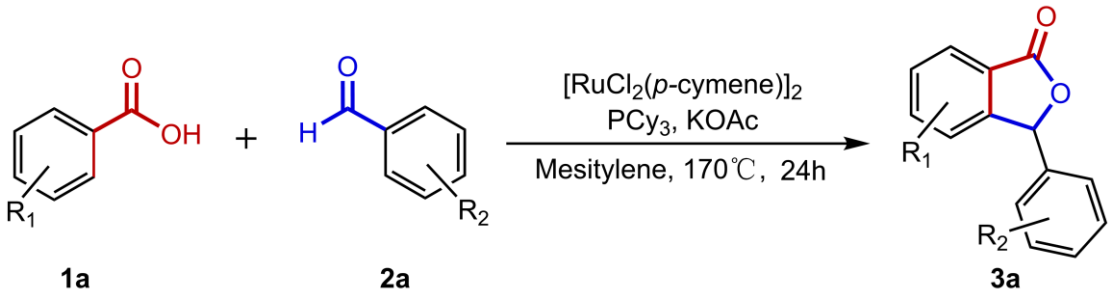
Scheme S2 The studied catalytic reaction schemes and numbering systems

M1:



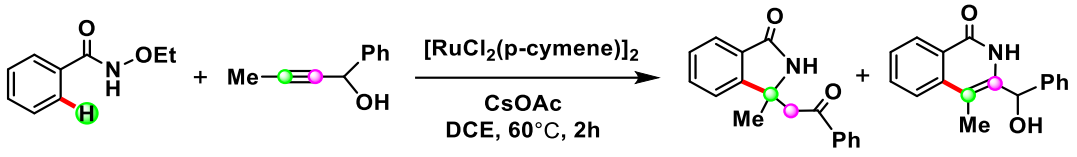
1a **2a** **3a**

M2:



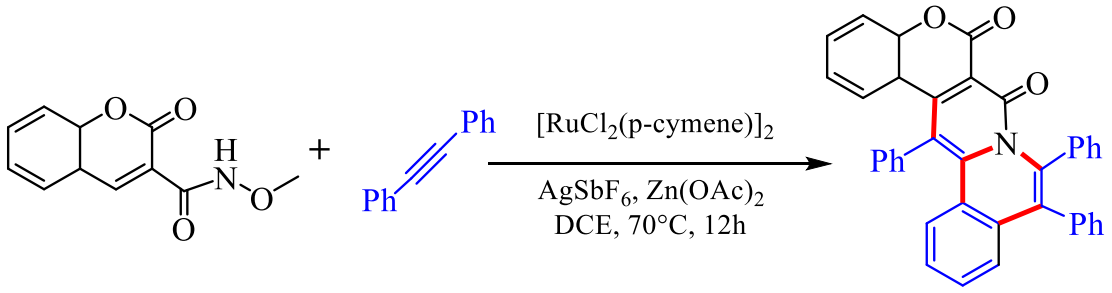
1a 2a 3a

M3:



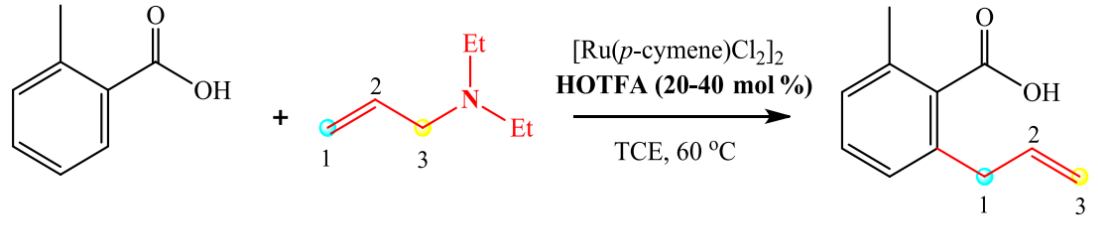
1a 2a 3a 98% 4a 2%

M4:



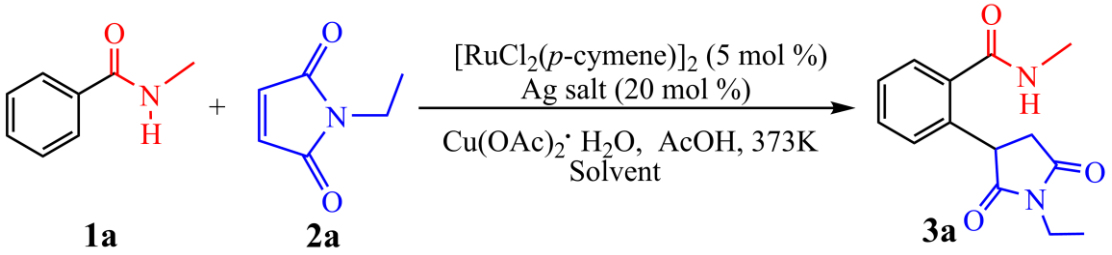
1a 2a 3aa

M5:



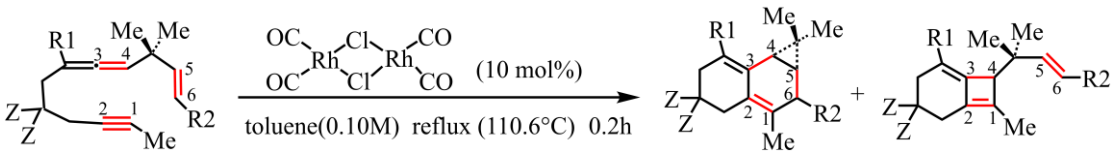
R1 R2 P (80%)

M6:



1a 2a 3a

M7:

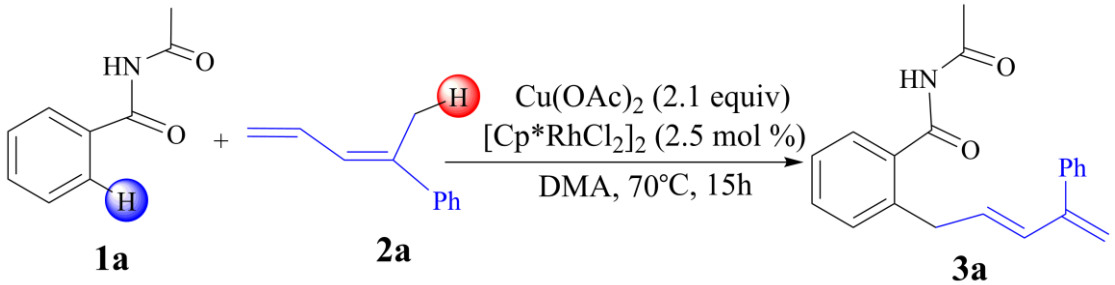


1a (R1=PhO_2S, R2=H) **2a** (R1=PhO_2S, R2=H) (100%) **3a** (R1=PhO_2S, R2=H) (0%)

1b (R1=PhO_2S, R2=npr(E)) **2b** (R1=PhO_2S, R2=npr(E)) (67%) **3b** (R1=PhO_2S, R2=npr(E)) (23%)

1c (R1=PhO_2S, R2=npr(Z)) **2c** (R1=PhO_2S, R2=npr(Z)) (100%) **3c** (R1=PhO_2S, R2=npr(Z)) (0%)

M8:



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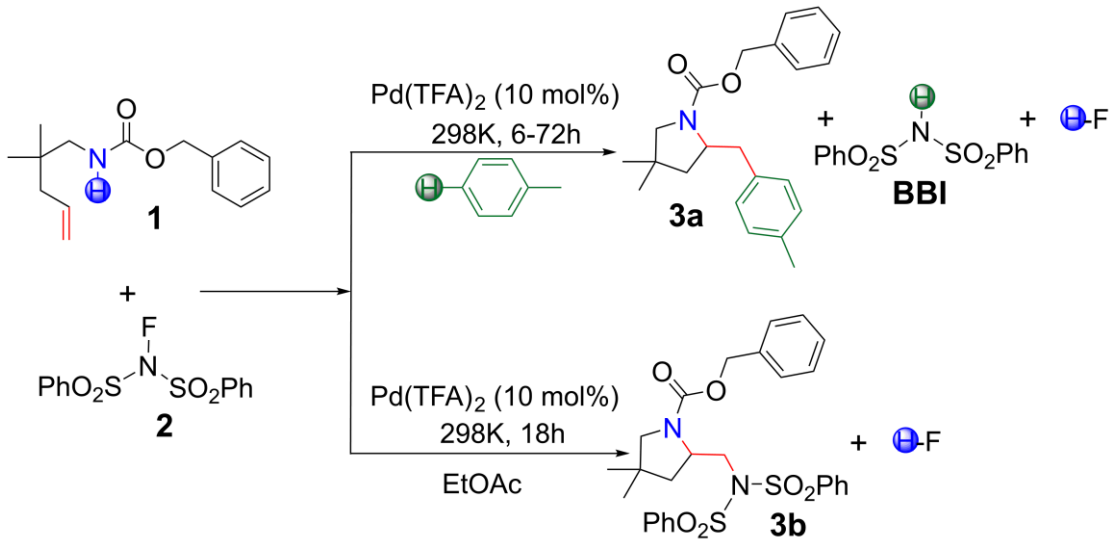

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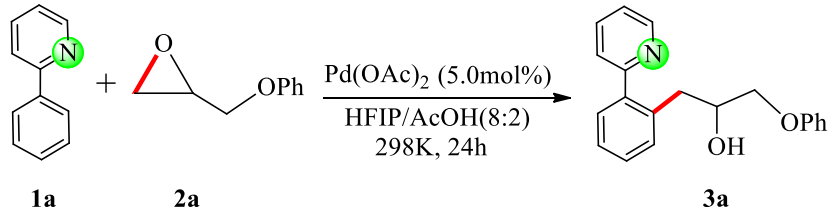
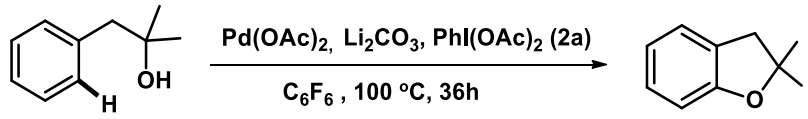


M11:



1a 3a

Table S2 The calculated total electronic energies, enthalpies, entropies and free energies in a.u.

Species	E_{elec}/a.u.	H/a.u.	S_g	S_l	G_g/a.u.	G_l/a.u.
1	-1619.08973[a]	-1618.46993	176.6	156.0	-1618.55382	-1618.54403
	-1619.06945[b]	-1618.44961	180.0	159.4	-1618.53512	-1618.52533
1a	-678.83562	-678.69346	115.8	93.7	-678.74845	-678.73798
	-678.82606	-678.68391	116.0	94.0	-678.73902	-678.72855
c1a	-2297.93892	-2297.17405	255.2	234.6	-2297.29529	-2297.28552
	-2297.91631	-2297.15139	257.1	236.5	-2297.27355	-2297.26377
1b	-416.89341	-416.78711	85.0	62.4	-416.82751	-416.81676
	-416.88637	-416.78009	85.4	62.7	-416.82065	-416.80990
c1b	-2035.99104	-2035.26242	229.0	208.4	-2035.37122	-2035.36143
	-2035.96922	-2035.24050	230.5	209.8	-2035.35000	-2035.34020
2	-2639.05148	-2638.21988	287.7	267.1	-2638.35659	-2638.34681
	-2639.02817	-2638.19641	284.6	264.0	-2638.33165	-2638.32187
2a	-1189.36857	-1189.17465	138.5	116.0	-1189.24046	-1189.22975
	-1189.35412	-1189.16020	139.1	116.6	-1189.22631	-1189.21560
c2a	-3828.42767	-3827.40012	377.0	356.5	-3827.57926	-3827.56950
	-3828.39892	-3827.37126	379.8	359.2	-3827.55172	-3827.54195
2b	-1079.83974	-1079.74415	100.0	77.1	-1079.79165	-1079.78077
	-1079.83003	-1079.73446	99.9	77.0	-1079.78192	-1079.77104
c2b	-3718.89891	-3717.96995	341.4	320.9	-3718.13218	-3718.12244
	-3718.87197	-3717.94299	344.0	323.5	-3718.10643	-3718.09669
3	-2304.16371	-2303.44971	218.6	198.4	-2303.55183	-2303.54241
	-2304.12955	-2303.41542	220.8	200.7	-2303.51858	-2303.50916
3a	-2286.95843	-2286.56091	132.5	110.9	-2286.62281	-2286.61273
	-2286.93287	-2286.53563	132.6	111.0	-2286.59757	-2286.58749
c3a	-4591.12687	-4590.01342	304.2	284.3	-4590.15555	-4590.14623
	-4591.08186	-4589.96847	313.2	293.3	-4590.11481	-4590.10549
3b	-2668.21737	-2667.75255	145.3	123.9	-2667.82041	-2667.81043
	-2668.18878	-2667.72370	143.9	122.5	-2667.79092	-2667.78094
c3b	-4972.38590	-4971.20456	319.0	299.2	-4971.35360	-4971.34432
	-4972.33881	-4971.15840	315.2	295.3	-4971.30563	-4971.29634
4	-2878.18972	-2877.03754	339.3	319.6	-2877.19874	-2877.18939
	-2878.15446	-2877.00175	339.5	319.8	-2877.16305	-2877.15370

4a	-416.18593 -416.17450	-416.06868 -416.05707	83.0 83.3	59.5 59.8	-416.10812 -416.09664	-416.09698 -416.08550
c4a	-3294.39810 -3294.36242	-3293.12507 -3293.08891	372.1 373.7	352.2 353.9	-3293.30184 -3293.26649	-3293.29243 -3293.25707
4b	-381.60431 -381.59592	-381.51230 -381.50382	77.0 76.6	53.6 53.3	-381.54888 -381.54024	-381.53777 -381.52913
c4b	-3259.80588 -3259.77070	-3258.55848 -3258.52279	372.5 377.2	352.8 357.4	-3258.73549 -3258.70201	-3258.72610 -3258.69261
5	-4213.91033 -4213.86808	-4212.87936 -4212.83689	317.0 320.5	296.6 300.1	-4213.02998 -4212.98918	-4213.02027 -4212.97948
5a	-2075.40531 -2075.38981	-2074.92489 -2074.90928	143.01 45.7	121.6 124.3	-2074.99283 -2074.97852	-2074.98265 -2074.96835
c5a	-6289.34160 -6289.29996	-6287.82565 -6287.78372	415.3 414.9	394.9 394.5	-6288.02297 -6287.98088	-6288.01325 -6287.97116

a) eqn. 12; b) eqn. 13

Table S3 The calculated solvation energies(kcal mol^{-1}), along with the experimental solvation energies.

quantity	solvent	E_{SSD} SMSSP	ΔE^{sol} PCM	ΔE^{sol} IDSCRF	ΔG_S*
C_3H_8	cyclohexane	-2.80	-4.10	-2.65	-2.1
C_4H_{10}	cyclohexane	-3.65	-4.91	-3.69	-2.86
C_5H_{12}	cyclohexane	-4.51	-5.68	-4.25	-3.50
C_8H_{18}	cyclohexane	-7.13	-8.04	-6.04	-5.63
cyclohexane	cyclohexane	-4.90	-5.86	-4.44	-4.43
benzene	cyclohexane	-4.69	-5.18	-4.09	-4.19
toluene	cyclohexane	-5.64	-5.95	-4.53	-4.90
ethylbenzene	cyclohexane	-6.53	-6.64	-5.04	-4.97
o-xylene	cyclohexane	-6.53	-6.64	-5.07	-5.54
m-xylene	cyclohexane	-6.60	-6.57	-5.08	-5.52
naphthalene	cyclohexane	-8.19	-7.23	-5.67	-7.17
methanol	cyclohexane	-1.29	-2.36	-1.97	-1.38
ethanol	cyclohexane	-2.25	-3.76	-2.74	-2.42
1-propanol	cyclohexane	-3.09	-4.58	-3.40	-2.73
isopropanol	cyclohexane	-3.11	-4.51	-3.23	-2.37
1-butanol	cyclohexane	-3.95	-5.40	-4.02	-3.52
t-butanol	cyclohexane	-3.94	-5.19	-3.52	-2.93
1-pentanol	cyclohexane	-4.81	-6.16	-4.63	-3.61
phenol	cyclohexane	-5.07	-5.63	-4.62	-5.57
1-hexanol	cyclohexane	-5.68	-6.99	-5.27	-5.31
o-cresol	cyclohexane	-5.99	-6.38	-4.91	-6.02
m-cresol	cyclohexane	-6.02	-6.41	-4.95	-5.20
p-cresol	cyclohexane	-6.02	-6.43	-4.95	-5.89
1-heptanol	cyclohexane	-6.56	-7.73	-5.89	-6.02
1,4-dioxane	cyclohexane	-3.88	-5.37	-4.03	-4.17
diethylether	cyclohexane	-3.95	-5.45	-3.61	-3.03
anisol	cyclohexane	-6.02	-6.45	-4.96	-5.38
benzaldehyde	cyclohexane	-5.87	-7.13	-5.14	-5.71
acetone	cyclohexane	-2.86	-4.21	-2.78	-2.67
2-butanone	cyclohexane	-3.68	-5.28	-3.74	-3.48

2-pentanone	cyclohexane	-4.54	-5.81	-4.00	-4.19
3-pentanone	cyclohexane	-4.50	-5.79	-3.99	-4.30
2-hexanone	cyclohexane	-5.41	-6.57	-4.62	-4.77
3,3-dimethylbutanone	cyclohexane	-5.32	-6.46	-4.30	-4.42
2-heptanone	cyclohexane	-6.28	-7.38	-5.23	-5.47
acetophenone	cyclohexane	-6.69	-6.83	-5.08	-6.29
aceticacid	cyclohexane	-2.28	-3.89	-2.99	-1.73
propanoicacid	cyclohexane	-3.10	-4.69	-3.65	-3.78
methylacetate	cyclohexane	-3.12	-4.75	-3.08	-3.06
methylpropanoate	cyclohexane	-3.95	-5.53	-3.71	-3.71
ethylacetate	cyclohexane	-3.99	-5.04	-3.72	-3.56
propylacetate	cyclohexane	-4.85	-6.34	-4.35	-4.36
methylpentanoate	cyclohexane	-5.70	-7.11	-4.95	-5.04
butylacetate	cyclohexane	-5.73	-7.11	-4.97	-4.94
methylhexanoate	cyclohexane	-6.57	-7.89	-5.56	-5.75
pentylacetate	cyclohexane	-6.61	-7.90	-5.58	-5.71
ethylamine	cyclohexane	-2.60	-3.96	-2.87	-2.04
trimethylamine	cyclohexane	-3.51	-4.73	-2.92	-2.63
diethylamine	cyclohexane	-4.27	-5.58	-3.79	-3.61
pyridine	cyclohexane	-4.33	-5.02	-3.95	-4.30
aniline	cyclohexane	-5.52	-5.83	-5.03	-5.52
2-methylpyridine	cyclohexane	-5.29	-5.83	-4.24	-5.05
3-methylpyridine	cyclohexane	-5.27	-5.80	-4.24	-5.14
4-methylpyridine	cyclohexane	-5.27	-5.80	-4.25	-5.23
N-methylaniline	cyclohexane	-6.49	-6.61	-4.91	-6.33
2,6-dimethylpyridine	cyclohexane	-6.26	-6.59	-4.48	-5.51
Acetonitrile	cyclohexane	-1.95	-3.19	-2.16	-1.87
Benzonitrile	cyclohexane	-5.89	-5.90	-4.68	-5.54
1-nitropropane	cyclohexane	-3.80	-5.28	-4.02	-4.06
Nitrobenzene	cyclohexane	-5.92	-6.35	-5.16	-6.62
2-methyl-1-nitrobenzene	cyclohexane	-6.84	-7.00	-5.37	-6.71
1-propanethiol	cyclohexane	-4.27	-5.56	-4.01	-3.12
Thioanisole	cyclohexane	-7.33	-7.26	-5.24	-5.66
m-hydroxybenzaldehyde	cyclohexane	-6.26	-6.51	-5.27	-6.88
p-hydroxybenzaldehyde	cyclohexane	-6.39	-6.55	-5.33	-7.19
Fluorobenzene	cyclohexane	-4.69	-5.46	-4.35	-3.59
1,1,1-trichloroethane	cyclohexane	-4.78	-6.08	-4.20	-4.08
Trichloroethene	cyclohexane	-4.79	-6.01	-4.34	-4.29
Chlorobenzene	cyclohexane	-5.76	-6.15	-4.72	-5.10
1,4-dichlorobenzene	cyclohexane	-6.91	-7.12	-5.35	-5.89
bromobenzene	cyclohexane	-6.26	-6.50	-4.92	-5.29
2,2,2-trifluoroethanol	cyclohexane	-2.28	-4.66	-3.86	-1.53
p-bromophenol	cyclohexane	-6.65	-6.97	-5.43	-7.14
water	cyclohexane	-0.57	-1.77	-1.61	-0.39
trimethylphosphate	cyclohexane	-5.02	-7.01	-5.46	-5.67
triethylphosphate	cyclohexane	-7.64	-8.89	-6.80	-7.60
tripropylphosphate	cyclohexane	-10.23	-10.58	-8.16	-7.71
methylbenzoate	cyclohexane	-7.02	-7.35	-5.70	-7.01
tetrahydropyran	cyclohexane	-4.39	-5.63	-4.25	-4.41
ethylphenylether	cyclohexane	-6.96	-7.24	-5.32	-6.00
difluorodichloromethane	cyclohexane	-3.02	-5.08	-3.82	-1.18
fluorotrichloromethane	cyclohexane	-3.96	-5.71	-4.17	-2.63
3,5-dibromo-4-hydroxyben	cyclohexane	-9.58	-8.72	-6.71	-6.83

zonitrile					
nitromethane	cyclohexane	-2.13	-3.67	-2.71	-2.86
N,N-dimethylformamide	cyclohexane	-3.53	-4.87	-3.30	-3.83
pyrrole	cyclohexane	-3.67	-4.58	-3.66	-3.77
quinoline	cyclohexane	-7.82	-7.10	-5.57	-7.38
benzamide	cyclohexane	-6.43	-7.15	-5.82	-8.72
2-methylaniline	cyclohexane	-6.42	-6.49	-4.95	-6.44
3-methylaniline	cyclohexane	-6.48	-6.56	-4.97	-6.47
4-methylaniline	cyclohexane	-6.49	-6.57	-4.98	-6.30
iodobenzene	cyclohexane	-7.23	-7.27	-5.63	-6.26
n-octane	CCl_4	-7.61	-6.58	-5.15	-5.39
2-methylpropene	CCl_4	-3.86	-3.75	-2.93	-2.63
1-butene	CCl_4	-3.78	-3.79	-2.96	-2.48
E-2-pentene	CCl_4	-4.86	-4.47	-3.48	-3.46
benzene	CCl_4	-5.01	-4.30	-3.38	-4.50
toluene	CCl_4	-6.02	-4.96	-3.86	-5.12
ethylbenzene	CCl_4	-6.97	-5.48	-4.28	-5.67
o-xylene	CCl_4	-6.98	-5.50	-4.32	-6.07
m-xylene	CCl_4	-7.04	-5.52	-4.32	-5.71
naphthalene	CCl_4	-8.75	-5.98	-4.86	-7.55
methanol	CCl_4	-1.48	-2.34	-1.88	-2.25
ethanol	CCl_4	-2.40	-3.08	-2.44	-2.96
1-propanol	CCl_4	-3.30	-3.75	-2.98	-3.64
isopropanol	CCl_4	-3.32	-3.70	-2.95	-3.15
1-butanol	CCl_4	-4.22	-4.40	-3.49	-4.20
t-butanol	CCl_4	-4.21	-4.33	-3.43	-3.40
1-pentanol	CCl_4	-5.14	-5.06	-4.00	-4.73
phenol	CCl_4	-5.41	-4.64	-3.92	-6.14
1-hexanol	CCl_4	-6.07	-5.67	-4.50	-5.04
o-cresol	CCl_4	-6.40	-5.27	-4.18	-6.51
p-cresol	CCl_4	-6.43	-5.47	-4.52	-6.32
1-heptanol	CCl_4	-7.00	-5.70	-4.50	-6.49
1,4-dioxane	CCl_4	-4.15	-4.43	-3.56	-4.97
anisole	CCl_4	-6.43	-5.31	-4.22	-5.49
benzaldehyde	CCl_4	-6.27	-5.03	-4.22	-6.11
acetone	CCl_4	-3.06	-3.46	-2.79	-3.35
2-butanone	CCl_4	-3.93	-4.11	-3.28	-4.09
cyclopentanone	CCl_4	-4.43	-4.49	-3.54	-5.56
2-pentanone	CCl_4	-4.85	-4.76	-3.79	-4.81
2-hexanone	CCl_4	-5.78	-5.40	-4.29	-5.47
2-heptanone	CCl_4	-6.71	-6.05	-4.79	-6.12
acetophenone	CCl_4	-7.14	-5.63	-4.51	-7.10
aceticacid	CCl_4	-2.43	-3.20	-2.63	-3.64
propanoicacid	CCl_4	-3.31	-3.86	-3.14	-4.09
butanoicacid	CCl_4	-4.23	-4.49	-3.63	-4.81
hexanoicacid	CCl_4	-6.08	-5.80	-4.69	-6.99
methylacetate	CCl_4	-3.33	-3.90	-3.14	-3.82
methylpropanoate	CCl_4	-4.22	-4.54	-3.62	-4.43
ethylacetate	CCl_4	-4.26	-4.53	-3.61	-4.40
propylacetate	CCl_4	-5.18	-5.17	-4.11	-5.03
methylpentanoate	CCl_4	-6.07	-6.45	-5.11	-5.71
butylacetate	CCl_4	-6.12	-5.81	-4.61	-5.59
methylhexanoate	CCl_4	-7.02	-6.46	-5.12	-6.36

pentylacetate	CCl_4	-7.06	-6.45	-5.12	-6.35
ethylamine	CCl_4	-2.78	-3.25	-2.54	-2.77
dimethylamine	CCl_4	-2.78	-3.27	-2.55	-2.75
propylamine	CCl_4	-3.67	-3.90	-3.06	-3.59
trimethylamine	CCl_4	-3.75	-3.89	-3.05	-3.09
butylamine	CCl_4	-4.59	-4.56	-3.58	-5.35
diethylamine	CCl_4	-4.56	-4.56	-3.57	-4.12
pyridine	CCl_4	-4.62	-4.16	-3.38	-5.01
aniline	CCl_4	-5.89	-4.83	-3.99	-6.10
N-methylaniline	CCl_4	-6.93	-5.45	-4.29	-6.58
benzonitrile	CCl_4	-6.29	-4.88	-4.00	-6.28
1-nitropropane	CCl_4	-4.06	-3.98	-3.23	-4.49
nitrobenzene	CCl_4	-6.32	-4.89	-4.06	-6.92
2-methyl-1-nitrobenzene	CCl_4	-7.31	-5.46	-4.27	-7.39
thioanisole	CCl_4	-7.83	-5.97	-4.63	-5.66
p-hydroxybenzaldehyde	CCl_4	-6.82	-5.33	-4.55	-8.16
fluorobenzene	CCl_4	-5.01	-4.53	-3.71	-3.64
chlorobenzene	CCl_4	-6.15	-5.11	-4.05	-5.21
1,4-dichlorobenzene	CCl_4	-7.38	-5.95	-4.59	-6.28
bromobenzene	CCl_4	-6.68	-5.40	-4.23	-5.85
p-bromophenol	CCl_4	-7.11	-5.78	-4.64	-7.86
ammonia	CCl_4	-0.94	-1.67	-1.35	-1.06
water	CCl_4	-0.61	-1.44	-1.32	-0.85
trimethylphosphate	CCl_4	-5.36	-5.80	-4.62	-7.24
triethylphosphate	CCl_4	-8.16	-7.25	-5.75	-7.51
tripropylphosphate	CCl_4	-10.92	-8.75	-6.89	-8.60
methylamine	CCl_4	-1.82	-2.52	-1.97	-2.53
methylbenzoate	CCl_4	-7.50	-6.06	-4.83	-7.19
nitromethane	CCl_4	-2.28	-3.02	-2.55	-3.52
carbontetrachloride	CCl_4	-5.22	-5.26	-3.90	-4.35
benzamide	CCl_4	-6.86	-5.42	-4.36	-9.13
2-methylaniline	CCl_4	-6.86	-5.35	-4.21	-7.16
3-methylaniline	CCl_4	-6.92	-5.40	-4.25	-7.23
4-methylaniline	CCl_4	-6.94	-5.40	-4.25	-7.24
hydrogenperoxide	CCl_4	-1.00	-1.98	-1.66	-3.14
iodobenzene	CCl_4	-7.72	-6.10	-4.77	-6.50
n-heptane	heptane	-5.75	-6.71	-5.06	-4.65
benzene	heptane	-4.31	-4.80	-3.67	-4.00
toluene	heptane	-5.19	-5.52	-4.19	-4.78
o-xylene	heptane	-6.01	-6.16	-4.69	-5.52
m-xylene	heptane	-6.07	-6.21	-4.70	-5.57
p-xylene	heptane	-6.09	-6.22	-4.71	-5.52
naphthalene	heptane	-7.53	-6.71	-5.12	-7.02
anthracene	heptane	-11.46	-8.57	-6.55	-10.0
methanol	heptane	-1.27	-2.65	-2.06	-1.29
ethanol	heptane	-2.07	-3.48	-2.67	-2.16
1-propanol	heptane	-2.84	-4.24	-3.25	-3.01
1-butanol	heptane	-3.63	-4.95	-3.81	-3.66
1-pentanol	heptane	-4.43	-5.73	-4.35	-4.00
phenol	heptane	-4.66	-5.21	-4.03	-5.32
1-hexanol	heptane	-5.23	-6.42	-4.90	-4.89
o-cresol	heptane	-5.51	-5.91	-4.55	-6.01
m-cresol	heptane	-5.53	-5.94	-4.58	-5.01

p-cresol	heptane	-5.53	-5.95	-4.59	-5.77
1-heptanol	heptane	-6.03	-6.46	-4.90	-5.06
anisole	heptane	-5.54	-5.98	-4.59	-5.35
benzaldehyde	heptane	-5.40	-5.64	-4.39	-5.50
acetone	heptane	-2.63	-3.90	-3.05	-2.61
2-butanone	heptane	-3.38	-4.64	-3.58	-3.36
2-pentanone	heptane	-4.17	-5.38	-4.13	-4.07
2-hexanone	heptane	-4.97	-6.08	-4.68	-4.55
3,3-dimethylbutanone	heptane	-4.89	-5.85	-4.51	-4.30
2-heptanone	heptane	-5.78	-6.84	-5.22	-5.22
acetophenone	heptane	-6.15	-6.33	-4.89	-6.14
propanoicacid	heptane	-2.85	-4.35	-3.43	-4.06
butanoicacid	heptane	-3.64	-5.07	-3.97	-5.05
pentanoicacid	heptane	-4.44	-5.82	-4.53	-5.23
hexanoicacid	heptane	-5.24	-6.50	-5.09	-6.54
methylacetate	heptane	-2.87	-4.40	-3.44	-2.97
methylpropanoate	heptane	-3.63	-5.13	-3.96	-3.63
ethylacetate	heptane	-3.67	-5.13	-3.96	-3.50
propylacetate	heptane	-4.46	-2.23	-4.50	-4.09
methylpentanoate	heptane	-5.24	-6.60	-5.06	-4.92
butylacetate	heptane	-5.27	-6.59	-5.05	-4.83
methylhexanoate	heptane	-6.04	-7.31	-5.61	-5.63
pentylacetate	heptane	-6.08	-7.32	5.60	-5.42
ethylamine	heptane	-2.39	-3.67	-2.76	-2.09
propylamine	heptane	-3.16	-4.40	-3.33	-3.03
butylamine	heptane	-3.95	-5.14	-3.89	-3.55
pyridine	heptane	-3.98	-4.66	-3.58	-4.28
aniline	heptane	-5.08	-5.40	-4.14	-5.38
acetonitrile	heptane	-1.80	-2.95	-2.29	-2.06
benzonitrile	heptane	-5.42	-5.47	-4.23	-5.33
nitrobenzene	heptane	-5.44	-5.88	-4.72	-6.14
fluorobenzene	heptane	-4.31	-5.06	-3.93	-4.13
chlorobenzene	heptane	-5.30	-5.70	-4.29	-5.10
1,2-dichlorobenzene	heptane	-6.23	-6.52	-4.83	-6.01
1,4-dichlorobenzene	heptane	-6.35	-6.65	-4.89	-5.81
bromobenzene	heptane	-5.75	-6.02	-4.44	-5.72
p-dibromobenzene	heptane	-7.32	-7.23	-5.22	-7.55
trimethylphosphate	heptane	-4.61	-6.50	-5.05	-5.59
triethylphosphate	heptane	-7.02	-8.24	-6.29	-6.67
tripropylphosphate	heptane	-9.40	-9.97	-7.55	-7.50
2-octanone	heptane	-6.59	-7.52	-5.77	-5.68
thiophene	heptane	-4.02	-4.45	-3.67	-4.09
2,2'-dichlorobiphenyl	heptane	-10.63	-9.09	-6.80	-9.22
N,N-dimethylacetamide	heptane	-4.00	-5.19	-4.01	-4.80
benzamide	heptane	-5.91	-6.10	-4.76	-7.26
2-methylaniline	heptane	-5.91	-6.02	-4.57	-6.28
3-methylaniline	heptane	-5.95	-6.09	-4.62	-6.35
4-methylaniline	heptane	-5.97	-6.09	-4.62	-6.15
N-methyl-2-pyrrolidinone	heptane	-4.44	-5.47	-4.23	-5.80
5-fluorouracil	heptane	-4.32	-6.61	-4.56	-11.3
6-fluorouracil	heptane	-5.68	-5.63	-4.57	-12.7
iodobenzene	heptane	-6.64	-6.73	-5.15	-6.27