Novel working solvent for the production of hydrogen peroxide

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Supplementary Information

Table A.1 Detailed information about materials used in this work

Chemical name	Souce	Purification method	Mass fraction purity	Analysis method
2-ethylanthraquinone	Energy Chemical	none	0.99	HPLC
2-tert-butylanthraquinone	Aladdin Industrial Co.	none	0.97	HPLC
trimethylbenzene	Qianyang Technology Co.	distillation	0.990	GC
trioctyl phosphate	Qianyang Technology Co.	none	0.992	none
N,N,N,N-tetrapropyl malonamide	Tianjin Guangfu Chemical Regent Co.	distillation	0.965	GC
Cyclohexane	Tianjin Guangfu Chemical Regent Co.	none	0.995	none
N-hexane	Tianjin Guangfu Chemical Regent Co.	none	0.995	none
Toluene	Qianyang Technology Co.	none	0.990	none
Hydrogen	Dalian Special Gases Co. Ltd.	none	0.9999	GC

Table A.2 Physicochemical nature of studied solvents used in this work

Properties	Liquids					
	TMB	TOP	TPMA	Cyclohexane	N-hexane	Toluene
Formula	C_9H_{12}	$C_{36}H_{75}O_4P$	$C_{15}H_{30}N_2O_2$	C_6H_{14}	C_6H_{14}	C_7H_8
M / (g.mol^{-1})	120.19	434.63	270.41	84.16	86.17	92.14
ρ / (g.cm^{-3})	0.86	0.92	0.91	0.78	0.66	0.86
$P^0_{293.15k}$/ (10^3. Pa)	1.33	0.28	1.64	13.10	5.34	4.89
μ / (mPa.s)	1.154	11.27	6.93	0.89	0.31	0.59
T_c / (K)	652.30	743.15	450.65	553.55	507.25	593.15
P_c/ (10^6. Pa)	3.23	18.9	16.3	4.07	3.03	4.05

Table B.1: Calculation method for H_2 mole fraction in each neat solvent

Following sample calculation is based on the data in Figure 3 [T = 328.15k, P = 7×10^5 Pa, f_{H2} = 1.092×10^6 Pa]. The mole fraction of hydrogen in the neat solvent at a given gas-phase solute fugacity is estimated using Henry's law constants obtained from Figure5. At 328.15k, H=25.34 $\times10^5$ Pa, $M_{trimethylbenzene}$ = 120.19 g/mol, $\rho_{trimethylbenzene}$ = 0.86 g.cm^{-3}.

$$H = \frac{f_{H_2}}{x_{H_2}} \qquad \text{Eq. (B.1)}$$

$$x_{H_2} = \frac{c_{H_2}}{c_{TMB} + c_{H_2}} \qquad \text{Eq. (B.2)}$$

$$x_{TMB} = 1 - x_{H_2} \qquad \text{Eq. (B.3)}$$

$$\frac{n_{H_2}}{n_{TMB}} = \frac{x_{H_2}}{1 - x_{H_2}} \qquad \text{Eq. (B.4)}$$

Assuming the volume of hydrogen in the liquid phase is negligible compared to trimethylbenzene (TMB),

$$n_{TMB} = \frac{V_{sample} * \rho_{TMB}}{M_{TMB}} \qquad \text{Eq. (B.5)}$$

$$n_{H_2} = \frac{(V_{sample} * \rho_{TMB})}{M_{TMB}} * \frac{x_{H_2}}{1 - x_{H_2}} \qquad \text{Eq. (B.6)}$$

$$c_{H_2} = \frac{n_{H_2}}{V_{sample}} = \frac{\rho_{TMB}}{M_{TMB,}} * \frac{x_{H_2}}{1 - x_{H_2}} \qquad \text{Eq. (B.7)}$$

The foregoing equation is solved to obtain x_{H_2} = 0.00269.