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APPENDICES

APPENDIX A

BASIC INFORMATION OF COBALT

A1. General [Young (1960), Othmer (1991)]

Cobalt, a transition series metallic element having atomic number 27, is similar to silver in appearance.

Cobalt and cobalt compounds have expanded from use colorants in glassed and ground coat frits for pottery to drying agent in paints and lacquers, animal and human nutrients, electroplating materials, high temperature alloys, hard facing alloys, high speed tools, magnetic alloys, alloys used for prosthetics, and used in radiology. Cobalt is also as a catalyst for hydrocarbon refining from crude oil for the synthesis of heating fuel.

A2. Physical Properties

The electronic structure of cobalt is $[\text{Ar}]3d^74s^2$. At room temperature the crystalline structure of the α (or ϵ) form, is close-packed hexagonal (cph) and lattice parameters are $a = 0.2501$ nm and $c = 0.4066$ nm. Above approximately 417 °C, a face-centered cubic (fcc) allotrope, the γ (or β) form, having a lattice parameter $a = 0.3544$ nm, becomes the stable crystalline form. Physical properties of cobalt are listed in Table A.1.

The scale formed on unalloyed cobalt during exposure to air or oxygen at high temperature is double-layered. In the range of 300 to 900 °C, the scale consists of a thin layer of mixed cobalt oxide, Co_3O_4 , on the outside and cobalt(II) oxide, CoO , layer next to metal. Cobalt (III) oxide, Co_2O_3 may be formed at temperature below 300 °C. Above 900 °C, Co_3O_4 decomposes and both layers, although of different appearance, are composed of CoO only. Scales formed below 600 °C and above 750 °C appear to crack on cooling, whereas those produced at 600 - 750 °C crack and flake off the surface.

Cobalt forms numerous compounds and complexes of industrial importance. Cobalt, atomic weight 58.933, is one of the members of the first transition series of Group 9 (VIII B). There are thirteen known isotopes, but only three are significant: ^{59}Co is the only stable and naturally occurring isotope; ^{60}Co has a half-life of 5.3 years and is a common source of γ -radioactivity; and ^{57}Co has a 270-d half-life and provides the source for Mössbauer spectroscopy.

Table A1 Physical properties of the cobalt [Othmer (1991)]

Property	Value
Atomic number	27
Atomic weight	58.93
Transformation temperature, °C	417
Heat of transformation, J/g ^a	251
melting point, °C	1493
latent heat of fusion, ΔH^{fus} J/g ^a	395
boiling point, °C	3100
latent heat of vaporization at bp, ΔH^{fus} J/g ^a	6276
specific heat, J/(g ⁰ C) ^a	
15-100 °C	0.442
Molten metal	0.560
coefficient of the thermalexpansion, °C ⁻¹	
cph at room temperature	12.5
fcc at 417 °C	14.2
thermal conductivity at 25 °C, W/(mK)	69.16
thermal neutron absorption, Bohr atom	34.8
resistivity, at 20 ⁰ C ^b , 10 ⁻⁸ Ω.m	6.24

Table A1 Physical properties of the cobalt [Othmer (1991)] (cont.)

Property	Value		
Curie temperature, °C	1121		
Saturation induction, $4\pi I_s, T^c$	1.870		
Permeability, μ			
Initial	68		
max	245		
Residual induction, T^c	0.490		
Coercive force, A/m	708		
Young's modulus, Gpac	211		
Poisson's ratio	0.32		
Hardness ^f , diamond pyramid, of % Co	99.9	99.98 ^e	
At 20 °C	225	253	
At 300 °C	141	145	
At 600 °C	62	43	
At 900 °C	22	17	
Strength of 99.99 % cobalt, Mpa ^g	as cast	annealed	sintered
Tensile	237	588	679
Tensile yield	138	193	302
Compressive	841	808	
Compressive yield	291	387	

^aTo convert J to cal, divided by 4.184.

^bconductivity = 27.6 % of International Annealed Copper standard.

^cTo convert T to gauss, multiply by 10^4 .

^dTo convert GPa to psi, multiply by 145,000.

^eZone refined.

^fVickers.

^gTo convert MPa to psi, multiply by 145.

Cobalt exists in the +2 or +3 valance states for the major of its compounds and complexes. A multitude of complexes of the cobalt (III) ion exists, but few stable simple salt are known. Octahedral stereochemistries are the most common for cobalt (II) ion as well as for cobalt (III). Cobalt (II) forms numerous simple compounds and complexes, most of which are octahedral or tetrahedral in nature; cobalt (II) forms more tetrahedral complex than other transition-metal ions. Because of the small stability difference between octahedral and tetrahedral complexes of cobalt (II), both can be found equilibrium for a number of complexes. Typically, octahedral cobalt (II) salts and complexes are pink to brownish red; most of the tetrahedral Co(II) species are blue.

A3. Cobalt Oxides

Cobalt has three well-known oxides:

Cobalt (II) oxide, CoO , is olive green, cubic crystalline material. Cobalt (II) oxide is the final product formed when the carbonate or the other oxides are calcined to a sufficiently high temperature, preferably in a neutral or slightly reducing atmosphere. Pure cobalt (II) oxide is a difficult substance to prepare, since it readily takes up oxygen even at room temperature to re-form a higher oxide. Above about 850°C , cobalt (II) oxide form is the stable oxide. The product of commerce is usually dark gray and contain 75-78 wt% cobalt. Cobalt (II) oxide is soluble in water, ammonia solution, and organic solvents, but dissolves in strong mineral acids. It is used in glass decorating and coloring and is a precursor for the production of cobalt chemical.

Cobalt(III) oxide, Co_2O_3 , is form when cobalt compounds are heated at a low temperature in the presence of an excess of air. Some authorities told that cobalt (III) oxide exists only in the hydrate form. The lower hydrate may be made as a black power by oxidizing neutral cobalt solutions with substance with substance like sodium hypochlorite. Co_2O_3 or $\text{Co}_2\text{O}_3 \cdot \text{H}_2\text{O}$ is completely converted to Co_2O_3 at temperature above 265°C . Co_2O_3 will absorb oxygen in a sufficient quantity to correspond to the higher oxide Co_2O_3

Cobalt oxide, Co_2O_3 , is formed when cobalt compound, such as the carbonate or the hydrate sesquioxide, are heated in air at temperature above approximately $265\text{ }^\circ\text{C}$ and not exceeding $800\text{ }^\circ\text{C}$.

A4. Co-based Catalysts

Support cobalt (Co) catalysts are the preferred catalysts for the synthesis of hydrocarbons from natural gas based syngas (CO and H_2) because of their high Fischer-Tropsch (FT) activity, high selectivity for linear hydrocarbons and low activity for the water-gas shift reaction. It is known that reduced cobalt metal, rather than its oxides or carbides, is the most active phase for CO hydrogenation in such catalysts. Investigations have been done to determine the nature of cobalt species on various supports such as alumina, silica, titania, magnesia, carbon, and zeolites. The influence of various types of cobalt precursor used was also investigated. It was found that the use of organic precursors such as Co(III) acetate resulting in an increase of Co conversion compared to that of cobalt nitrate.

A5. Cobalt-Support Compound Formation (Co-SCF)

Compound formation between cobalt metal and the support can occur under pretreatment and/or reaction conditions, leading to catalyst deactivation. The compound formation of cobalt metal with support materials, however, is difficult to predict because of the lack of sufficient thermodynamic data. Co-Support compound formation can be detected evidentially.

A6. Co-Aluminate Formation

Interaction of cobalt with its alumina support has been observed by many authors using various techniques including TPR, XRD, EXAFS, and XPS. The migration of cobalt ions into alumina lattice sites of octahedral or tetrahedral symmetry is limited to the first few layers of the support under normal calcination conditions. The reaction of Co with $\gamma\text{-Al}_2\text{O}_3$ can form a surface spinel in $\text{Co}/\gamma\text{-Al}_2\text{O}_3$ catalysts. The surface spinel structure can not be observed by X-ray diffraction because it does not have long range, three dimensional order. It has been suggested

that cobalt ions occupying surface octahedral site of $\gamma\text{-Al}_2\text{O}_3$ are reducible while cobalt ions occupying tetrahedral sites are non-reducible, at least at temperature ≤ 900 °C. At lower calcinations temperatures, filling of the octahedral sites is more favorable. Filling of the tetrahedral site of $\gamma\text{-Al}_2\text{O}_3$ may be enhanced by an increase in calcinations temperature.

A7. Co-silicate Formation

The formation of cobalt silicates on Co/SiO_2 under hydrothermal conditions has been extensively studied by Kogelbauer et al. (1995). Hydrothermal treatment at 200 °C led to a catalyst with lower reducibility due to the formation of both reducible and non-reducible (at-temperature ≤ 900 °C) cobalt silicates. It was found that hydrothermal treatment of the reduced catalyst or hydrothermal treatment of the calcinations catalyst in the presence of hydrogen produces cobalt silicates, while hydrothermal treatment of the calcined catalyst in air does not result in their formation. Hydrothermal treatment of the calcined catalyst in inert gas also has little effect.

APPENDIX B

CALCULATION FOR CATALYST PREPARATION

The calculations is base on weight of Sodium Silicate ($\text{Na}_2\text{O} \cdot \text{SiO}_2 \cdot \text{H}_2\text{O}$) in B1 and B2 solution.

$$\begin{aligned}\text{Molecular weight of Si} &= 28.0855 \\ \text{Molecular weight of SiO}_2 &= 60.0843 \\ \text{Weight present of SiO}_2 \text{ in Sodium Silicate} &= 28.5 \%\end{aligned}$$

Using Sodium Silicate 69g with 45 g of water as a B1 and B2 solution.

$$\begin{aligned}\text{Mole of Si used} &= \frac{\text{wt.} \times (\%) \times (\text{M.W. of Si}) \times (1 \text{ mole})}{100 (\text{M.W. of SiO}_2) (\text{M.W. of Si})} \\ &= 69 \times (28.5/100) \times (1/60.0843) \\ &= 0.3273 \text{ mole}\end{aligned}$$

For example , to prepare Si/Ti atomic ratio of 50 by using titanium butoxide 97%, $\text{Ti}[\text{O}(\text{CH}_2)_3\text{CH}_3]_4$, for titanium source.

$$\begin{aligned}\text{Molecular weight of Ti} &= 47.88 \\ \text{Molecular weight of Ti}[\text{O}(\text{CH}_2)_3\text{CH}_3]_4 &= 340.36 \\ \text{Weight \% purities of Ti}[\text{O}(\text{CH}_2)_3\text{CH}_3]_4 &= 97\end{aligned}$$

Si/Ti atomic ratio = 50

$$\begin{aligned}\text{Mole of Ti}[\text{O}(\text{CH}_2)_3\text{CH}_3]_4 \text{ required} &= 0.3273/50 \\ &= 6.546 \times 10^{-3} \text{ mole} \\ \text{amount of Ti}[\text{O}(\text{CH}_2)_3\text{CH}_3]_4 &= (6.546 \times 10^{-3}) \times (340.36) \times (100/97) \\ &= 2.2970 \text{ g}\end{aligned}$$

For preparing Si/Co atomic ratio of 150 by using $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ for cobalt source.

$$\begin{aligned}\text{Molecular weight of Co} &= 58.93 \\ \text{Molecular weight of Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O} &= 291.03\end{aligned}$$



Si/Ti atomic ratio = 150

$$\begin{aligned}
 \text{Mole of } \text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O} \text{ required} &= 0.3273/150 \\
 &= 2.182 \times 10^{-3} \text{ mole} \\
 \text{amount of } \text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O} &= (2.182 \times 10^{-3}) \times (291.03) \\
 &= 0.635027 \text{ g}
 \end{aligned}$$

Because of the addition of cobalt salts in either gel solution or decantation solution in amount of 2X but adding of cobalt salts in both of solutions (A1 and A2) is X.

$$\begin{aligned}
 \text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O} \text{ used in A1 and A2 solutions (X)} &= 0.635027 \text{ g} \\
 \text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O} \text{ used in either gel solution or decantation solution (2X)} &= 2 \times 0.635027 \\
 &= 1.270054 \text{ g}
 \end{aligned}$$

which is used in Table 3.3

For preparing Si/Co atomic ratio of 150 by using $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ for cobalt source.

$$\begin{aligned}
 \text{Molecular weight of Co} &= 58.93 \\
 \text{Molecular weight of } \text{CoCl}_2 \cdot 6\text{H}_2\text{O} &= 237
 \end{aligned}$$

Si/Ti atomic ratio = 150

$$\begin{aligned}
 \text{Mole of } \text{CoCl}_2 \cdot 6\text{H}_2\text{O} \text{ required} &= 0.3273/150 \\
 &= 2.182 \times 10^{-3} \text{ mole} \\
 \text{amount of } \text{CoCl}_2 \cdot 6\text{H}_2\text{O} &= (2.182 \times 10^{-3}) \times (237) \\
 &= 0.5171 \text{ g}
 \end{aligned}$$

Because of the addition of cobalt salts in either gel solution or decantation solution in amount of 2X but adding of cobalt salts in both of solutions (A1 and A2) is X.

$$\begin{aligned}
 \text{CoCl}_2 \cdot 6\text{H}_2\text{O} \text{ used in A1 and A2 solutions (X)} &= 0.5171 \text{ g} \\
 \text{CoCl}_2 \cdot 6\text{H}_2\text{O} \text{ used in either gel solution or decantation solution (2X)} &= 2 \times 0.5171 \\
 &= 1.0342 \text{ g}
 \end{aligned}$$

which is also used in Table 3.3

For preparing Si/Co atomic ratio of 150 by using $\text{Co}(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot 4\text{H}_2\text{O}$ for cobalt source.

$$\begin{aligned} \text{Molecular weight of Co} &= 58.93 \\ \text{Molecular weight of } \text{Co}(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot 4\text{H}_2\text{O} &= 249.08 \end{aligned}$$

Si/Ti atomic ratio = 150

$$\begin{aligned} \text{Mole of } \text{Co}(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot 4\text{H}_2\text{O} \text{ required} &= 0.3273/150 \\ &= 2.182 \times 10^{-3} \text{ mole} \\ \text{amount of } \text{Co}(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot 4\text{H}_2\text{O} &= (2.182 \times 10^{-3}) \times (249.08) \\ &= 0.54349 \text{ g} \end{aligned}$$

Because of the addition of cobalt salts in either gel solution or decantation solution in amount of 2X but adding of cobalt salts in both of solutions (A1 and A2) is X.

$$\begin{aligned} \text{Co}(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot 4\text{H}_2\text{O} \text{ used in A1 and A2 solutions (X)} &= 0.54349 \text{ g} \\ \text{Co}(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot 4\text{H}_2\text{O} \text{ used in either gel solution or decantation solution (2X)} & \\ &= 2 \times 0.54349 \\ &= 1.0870 \text{ g} \end{aligned}$$

which is also used in Table 3.3

APPENDIX C

THE DATA OF X-RAY FLUORESCENCE (XRF)

C1. Calculation of Chemical Composition by base on standard solution

Sample: Co/TS-1 (Co(NO₃)₂·6H₂O loading to A1)
Wed 2/14/2007 at 4:49:06 PM
Method Name: Method494139

FCD Name

- 1 Liquids A (S,Cl)
- 2 Medium Elmts - Liquids
- 3 V. Heavy Elmts - Liquids
- 4 V. Light Elmts - Liquids

FCD	LT,s	Zero	FWHM	Gain
1	30	-0.1	89.1	100.01
2	30	-0.8	121.1	100.01
3	30	-1.7	122.1	100.01
4	30	-0.4	89.2	100.01

Total: 27.27%

El Line	Concentration	+/- Err	Fit	Intensity
TiO2K	0.95 Wt %	4.70E-3	8.9	4187.7
Fe2O3Ka	153 ppm	8.25E-4	0.9	53.9
CoO Ka	0.96 Wt %	0.01	1.3	1495.8
Cu2OKa	87 ppm	8.70E-4	272.7	24.3
ZnO Ka	58 ppm	6.42E-4	65.1	20.4
Br Ka	7 ppm	3.07E-4	0.5	9.6
ZrO2Ka	30 ppm	3.11E-4	0.2	23.3
SiO2K	25.33 Wt %	0.07	42.7	13910.9

Sample: Co/TS-1 (Co(NO₃)₂·6H₂O loading to A2)
Wed 2/14/2007 at 5:03:51 PM
Method Name: Method494139

FCD Name

- 1 Liquids A (S,Cl)
- 2 Medium Elmts - Liquids
- 3 V. Heavy Elmts - Liquids
- 4 V. Light Elmts - Liquids

FCD	LT,s	Zero	FWHM	Gain
1	30	-0.1	89.1	100.01
2	30	-0.9	121.2	100.01
3	30	-1.6	122.0	100.01
4	30	-0.4	89.2	100.01

Total: 24.78%

El Line	Concentration	+/- Err	Fit	Intensity
TiO2K	1.30 Wt %	4.91E-3	20.6	7149.9
Fe2O3Ka	118 ppm	6.71E-4	2.0	43.1
CoO Ka	1 ppm	9.88E-4	1.6	0.1
Cu2OKa	48 ppm	5.83E-4	0.9	16.9
ZnO Ka	57 ppm	5.01E-4	0.1	25.4
Br Ka	15 ppm	2.72E-4	0.4	28.4
ZrO2Ka	41 ppm	2.94E-4	0.2	37.1
SiO2K	23.45 Wt %	0.06	40.3	13836.1

Sample: Co-TS-1 (Co(NO₃)₂·6H₂O loading to C1)
 Wed 2/14/2007 at 5:11:16 PM
 Method Name: Method494139

FCD Name

- 1 Liquids A (S,C1)
- 2 Medium Elmts - Liquids
- 3 V. Heavy Elmts - Liquids
- 4 V. Light Elmts - Liquids

FCD	LT,s	Zero	FWHM	Gain
1	30	-0.1	89.1	100.01
2	30	-1.0	121.1	100.01
3	30	-1.6	122.1	100.01
4	30	-0.4	89.3	100.01

Total: 27.55%

El Line	Concentration	+/- Err	Fit	Intensity
TiO2K	0.85 Wt %	4.26E-3	9.6	4108.5
Fe2O3Ka	146 ppm	7.38E-4	0.8	59.7
CoO Ka	0.60 Wt %	0.01	1.2	1082.4
Cu2OKa	62 ppm	6.72E-4	177.6	21.5
ZnO Ka	37 ppm	4.37E-4	43.1	16.4
Br Ka	9 ppm	2.60E-4	0.9	16.7
ZrO2Ka	21 ppm	2.29E-4	0.2	18.0
SiO2K	26.08 Wt %	0.07	44.1	14922.0

Sample: Co-TS-1 (Co(NO₃)₂·6H₂O loading to A1 and A2)
 Tue 3/06/2007 at 11:21:30 AM
 Method Name: Method494139

FCD Name

- 1 Liquids A (S,C1)
- 2 Medium Elmts - Liquids
- 3 V. Heavy Elmts - Liquids
- 4 V. Light Elmts - Liquids

FCD	LT,s	Zero	FWHM	Gain
1	30	-0.1	88.9	100.01
2	30	-0.8	120.8	100.01
3	30	-1.6	121.7	100.01
4	30	-0.5	89.2	100.01

Total: 27.48%

El Line	Concentration	+/- Err	Fit	Intensity
TiO2K	1.06 Wt %	4.63E-3	13.6	5440.7
Fe2O3Ka	142 ppm	7.47E-4	1.3	56.7
CoO Ka	0.42 Wt %	4.97E-3	1.9	738.9
Cu2OKa	68 ppm	6.69E-4	107.8	24.1
ZnO Ka	47 ppm	5.15E-4	23.9	21.0
Br Ka	16 ppm	2.68E-4	0.7	29.4
ZrO2Ka	37 ppm	2.87E-4	0.1	32.1
SiO2K	98.48 Wt %	0.07	35.4	15023.0

Sample: Co-TS-1 (CoCl₂ · 6H₂O loading to Al)

Sun 11/19/2006 at 1:45:12 PM

Method Name: Method494139

FCD Name

- 1 Liquids A (S,Cl)
- 2 Medium Elmts - Liquids
- 3 V. Heavy Elmts - Liquids
- 4 V. Light Elmts - Liquids

FCD LT,s Zero FWHM Gain

1	30	-0.2	89.1	100.01
2	30	-0.8	121.2	100.01
3	30	-1.7	122.3	100.01
4	30	-0.5	89.2	100.01

Total: 29.69%

El Line	Concentration	+/- Err	Fit	Intensity
TiO2K	1.22 Wt %	0.01	14.3	5232.3
Fe2O3Ka	114 ppm	7.99E-4	1.4	34.5
CoO Ka	0.98 Wt %	0.01	3.9	1320.2
Cu2OKa	96 ppm	8.83E-4	222.4	23.5
ZnO Ka	37 ppm	6.16E-4	55.3	11.4
Br Ka	15 ppm	3.32E-4	0.1	18.5
ZrO2Ka	81 ppm	4.66E-4	0.1	53.4
SiO2K	27.44 Wt %	0.07	40.8	15331.6

Sample: Co-TS-1 (CoCl₂ · 6H₂O loading to Cl)

Sun 11/19/2006 at 1:52:31 PM

Method Name: Method494139

FCD Name

- 1 Liquids A (S,Cl)
- 2 Medium Elmts - Liquids
- 3 V. Heavy Elmts - Liquids
- 4 V. Light Elmts - Liquids

FCD LT,s Zero FWHM Gain

1	30	-0.1	89.0	100.01
2	30	-0.9	121.0	100.01
3	30	-2.0	122.4	100.01
4	30	-0.4	89.3	100.01

Total: 30.58%

El Line	Concentration	+/- Err	Fit	Intensity
TiO2K	1.22 Wt %	0.01	11.4	4582.4
Fe2O3Ka	107 ppm	8.20E-4	0.8	35.3
CoO Ka	1.56 Wt %	0.01	8.0	2264.9
Cu2OKa	86 ppm	9.47E-4	419.7	20.8
ZnO Ka	41 ppm	6.34E-4	110.2	12.5
Br Ka	43 ppm	3.86E-4	0.4	53.8
ZrO2Ka	79 ppm	4.34E-4	0.4	55.8
SiO2K	27.77 Wt %	0.07	39.9	14932.2

Sample: Co-TS-1 (CoCl₂ · 6H₂O loading to A1 and A2)

Tue 12/12/2006 at 11:37:38 AM

Method Name: Method494139

FCD Name

- 1 Liquids A (S,Cl)
- 2 Medium Elmts - Liquids
- 3 V. Heavy Elmts - Liquids
- 4 V. Light Elmts - Liquids

FCD LT,s Zero FWHM Gain

1	30	-0.1	89.3	100.01
2	30	-1.0	121.2	100.01
3	30	-1.7	122.0	100.01
4	30	-0.4	89.3	100.01

Total: 27.51%

El Line	Concentration	+/- Err	Fit	Intensity
TiO2K	1.28 Wt %	0.01	14.8	6148.9
Fe2O3Ka	100 ppm	7.08E-4	1.5	35.9
CoO Ka	0.47 Wt %	0.01	0.3	740.0
Cu2OKa	69 ppm	6.84E-4	113.4	21.8
ZnO Ka	38 ppm	5.21E-4	23.5	15.2
Br Ka	9 ppm	2.86E-4	0.2	14.1
ZrO2Ka	42 ppm	2.94E-4	0.2	34.9
SiO2K	25.73 Wt %	0.07	41.9	14769.7

Sample: Co-TS-1 (Co(C₂H₃O₂)₂ · 4H₂O loading to A1)

Tue 12/12/2006 at 11:14:17 AM

Method Name: Method494139

FCD Name

- 1 Liquids A (S,Cl)
- 2 Medium Elmts - Liquids
- 3 V. Heavy Elmts - Liquids
- 4 V. Light Elmts - Liquids

FCD LT,s Zero FWHM Gain

1	30	-0.1	89.1	100.01
2	30	-0.9	121.1	100.01
3	30	-1.8	122.5	100.01
4	30	-0.5	89.2	100.01

Total: 31.09%

El Line	Concentration	+/- Err	Fit	Intensity
TiO2K	1.13 Wt %	0.01	10.5	4642.6
Fe2O3Ka	177 ppm	8.84E-4	2.0	62.6
CoO Ka	1.47 Wt %	0.01	2.6	2299.6
Cu2OKa	79 ppm	9.07E-4	446.7	21.0
ZnO Ka	58 ppm	6.58E-4	111.0	19.2
Br Ka	12 ppm	3.04E-4	0.7	16.0
ZrO2Ka	61 ppm	3.91E-4	0.6	44.6
SiO2K	28.45 Wt %	0.07	43.9	15496.9

Sample: Co-TS-1 (Co(C₂H₃O₂)₂·4H₂O loading to Cl)

Tue 12/12/2006 at 11:22:53 AM

Method Name: Method494139

FCD Name

- 1 Liquids A (S,Cl)
- 2 Medium Elmts - Liquids
- 3 V. Heavy Elmts - Liquids
- 4 V. Light Elmts - Liquids

FCD LT,s Zero FWHM Gain

1	30	-0.1	89.2	100.01
2	30	-0.9	121.2	100.01
3	30	-1.7	122.4	100.01
4	30	-0.4	89.2	100.01

Total: 30.09%

El Line	Concentration	+/- Err	Fit	Intensity
TiO2K	1.31 Wt %	0.01	10.9	4755.7
Fe2O3Ka	123 ppm	7.62E-4	0.6	45.4
CoO Ka	1.64 Wt %	0.01	6.5	2671.1
Cu2OKa	86 ppm	9.19E-4	473.8	23.0
ZnO Ka	42 ppm	6.57E-4	130.2	14.3
Br Ka	15 ppm	3.37E-4	0.7	20.6
ZrO2Ka	53 ppm	3.90E-4	0.3	36.6
SiO2K	27.11 Wt %	0.07	44.7	14404.2

Sample: Co-TS-1 (Co(C₂H₃O₂)₂·4H₂O loading to A1 and A2)

Tue 12/12/2006 at 11:30:16 AM

Method Name: Method494139

FCD Name

- 1 Liquids A (S,Cl)
- 2 Medium Elmts - Liquids
- 3 V. Heavy Elmts - Liquids
- 4 V. Light Elmts - Liquids

FCD LT,s Zero FWHM Gain

1	30	-0.1	89.2	100.01
2	30	-0.9	121.2	100.01
3	30	-1.8	122.4	100.01
4	30	-0.4	89.3	100.01

Total: 27.96%

El Line	Concentration	+/- Err	Fit	Intensity
TiO2K	1.11 Wt %	4.96E-3	12.1	5154.3
Fe2O3Ka	115 ppm	7.62E-4	1.8	39.8
CoO Ka	0.73 Wt %	0.01	2.2	1123.8
Cu2OKa	73 ppm	7.86E-4	184.8	21.3
ZnO Ka	48 ppm	5.99E-4	42.3	17.5
Br Ka	6 ppm	2.90E-4	0.4	8.8
ZrO2Ka	44 ppm	3.39E-4	0.5	35.1
SiO2K	26.08 Wt %	0.07	44.2	14729.0

C2. Calculation of Chemical Composition from Information Library in Software of XRF Instrument

Sample: Co/TS-1 (Co(NO₃)₂·6H₂O loading to A1)

Wed 2/14/2007 at 4:49:06 PM

Method Name: Sample493105-4_Co TS1 Metal

Analyte	Concentration	Intensity
K2O	47 ppm	10.5
CaO	53 ppm	13.8
TiO2	0.72 Wt %	4187.5
Fe2O3	0.02 wt %	54.0
CoO	0.74 Wt %	1495.3
Cu2O	15 ppm	24.4
ZnO	13 ppm	20.4
ZrO2	5 ppm	23.3
SiO2	85.25 Wt %	13910.9

Sample: Co/TS-1 (Co(NO₃)₂·6H₂O loading to A2)

Wed 2/14/2007 at 5:03:51 PM

Method Name: Sample493105-4_Co TS1 Metal

Analyte	Concentration	Intensity
K2O	40 ppm	11.5
CaO	60 ppm	19.9
TiO2	0.97 Wt %	7149.7
Fe2O3	0.01 wt %	43.0
CoO	7E-3 ppm	1.5E-3
Cu2O	9 ppm	16.9
ZnO	14 ppm	25.2
ZrO2	7 ppm	37.1
SiO2	82.93 Wt %	13836.1

Sample: Co-TS-1 (Co(NO₃)₂·6H₂O loading to C1)

Wed 2/14/2007 at 5:11:16 PM

Method Name: Sample493105-4_Co TS1 Metal

Analyte	Concentration	Intensity
K2O	27 ppm	6.7
CaO	30 ppm	8.8
TiO2	0.63 Wt %	4108.5
Fe2O3	0.01 wt %	60.0

CoO	0.46 Wt %	1082.5
Cu2O	11 ppm	21.7
ZnO	9 ppm	16.2
ZrO2	4 ppm	18.0
SiO2	88.66 Wt %	14922.0

Sample: Co-TS-1 (Co(NO₃)₂·6H₂O loading to A1 and A2)

Tue 3/06/2007 at 11:21:30 AM

Method Name: Sample493105-4_Co TS1 Metal

Analyte	Concentration	Intensity
K2O	73 ppm	19.4
CaO	86 ppm	26.5
TiO2	0.79 Wt %	5440.5
Fe2O3	132 ppm	56.8
CoO	0.32 Wt %	738.6
Cu2O	12 ppm	24.0
ZnO	11 ppm	20.9
ZrO2	6 ppm	32.1
SiO2	88.69 Wt %	15023.0

Sample: Co-TS-1 (CoCl₂ ·6H₂O loading to A1)

Sun 11/19/2006 at 1:45:12 PM

Method Name: Sample493105-4_Co TS1 Metal

Analyte	Concentration	Intensity
K2O	49 ppm	10.8
CaO	58 ppm	15.0
TiO2	0.91 Wt %	5232.1
Fe2O3	0.01 Wt %	34.4
CoO	0.74 Wt %	1319.7
Cu2O	16 ppm	23.5
ZnO	8 ppm	11.4
ZrO2	13 ppm	53.4
SiO2	91.19 Wt %	15331.6

Sample: Co-TS-1 (CoCl₂ ·6H₂O loading to C1)

Sun 11/19/2006 at 1:52:31 PM

Method Name: Sample493105-4_Co TS1 Metal

Analyte	Concentration	Intensity
K2O	35 ppm	6.8
CaO	70 ppm	15.6
TiO2	0.92 Wt %	4582.3
Fe2O3	0.01 wt %	35.2
CoO	1.18 Wt %	2264.4
Cu2O	14 ppm	21.0
ZnO	9 ppm	12.6
ZrO2	12 ppm	55.8
SiO2	90.66 Wt %	14932.2

Sample: Co-TS-1 (CoCl₂ · 6H₂O loading to A1 and A2)

Tue 12/12/2006 at 11:37:38 AM

Method Name: Sample493105-4_Co TS1 Metal

Analyte	Concentration	Intensity
K2O	50 ppm	12.4
CaO	64 ppm	18.5
TiO2	0.95 Wt %	6148.7
Fe2O3	0.01 wt %	35.7
CoO	0.35 Wt %	740.2
Cu2O	12 ppm	21.6
ZnO	9 ppm	15.3
ZrO2	7 ppm	34.9
SiO2	87.77 Wt %	14769.7

Sample: Co-TS-1 (Co(C₂H₃O₂)₂ · 4H₂O loading to A1)

Tue 12/12/2006 at 11:14:17 AM

Method Name: Sample493105-4_Co TS1 Metal

Analyte	Concentration	Intensity
K2O	30 ppm	6.3
CaO	50 ppm	12.3
TiO2	0.84 Wt %	4642.5
Fe2O3	0.02 wt %	62.7
CoO	1.11 Wt %	2299.2
Cu2O	13 ppm	21.2
ZnO	13 ppm	19.3
ZrO2	10 ppm	44.6
SiO2	92.77 Wt %	15496.9

Sample: Co-TS-1 (Co(C₂H₃O₂)₂ · 4H₂O loading to C1)

Tue 12/12/2006 at 11:22:53 AM

Method Name: Sample493105-4_Co TS1 Metal

Analyte	Concentration	Intensity
K2O	55 ppm	10.2
CaO	66 ppm	14.1
TiO2	1.00 Wt %	4755.6
Fe2O3	0.01 wt %	45.2
CoO	1.24 Wt %	2670.6
Cu2O	14 ppm	23.2
ZnO	9 ppm	14.3
ZrO2	8 ppm	36.6
SiO2	88.54 Wt %	14404.2

Sample: Co-TS-1 (Co(C₂H₃O₂)₂ · 4H₂O loading to A1 and A2)

Tue 12/12/2006 at 11:30:16 AM

Method Name: Sample493105-4_Co TS1 Metal

Analyte	Concentration	Intensity
K2O	69 ppm	16.5
CaO	52 ppm	14.3
TiO2	0.83 Wt %	5154.2
Fe2O3	107 ppm	39.6
CoO	0.55 Wt %	1123.7
Cu2O	13 ppm	21.4
ZnO	11 ppm	17.4
ZrO2	7 ppm	35.1
SiO2	88.15 Wt %	14729.0

Table C1 Chemical composition of the synthesized Co-TS-1 samples

Sample	Types of Salts	Loading Solution	Chemical composition ratios by mole				
			Si (%)	Ti (%)	Co (%)	Si/Ti	Si/Co
batch 1	Co(NO ₃) ₂ ·6H ₂ O	A1	32.96	0.21	0.23	157.45	143.67
batch 2		A2	33.04	0.29	0	113.69	N/A
batch 3		C1	33.06	0.18	0.14	187.14	240.37
batch 4		A1andA2	32.87	0.35	0.15	94.58	218.99
batch 5	CoCl ₂ ·6H ₂ O	A1	32.94	0.25	0.21	133.26	153.68
batch 6		C1	32.85	0.25	0.34	131.04	95.82
batch 7		A1andA2	32.99	0.27	0.11	122.86	312.74
batch 8	Co(C ₂ H ₃ O ₂) ₂ ·4H ₂ O	A1	32.89	0.22	0.32	146.86	104.23
batch 9		C1	32.80	0.28	0.37	117.74	89.05
batch 10		A1andA2	32.98	0.23	0.17	141.23	199.88

APPENDIX D
DATA AND CALCULATION OF ACID SITE

Table D1 Reported total peak area from Micromeritics Chemisorb 2750

Sample	Types of Salts	Loading Solution	Reported total peak area
batch 1	Co(NO ₃) ₂ ·6H ₂ O	A1	0.05045
batch 2		A2	0.02638
batch 3		C1	0.04793
batch 4		A1 and A2	0.04661
batch 5	CoCl ₂ ·6H ₂ O	A1	0.04969
batch 6		C1	0.05439
batch 7		A1 and A2	0.05012
batch 8	Co(C ₂ H ₃ O ₂) ₂ ·4H ₂ O	A1	0.05428
batch 9		C1	0.05477
batch 10		A1 and A2	0.04925

D1. Calculation of Total Acid Sites

For example, TS-1, total acid site is calculated from the following step.

1. Conversion of total peak area to peak volume

Conversion factor from Micromeritics Chemisorb 2750 is equal to 77.57016 ml/area unit. Therefore, total peak volume is derived from

$$\begin{aligned}
 \text{Total peak volume} &= 77.57016 \times \text{total peak area} \\
 &= 77.57016 \times 0.05045 \\
 &= 3.91390 \text{ ml}
 \end{aligned}$$

2. Calculation for adsorbed volume of 15% NH₃

$$\begin{aligned} \text{adsorbed volume of 15\% NH}_3 &= 0.15 \times \text{total peak volume} \\ &= 0.15 \times 3.91390 \text{ ml} \\ &= 0.58709 \text{ ml} \end{aligned}$$

3. Total acid sites are calculated from the following equation

$$\text{Total acid sites} = \frac{(\text{Adsorbed volume, ml}) \times 101.325 \text{ Pa}}{\left(8.314 \times 10^{-3} \frac{\text{Pa} \cdot \text{ml}}{\text{K} \cdot \mu\text{mol}}\right) \times 298 \text{ K} \times (\text{weight of catalyst, g})}$$

For Co-TS-1 sample, 0.1004 g of this one was measured, therefore

$$\begin{aligned} \text{Total acid sites} &= \frac{0.58709 \text{ ml} \times 101.325 \text{ Pa}}{\left(8.314 \times 10^{-3} \frac{\text{Pa} \cdot \text{ml}}{\text{K} \cdot \mu\text{mol}}\right) \times 298 \text{ K} \times (0.1004 \text{ g})} \\ &= 239.1432 \mu\text{mol H}^+/\text{g} \end{aligned}$$

D2. Calculation of Acid Site Ratio

To calculate acid site ratio, experiment data from Micromeritics Chemisorb 2750 are transferred to peak fitting program to separate peak. As known, the first peak of desorption process is indicated as weak acid, relative with another peak, and the second one is strong acid. Ratio of each acid site on the catalyst surface is calculated from peak areas reported by peak fitting program as shown above.

For example, Co-TS-1(Batch1), the ratio of each acid site on catalyst surface is calculated from the following equation.

$$\text{The ratio of weak acid} = \frac{1^{\text{st}} \text{ peak area}}{\text{summation of both peak areas}} \times 100 \%$$

From Figure 5.5a-2, 1st peak area and 2nd peak area are equal to 0.043134 and 0.012361, respectively.

$$\begin{aligned}\text{The ratio of weak acid} &= \frac{0.043134}{0.043134 + 0.012361} \times 100 \% \\ &= 74.68 \%\end{aligned}$$

$$\begin{aligned}\text{therefore, the ratio of strong acid} &= 100 - 74.68 \% \\ &= 25.32 \%\end{aligned}$$

Note. Reported center values of both peaks from peak fitting program reveal times at the maximum of both peaks occur. Since, we know the relationship between time and temperature during desorption process from Micromeritics Chemisorb 2750, hence, the temperature at the maximum of both peaks as we state as desorption temperature of both acid sites can be located.

APPENDIX E

DATA OF EXPERIMENTS

E1. The Conversion and Selectivity Value

Table E1 Data of Figure 5.8a ($\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ loading to A1).

Reaction temperature (°C)	Component				
	% 2-propanol (C)	% propylene (S)	% isopropyl ether (S)	% acetone (S)	% CO ₂ (S)
200	0.04	5.19	0.00	94.81	0.00
250	1.48	16.05	0.00	83.95	0.00
300	17.23	23.06	0.63	74.33	1.98
350	37.85	26.97	0.55	67.65	4.83
400	70.26	28.71	0.41	56.86	14.03
450	87.59	25.69	0.24	51.89	22.18
500	93.73	22.60	0.21	54.22	22.98

Table E2 Data of Figure 5.8b ($\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ loading to A2).

Reaction temperature (°C)	Component				
	% 2-propanol (C)	% propylene (S)	% isopropyl ether (S)	% acetone (S)	% CO ₂ (S)
200	2.78	0.62	0.00	99.38	0.00
250	5.70	5.13	0.00	94.87	0.00
300	8.31	20.60	0.67	78.73	0.00
350	25.31	27.46	0.57	64.75	7.22
400	60.46	29.22	0.42	59.35	11.01
450	85.31	25.56	0.30	50.01	24.13
500	91.17	25.29	0.24	51.92	22.54

Table E3 Data of Figure 5.8c ($\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ loading to C1).

Reaction temperature (°C)	Component				
	% 2-propanol (C)	% propylene (S)	% isopropyl ether (S)	% acetone (S)	% CO ₂ (S)
200	2.26	1.35	0.00	98.65	0.00
250	0.87	9.75	0.72	89.54	0.00
300	1.29	18.04	1.36	77.07	3.54
350	22.37	23.13	1.36	71.39	4.12
400	67.63	32.09	0.81	56.66	10.44
450	90.41	36.83	0.00	52.34	10.83
500	94.17	30.63	0.31	47.28	21.78

Table E4 Data of Figure 5.8d ($\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ loading to A1 and A2).

Reaction temperature (°C)	Component				
	% 2-propanol (C)	% propylene (S)	% isopropyl ether (S)	% acetone (S)	% CO ₂ (S)
200	1.95	6.48	0.00	93.52	0.00
250	3.26	11.39	0.20	88.41	0.00
300	2.98	26.00	0.33	71.12	2.55
350	36.35	29.99	0.50	65.19	4.32
400	68.92	32.44	0.34	57.49	9.73
450	90.21	30.48	0.19	47.30	22.03
500	95.19	28.12	0.16	50.46	21.26

Table E5 Data of Figure 5.8e ($\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ loading to A1).

Reaction temperature (°C)	Component				
	% 2-propanol (C)	% propylene (S)	% isopropyl ether (S)	% acetone (S)	% CO ₂ (S)
200	0.21	2.59	0.00	97.41	0.00
250	2.72	7.04	0.27	92.69	0.00
300	10.82	13.15	0.80	86.05	0.00
350	34.04	27.81	0.90	66.35	4.94
400	75.02	40.69	0.77	57.98	0.55
450	95.11	32.13	0.31	34.98	32.58
500	98.42	29.47	0.19	39.15	31.19

Table E6 Data of Figure 5.8f ($\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ loading to C1).

Reaction temperature (°C)	Component				
	% 2-propanol (C)	% propylene (S)	% isopropyl ether (S)	% acetone (S)	% CO ₂ (S)
200	0.38	17.57	0.00	82.43	0.00
250	1.31	59.93	0.09	39.98	0.00
300	18.47	68.64	0.21	30.19	0.96
350	44.32	52.87	0.41	43.42	3.30
400	74.12	40.67	0.30	47.58	11.45
450	91.20	30.25	0.21	48.47	21.07
500	95.61	26.88	0.20	50.70	22.22

Table E7 Data of Figure 5.8g ($\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ loading to A1 and A2).

Reaction temperature (°C)	Component				
	% 2-propanol (C)	% propylene (S)	% isopropyl ether (S)	% acetone (S)	% CO ₂ (S)
200	1.72	4.26	0.00	95.74	0.00
250	0.95	20.41	0.42	79.17	0.00
300	5.28	32.52	1.02	66.46	0.00
350	22.88	24.92	0.57	70.12	4.39
400	70.48	32.38	0.46	55.52	11.64
450	91.70	28.12	0.25	50.01	21.62
500	95.27	25.84	0.20	50.32	23.64

Table E8 Data of Figure 5.8h ($\text{Co}(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot 4\text{H}_2\text{O}$ loading to A1).

Reaction temperature (°C)	Component				
	% 2-propanol (C)	% propylene (S)	% isopropyl ether (S)	% acetone (S)	% CO ₂ (S)
200	2.27	6.05	0.00	93.95	0.00
250	3.03	11.75	0.00	88.25	0.00
300	5.77	22.54	0.43	77.03	0.00
350	27.34	28.34	0.58	66.14	4.94
400	67.99	34.52	0.40	50.30	14.78
450	89.31	32.40	0.28	46.96	20.36
500	94.45	29.87	0.20	48.25	21.67

Table E9 Data of Figure 5.8i ($\text{Co}(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot 4\text{H}_2\text{O}$ loading to C1).

Reaction temperature (°C)	Component				
	% 2-propanol (C)	% propylene (S)	% isopropyl ether (S)	% acetone (S)	% CO ₂ (S)
200	-0.33	1.47	0.00	98.53	0.00
250	1.86	6.41	0.35	93.24	0.00
300	12.77	16.47	0.60	82.93	0.00
350	28.59	27.50	0.63	69.32	2.54
400	69.78	35.04	0.53	54.89	9.55
450	93.14	29.03	0.34	48.45	22.18
500	94.91	28.98	0.28	51.39	19.34

Table E10 Data of Figure 5.8j ($\text{Co}(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot 4\text{H}_2\text{O}$ loading to A1 and A2).

Reaction temperature (°C)	Component				
	% 2-propanol (C)	% propylene (S)	% isopropyl ether (S)	% acetone (S)	% CO ₂ (S)
200	0.58	1.20	0.00	98.80	0.00
250	7.40	9.57	0.00	90.43	0.00
300	23.61	23.97	0.54	74.76	0.73
350	27.14	31.28	0.56	64.74	3.43
400	68.67	38.73	0.39	50.98	9.90
450	88.65	35.55	0.25	49.09	15.12
500	95.42	31.83	0.19	48.69	19.29

E2. The Grams Mole of Products from 2-Propanol Oxidation Reaction over Co-TS-1.

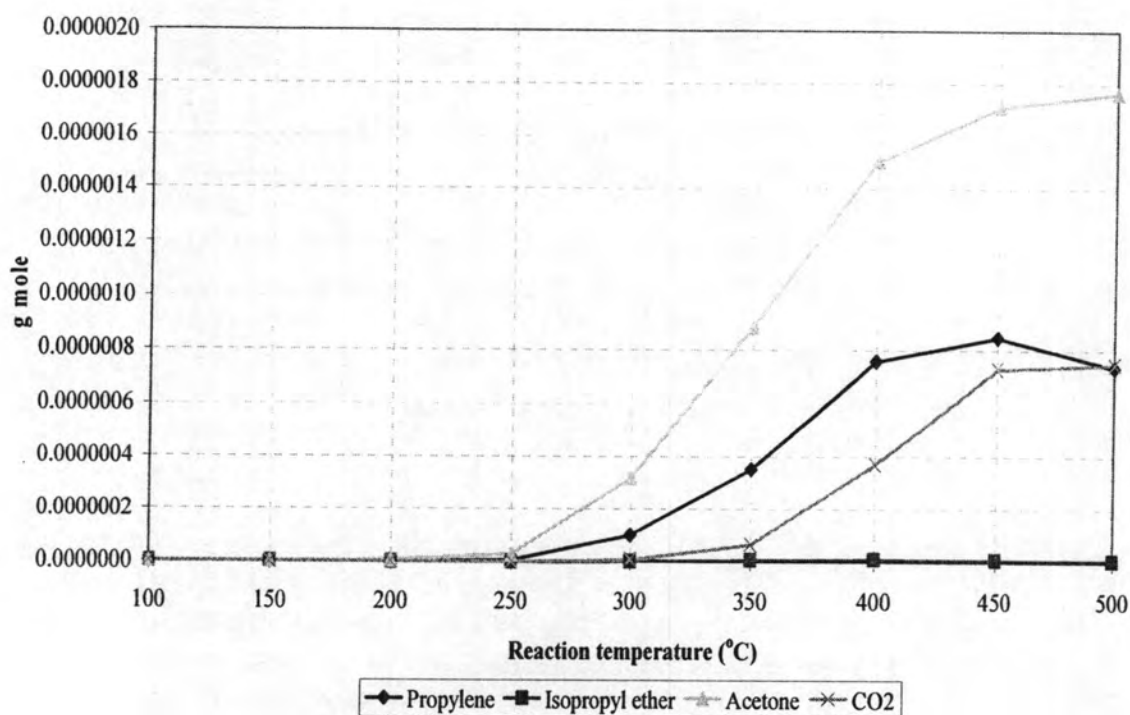


Figure E1 The amount of product of 2-propanol over Co-TS-1 for 8 Vol% O₂ system (Co(NO₃)₂·6H₂O loading to A1).

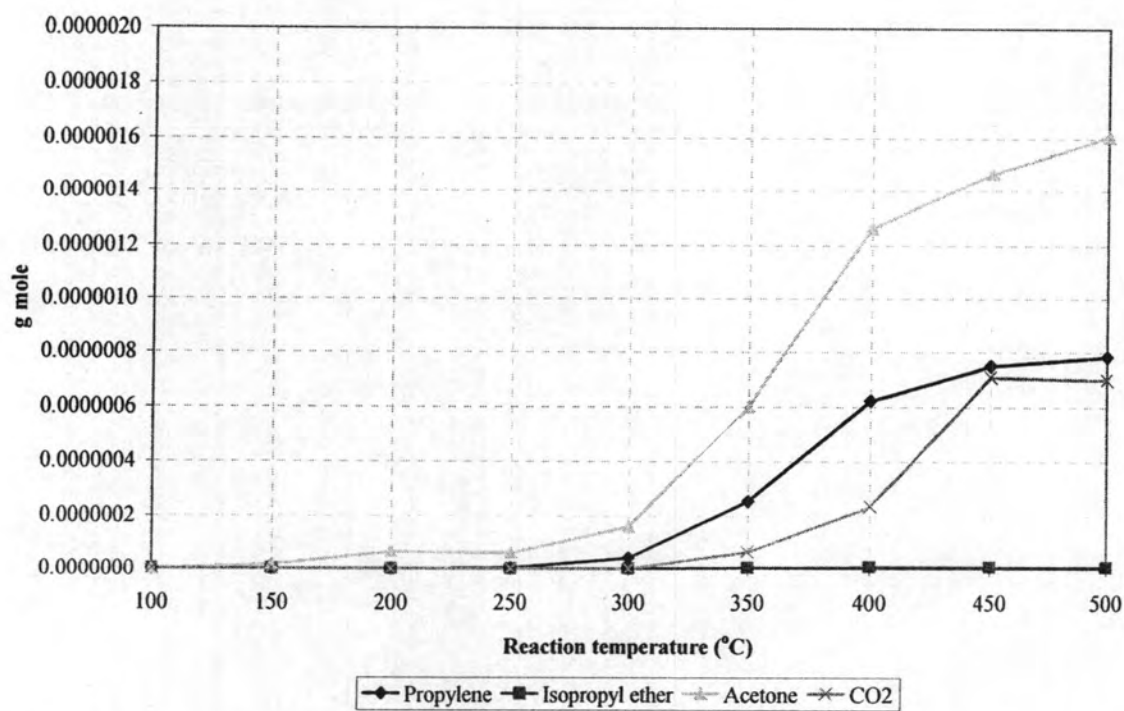


Figure E2 The amount of product of 2-propanol over Co-TS-1 for 8 Vol% O₂ system (Co(NO₃)₂·6H₂O loading to A2).

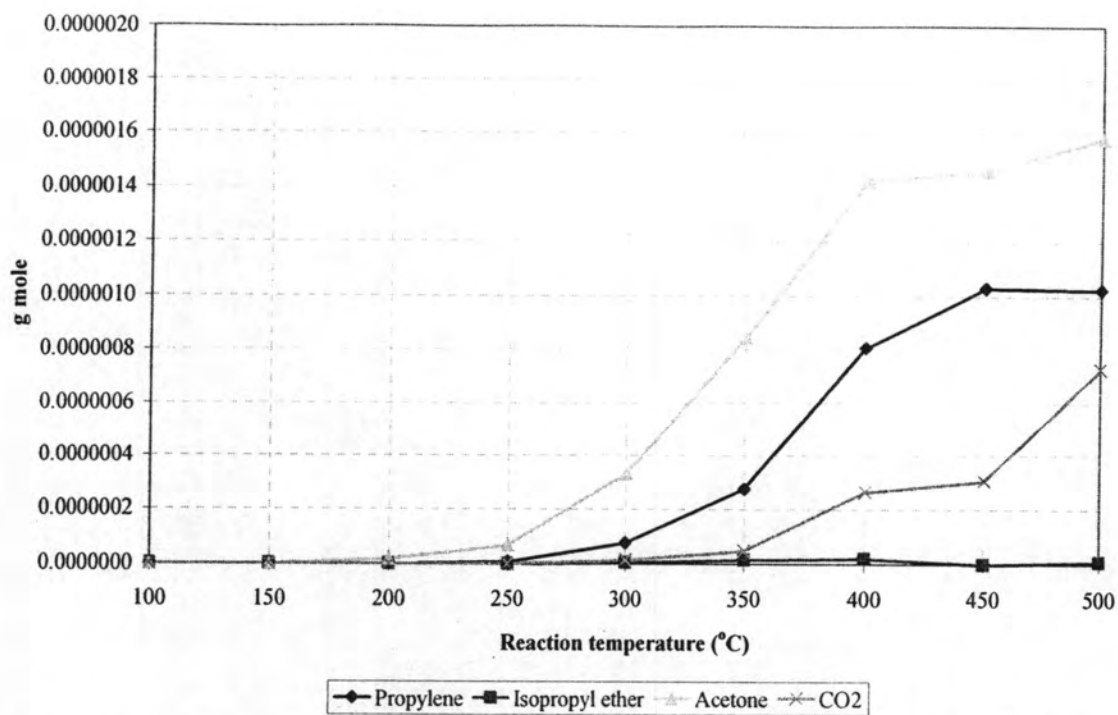


Figure E3 The amount of product of 2-propanol over Co-TS-1 for 8 Vol% O₂ system (Co(NO₃)₂·6H₂O loading to C1).

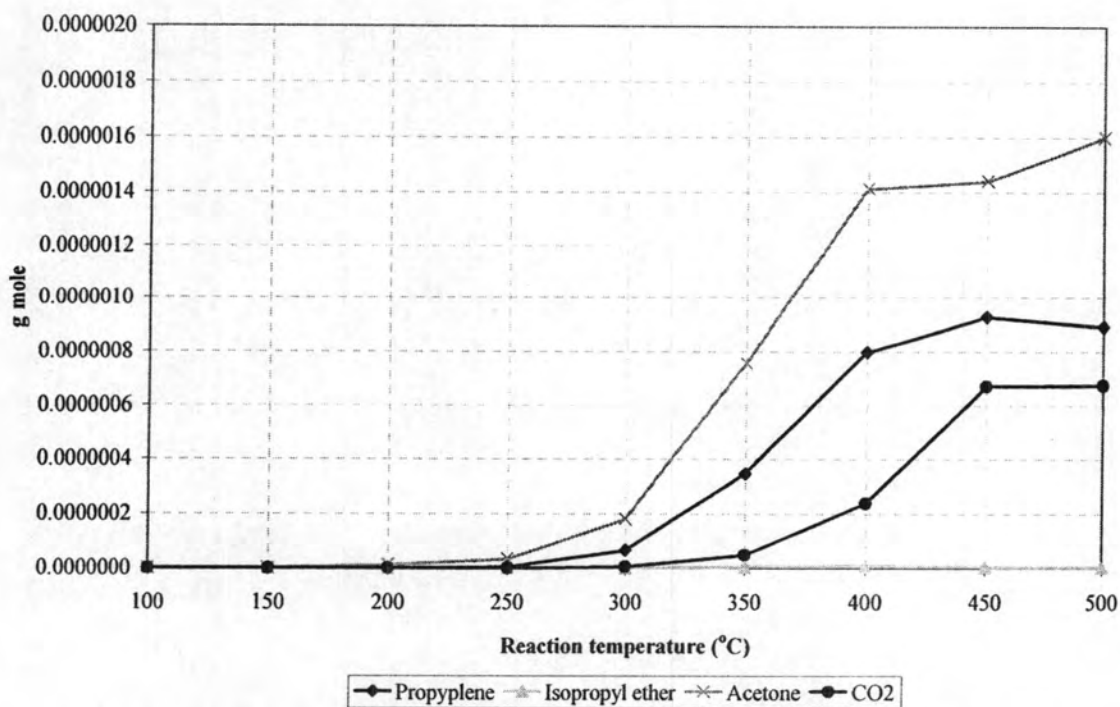


Figure E4 The amount of product of 2-propanol over Co-TS-1 for 8 Vol% O₂ system (Co(NO₃)₂·6H₂O loading to A1 and A2).

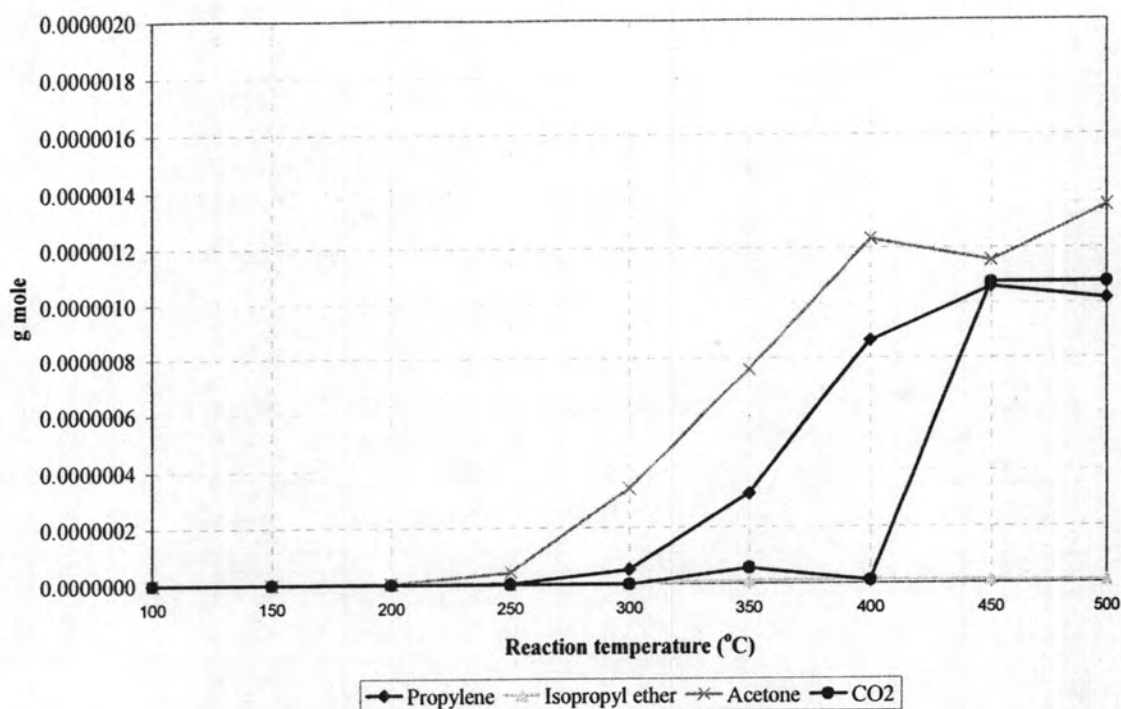


Figure E5 The amount of product of 2-propanol over Co-TS-1 for 8 Vol% O₂ system (CoCl₂ · 6H₂O loading to A1).

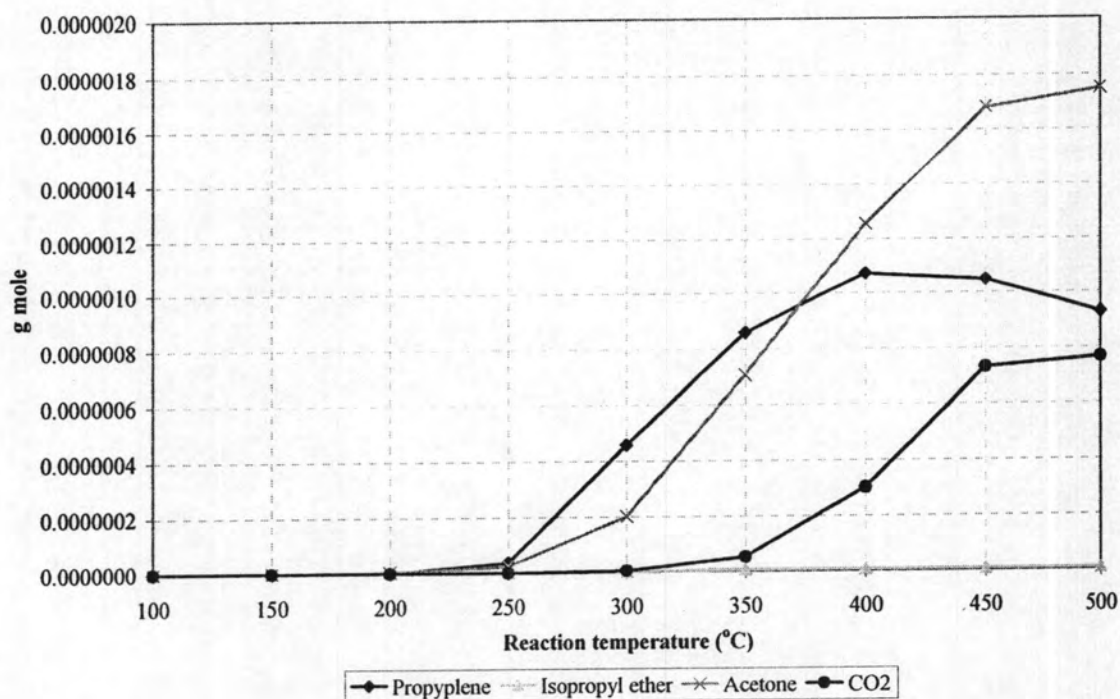


Figure E6 The amount of product of 2-propanol over Co-TS-1 for 8 Vol% O₂ system (CoCl₂ · 6H₂O loading to C1).

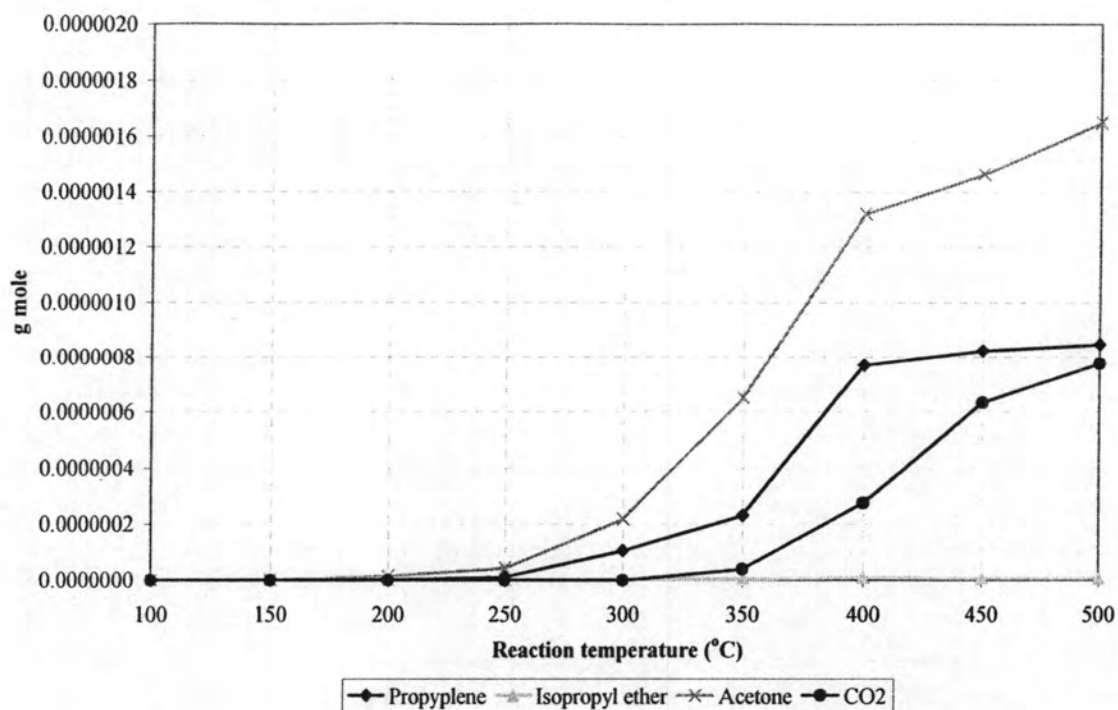


Figure E7 The amount of product of 2-propanol over Co-TS-1 for 8 Vol% O₂ system (CoCl₂ · 6H₂O loading to A1 and A2).

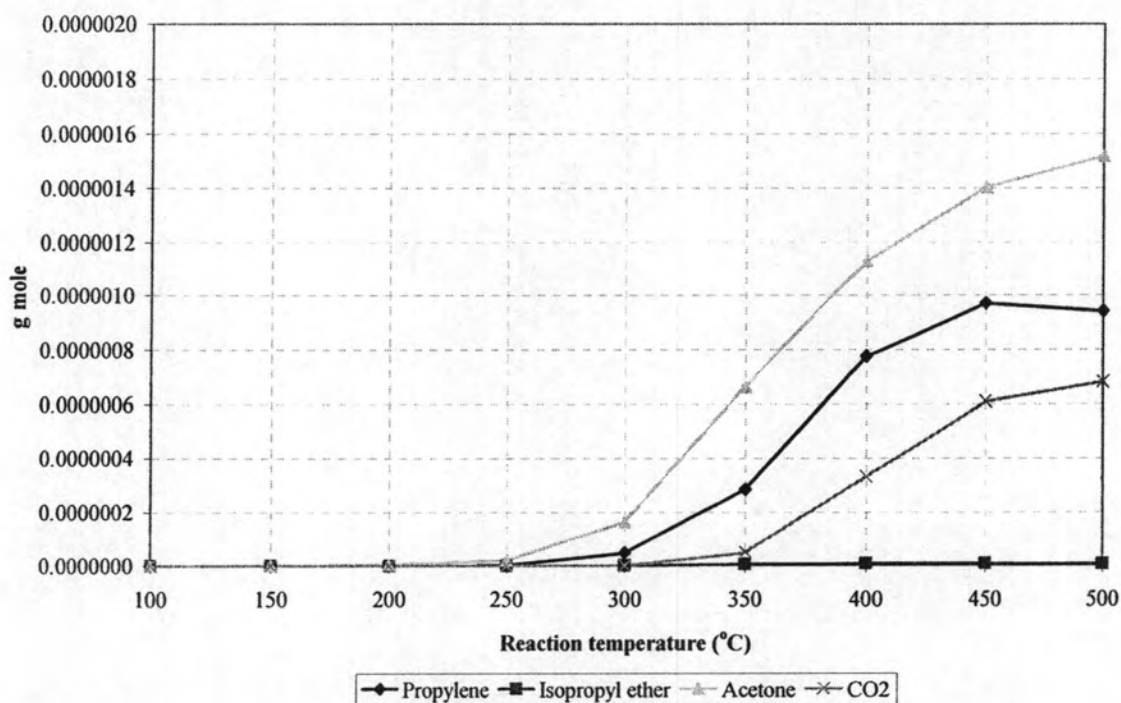


Figure E8 The amount of product of 2-propanol over Co-TS-1 for 8 Vol% O₂ system (Co(C₂H₃O₂)₂ · 4H₂O loading to A1).

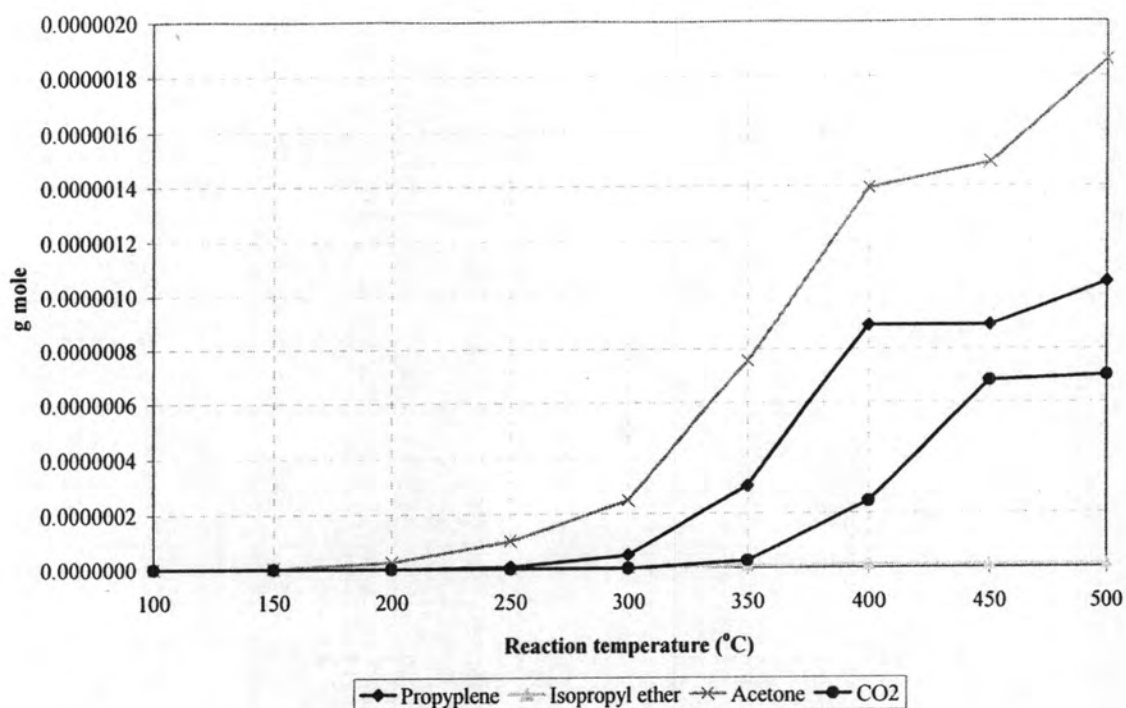


Figure E9 The amount of product of 2-propanol over Co-TS-1 for 8 Vol% O₂ system (Co(C₂H₃O₂)₂·4H₂O loading to A1).

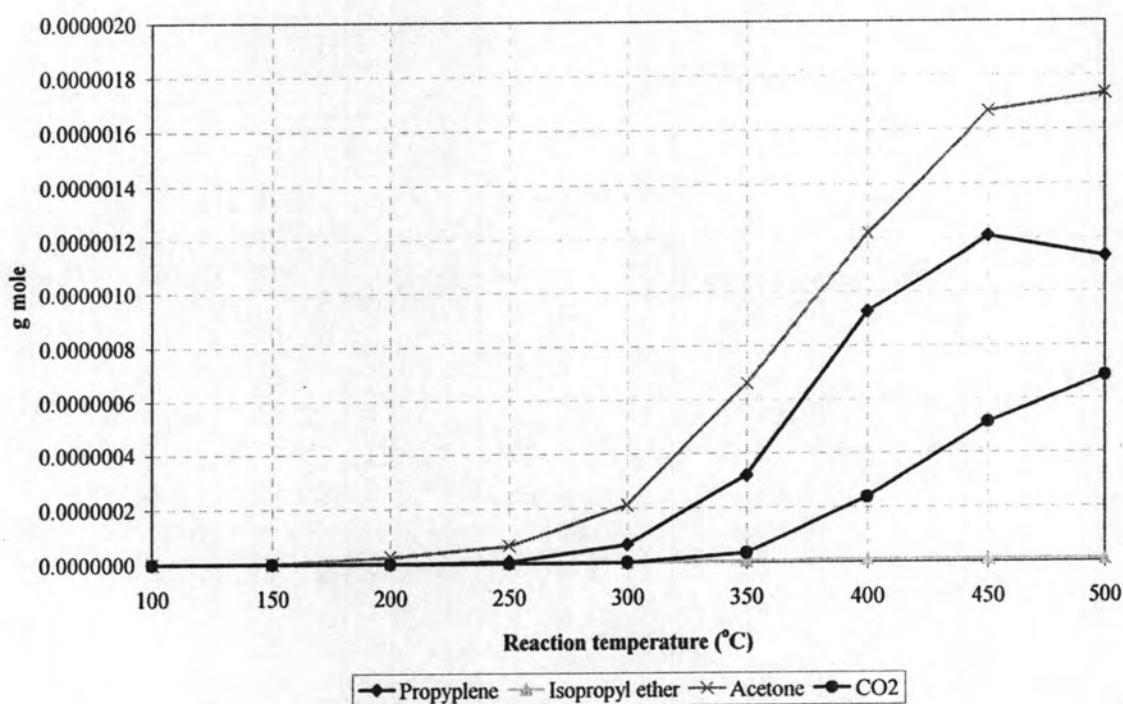


Figure E10 The amount of product of 2-propanol over Co-TS-1 for 8 Vol% O₂ system (Co(C₂H₃O₂)₂·4H₂O loading to A1 and A2).

APPENDIX F

CALIBRATION CURVES

Flame ionization detector gas chromatograph, model 8A, was used to analyze the concentrations of oxygenated compounds. 2-propanol, acetone, propylene, and isopropyl ether were analyzed by GC model 8A with using 15% Carbowax 1000.

Gas chromatograph with the thermal conductivity detector, model 8A, was used to analyze the concentration of CO, CO₂ by using Molecular Sieve 5A and Porapak-Q columns respectively.

The calibration curves 2-propanol, acetone, propylene, isopropyl ether, and CO₂ are illustrated in the following figures.

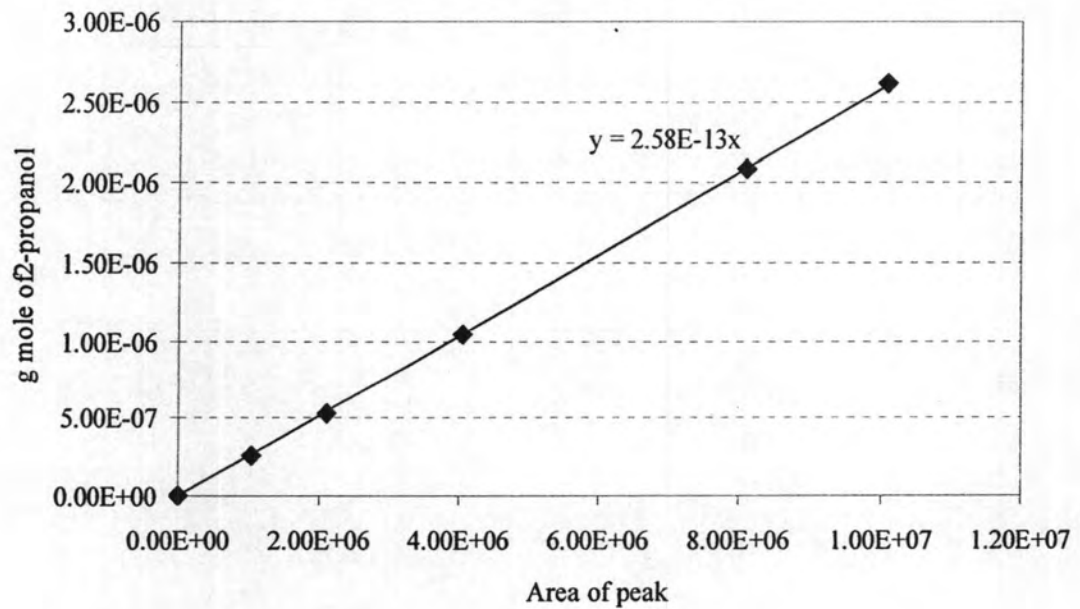


Figure F1 The calibration curve of 2-propanol.

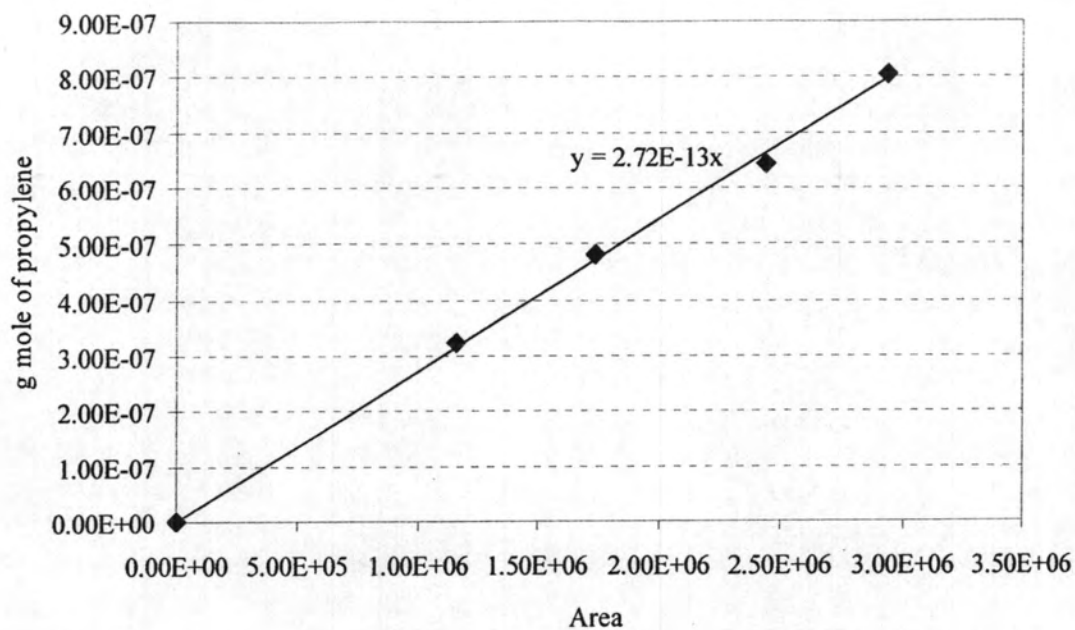


Figure F2 The calibration curve of propylene.

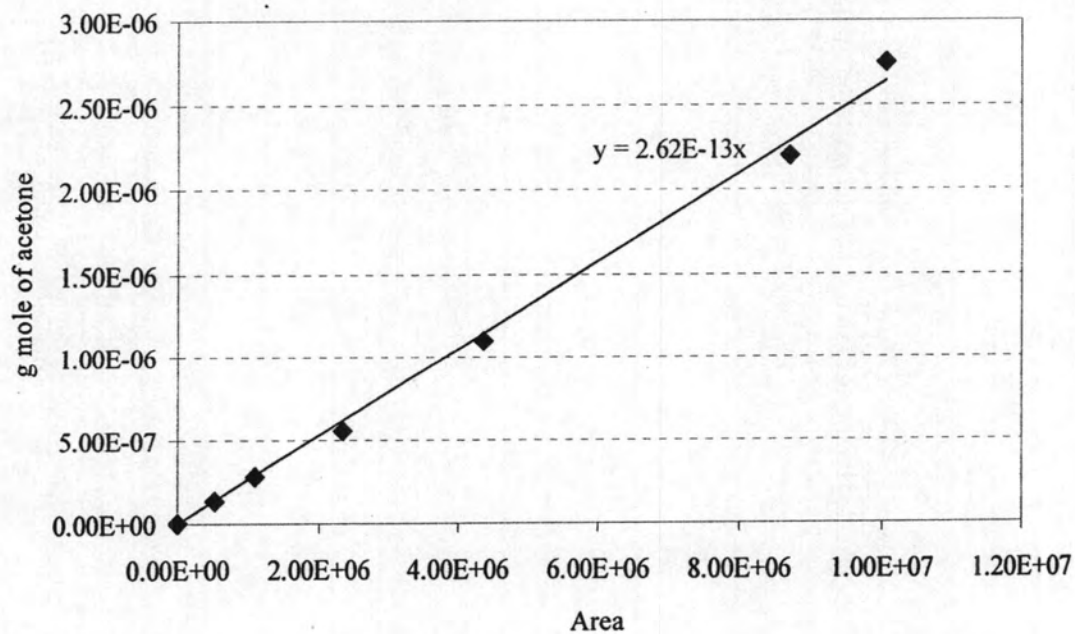


Figure F3 The calibration curve of acetone.

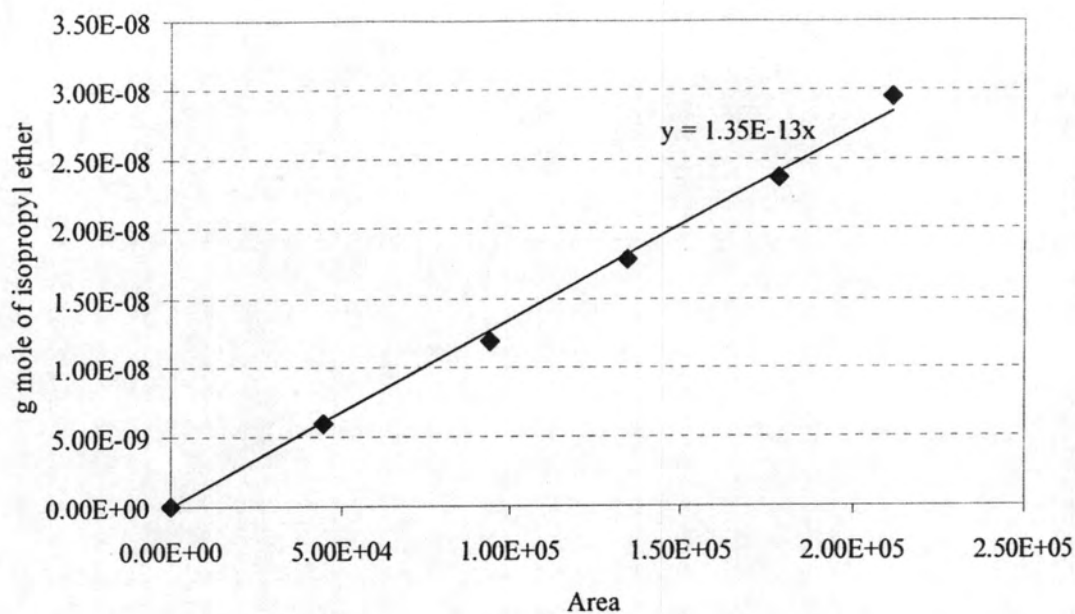


Figure F4 The calibration curve of isopropyl ether.

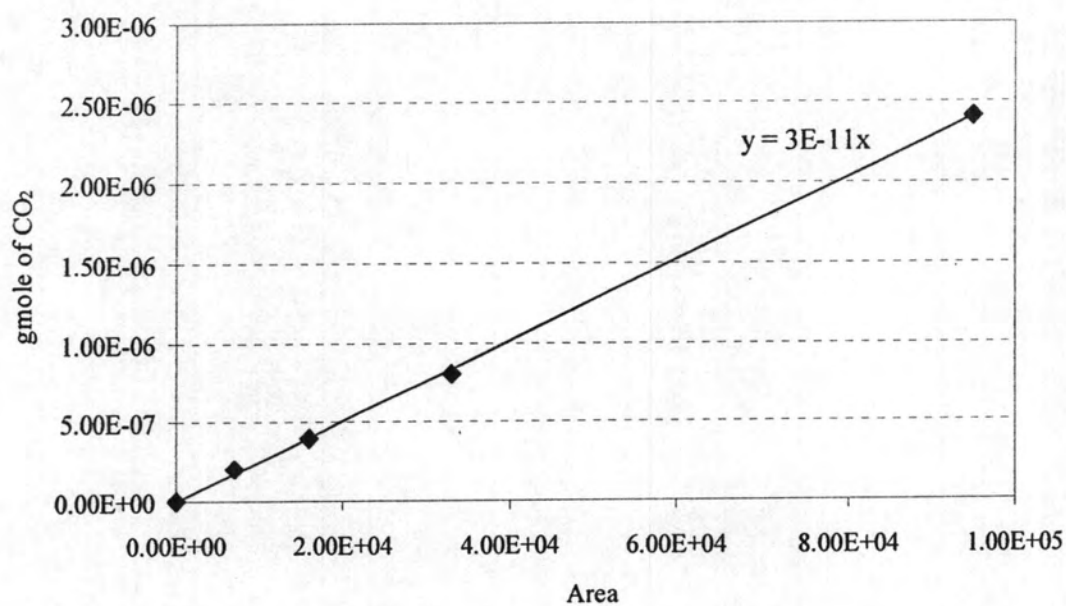


Figure F5 The calibration curve of CO₂.

APPENDIX G

MATERIAL SAFETY DATA SHEETS

G1. Titanium (IV) n-butoxide

General

Synonyms: Tetra-n-butyl titanate; TNBT; Titanium(IV) n-butoxide (TYZOR TNBT); Tetra-n-butyl orthotitanate for synthesis; titanium tetrabutanolate; Titanium(IV)n-butoxide (TYZOR TBT); Butyl Titanate; Titaniumbutoxidecolorlessliq; Titanium n-butoxide; Titanium (IV) n-butoxide, 99+%; Tetra-n-butoxytitanium(IV)~Tetra-n-butyl orthotitanate; Titanium tetrabutoxide; Triethoxy Methane; Titanium tetrabutylate; Orthotitanic acid tetrabutyl ester

Molecular formula: $C_{16}H_{36}O_4Ti$

Chemical formula: $Ti[O(CH_2)_3CH_3]_4$

Physical data

Boiling point	:	310-314 °C
Flash point	:	78 °C
Density	:	1.486 g/cm ³

Toxicology

Irritating to eyes, respiratory system and skin.

Personal protection

Avoid contact with skin and eyes.

G2. Tetrapropylammonium bromide

General

Synonyms: 1-Propanaminium, N, N, N-tripropyl, bromide or Tetra-n-propylammonium bromide or TPBr or TPABr

Molecular formula: $C_{12}H_{28}N.Br$

Chemical formula: $(C_3H_7)_4NBr$

Physical data

Solubility in Water	:	60% (20 °C)
pH	:	5 - 10 for solution
Melting Point	:	275-278 °C (decomposes)

Stability and reactivity

Stable at ambient temperatures. Do not expose to high temperatures.
Oxidizers should be tested for compatibility before use.

Hazardous decomposition

In fire conditions: Carbon monoxide, Hydrobromic acid and Nitrogen oxides.
If heated to decomposition, tripropylamine may be released.

Potential health effect

Inhalation	:	May cause irritation.
Eye Contact	:	May cause irritation.
Skin Contact	:	May cause irritation.
Ingestion	:	No toxicity or other health effects information available.
Chronic	:	May cause irritation. No additional information

available.

First aid measure

Inhalation: Remove to fresh air. If breathing has stopped, give artificial respiration. Consult a physician.

Eye Contact: Immediately flush with water until no evidence of chemical remains (at least 15-20 minutes) and consult a physician.

Skin Contact: Immediately flush with water with sufficient volume until there is no evidence of the chemical on the affected area.

Ingestion: If person is conscious and able to swallow, have them drink a large volume of water and milk and induce vomiting. Contact a physician.

Fire fighting measures

Wear S.C.B.A. May use water spray, carbon dioxide, dry chemical or chemical foam to fight fire.

Hazardous product combustion

May emit Nitrogen oxides, Hydrobromic acid and Carbon monoxide.

G3. Sodium chloride

General

Synonyms: extra fine 200 salt, extra fine 325 salt, H.G. blending, salt, sea salt, table salt, common salt, dendritis, rock salt, top flake, white crystal, saline, halite, purex, USP sodium chloride

Molecular formula: NaCl

Physical data

Appearance	:	colourless crystals or white powder
Melting point	:	804 °C
Boiling point	:	1413 °C
Vapour pressure	:	1 mm Hg at 865 °C
Specific gravity	:	2.16 g cm ⁻³
Solubility in water	:	35.7 g/100g at °C

Stability

Stable. Incompatible with strong oxidizing agents.

Toxicology

May cause skin, eye or respiratory irritation.

Personal protection

Not believed to present a significant hazard to health.

G4. Sodium hydroxide

General

Synonyms: caustic soda, soda lye, lye, white caustic, aetznatron, ascarite, Collo-Grillrein, Collo-Tapetta, sodium hydrate, fotofoil etchant, NAOH, STCC 4935235, sodium hydroxide pellets, Lewis red devil lye

Molecular formula: NaOH

Physical data

Appearance	:	odourless white solid (often sold as pellets)
Melting point	:	318 °C
Boiling point	:	1390 °C
Vapour pressure	:	1 mm Hg at 739 °C
Specific gravity	:	2.12
Water solubility	:	High (Note: dissolution in water is highly exothermic)

Stability

Stable. Incompatible with a wide variety of materials including many metals, ammonium compounds, cyanides, acids, nitro compounds, phenols, combustible organics. Hygroscopic. Heat of solution is very high and may lead to a dangerously hot solution if small amounts of water are used. Absorbs carbon dioxide from the air.

Toxicology

Very corrosive. Causes severe burns. May cause serious permanent eye damage. Very harmful by ingestion. Harmful by skin contact or by inhalation of dust. Typical TLV 2 mg m⁻¹.

Personal protection

Safety glasses, adequate ventilation, Neoprene or PVC gloves.

G5. Sodium silicate

General

Synonyms: silicic acid sodium salt, water glass, sodium water glass, soluble glass, silicate of soda, silicon sodium oxide, sodium orthosilicate, sodium sesquisilicate, sodium silicate glass, agrosil S, barasil S, britesil, carsil 2000, chemfin 60, chemsilicate, crystal 79, crystal 96, ineos 140, inosil Na 4237, portil A, pyramid 8, vitrosol N40, ZhS 3, very large number of further trade names

Molecular formula: $\text{Na}_4\text{O}_4\text{Si}$

Physical data

Appearance	:	colourless liquid as usually supplied (solution)
Boiling point	:	ca. 102 °C for a 40% aqueous solution
Specific gravity	:	approximately 1.3 for a ca. 40% solution

Stability

Stable. Incompatible with acids, most metals, many organic materials.

Toxicology

Harmful by ingestion. Corrosive - may cause burns through skin or eye contact. Very destructive of mucous membranes.

Personal protection

Safety glasses, gloves.

G6. Sulfuric acid

General

Synonyms: oil of vitriol, mattling acid, vitriol, battery acid, dipping acid, electrolyte acid, vitriol brown oil, sulphuric acid

Molecular formula: H_2SO_4

Physical data

Appearance	:	Colourless oily liquid
Melting point	:	-2 °C
Boiling point	:	327 °C
Specific gravity	:	1.84
Vapour pressure	:	<0.3 mm Hg at 20 °C (vapour density 3.4)
Water solubility	:	miscible in all proportions

Stability

Stable, but reacts with moisture very exothermically, which may enhance its ability to act as an oxidizing agent. Substances to be avoided include water, most common metals, organic materials, strong reducing agents, combustible materials, bases, oxidising agents. Reacts violently with water - when diluting concentrated acid, carefully and slowly add acid to water, not the reverse. Reaction with many metals is rapid or violent, and generates hydrogen (flammable, explosion hazard).

Toxicology

Extremely corrosive, causes serious burns. Highly toxic. Harmful by inhalation, ingestion and through skin contact. Ingestion may be fatal. Skin contact can lead to extensive and severe burns. Chronic exposure may result in lung damage and possibly cancer.

Personal protection

Safety glasses or face mask; acid-resistant gloves. Suitable ventilation. In the UK use of this material must be assessed under the COSHH regulations.

G7. Cobalt (II) Nitrate Hexahydrate

General

Synonyms: cobalt dinitrate hexahydrate, cobalt nitrate hexahydrate, nitric acid cobalt (+2) salt, cobaltous nitrate hexahydrate

Molecular formula: $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$

Physical data

Physical State	:	Solid
Appearance	:	red
Odor	:	odorless
pH	:	Not available.
Vapor Pressure	:	Negligible.
Vapor Density	:	Not available.
Evaporation Rate	:	Negligible.
Viscosity	:	Not applicable.
Boiling Point	:	Not available.
Freezing/Melting Point	:	55-56 °C
Autoignition Temperature	:	Not applicable.
Flash Point	:	Noncombustible.
Decomposition Temperature	:	74 deg C
NFPA Rating	:	(estimated) Health: 2; Flammability: 0; Reactivity: 1
Explosion Limits, Lower	:	Not available.
Upper	:	Not available.
Solubility	:	Soluble.
Specific Gravity/Density	:	2.49
Molecular Formula	:	$\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$
Molecular Weight	:	291.0234



Stability

Chemical Stability: Stable. However, may decompose if heated.

Conditions to Avoid: Incompatible materials, excess heat, combustible materials, reducing agents, temperatures above 100°C.

Incompatibilities with Other Materials: Reacts violently if mixed with reducing agents, organic matter, and other flammable and combustible materials including wood, paper, sulfur, aluminum, phosphorus, hydroxylamine, phosphinates, alky esters, ammonium hexacyanoferrate (4-), carbon, tin (II) chloride, and flammable liquids.

Hazardous Decomposition Products: Nitrogen oxides, irritating and toxic fumes and gases.

Hazardous Polymerization: Has not been reported. Stable. Strong oxidizer - incompatible with reducing agents.

Toxicology

Harmful if swallowed or inhaled.

Eye: Causes eye irritation.

Skin: Prolonged and/or repeated contact may cause irritation and/or dermatitis. May cause skin sensitization, an allergic reaction, which becomes evident upon re-exposure to this material.

Ingestion: Causes gastrointestinal irritation with nausea, vomiting and diarrhea. May be harmful if swallowed. Excessive ingestion may increase red blood cells and decrease blood pressure. May cause sensation of heat and enlargement of the thyroid.

Inhalation: Dust is irritating to the respiratory tract. May cause methemoglobinemia, cyanosis, convulsions, tachycardia, dyspnea (labored breathing), and death. May cause asthmatic attacks due to allergic sensitization of the respiratory tract.

Chronic: Repeated exposure may cause allergic respiratory reaction (asthma).

Personal protection

- Eyes : Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations
- Skin : Wear appropriate gloves to prevent skin exposure.
- Clothing : Wear appropriate protective clothing to prevent skin exposure

G8. Cobalt (II) Chloride Hexahydrate

General

Synonyms: cobaltous chloride, cobalt muriate

Molecular formula: $\text{Co}(\text{Cl})_2 \cdot 6\text{H}_2\text{O}$

Physical data

Physical State	:	Solid
Appearance	:	purple
Odor	:	Not available.
pH	:	4.6 @ M solution
Vapor Pressure	:	Negligible.
Vapor Density	:	Not available.
Evaporation Rate	:	Negligible.
Viscosity	:	Not available.
Boiling Point	:	1920 °F
Freezing/Melting Point	:	87 °C
Autoignition Temperature	:	Not applicable.
Flash Point	:	Noncombustible.
Decomposition Temperature	:	230 °C
NFPA Rating	:	(estimated) Health: 2; Flammability: 0; Reactivity: 0
Explosion Limits, Lower	:	Not available.
Upper	:	Not available.
Solubility	:	77 g/100 ml (0 °C)
Specific Gravity/Density	:	1.924
Molecular Formula	:	$\text{Co}(\text{Cl})_2 \cdot 6\text{H}_2\text{O}$
Molecular Weight	:	237.9196

Stability

Chemical Stability: Stable at room temperature in closed containers under normal storage and handling conditions.

Conditions to Avoid: Incompatible materials, dust generation, moisture, excess heat.

Incompatibilities with Other Materials: Strong oxidizers and alkali metals.

Hazardous Decomposition Products: Hydrogen chloride, irritating and toxic fumes and gases, cobalt/cobalt oxides.

Hazardous Polymerization: Has not been reported.

Toxicology

Harmful if swallowed or inhaled

Eye: Causes eye irritation.

Skin: Prolonged and/or repeated contact may cause irritation and/or dermatitis. May cause skin sensitization, an allergic reaction, which becomes evident upon re-exposure to this material.

Ingestion: May causes gastrointestinal irritation with nausea, vomiting and diarrhea. May be harmful if swallowed.

Inhalation: Dust: Cause delayed lung injury. Causes respiratory tract irritation. May cause asthmatic attacks due to allergic sensitization of the respiratory tract. May cause asthma and shortness of breath.

Chronic: Cobalt compounds may cause cancer based upon animal studies.

Personal protection

- | | |
|----------|--|
| Eyes | : Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations |
| Skin | : Wear appropriate gloves to prevent skin exposure. |
| Clothing | : Wear appropriate protective clothing to prevent skin exposure |

G9. Cobalt (II) Acetate Tetrahydrate

General

Synonyms: Cobalt (II) acetate tetrahydrate, Cobalt diacetate tetrahydrate, Cobaltous acetate tetrahydrate

Molecular formula: $\text{Co}(\text{CH}_3\text{COO}) \cdot 4\text{H}_2\text{O}$

Physical data

Physical State	:	Solid
Appearance	:	Light-pink crystals.
Odor	:	Vinegar-like odor.
pH	:	7 (1% Soln/water)
Vapor Pressure	:	Not applicable.
Vapor Density	:	Not available.
Viscosity	:	Not available.
Boiling Point	:	Not available.
Flash Point	:	Noncombustible.
Decomposition Temperature	:	100 °C
Explosion Limits, Lower	:	Not available.
Upper	:	Not available.
Solubility	:	Soluble in cold water.
Specific Gravity/Density	:	1.705
Molecular Formula	:	$\text{Co}(\text{CH}_3\text{COO}) \cdot 4\text{H}_2\text{O}$
Molecular Weight	:	249.0264

Stability

Chemical Stability: Stable under normal temperatures and pressures.

Conditions to Avoid: Not available.

Incompatibilities with Other Materials: Moisture - heat.

Hazardous Decomposition Products: Carbon monoxide, carbon dioxide

Hazardous Polymerization: Has not been reported.

Toxicology

Harmful if swallowed.

Eye: Causes eye irritation.

Skin: Prolonged and/or repeated contact may cause irritation and/or dermatitis.

May cause skin sensitization, an allergic reaction, which becomes evident upon re-exposure to this material.

Ingestion: May causes gastrointestinal irritation with nausea, vomiting and diarrhea. May be harmful if swallowed.

Inhalation: Dust: Cause delayed lung injury. Causes respiratory tract irritation. May cause asthmatic attacks due to allergic sensitization of the respiratory tract. May cause asthma and shortness of breath.

Chronic: Cobalt compounds may cause cancer based upon animal studies.

Personal protection

- Eyes : Wear safety glasses and chemical goggles if splashing is possible.
- Skin : Wear appropriate protective gloves and clothing to prevent skin exposure.
- Clothing : Wear appropriate protective clothing to minimize contact with skin.

G10. 2-Propanol**General**

Synonyms	:	Isopropanol, Isopropyl alcohol
Molecular formula	:	C ₃ H ₈ O
Chemical formula	:	CH ₃ CH(OH)CH ₃

Physical data

Melting point	:	-89.5 °C
Boiling point	:	82.4 °C
Ignition temperature	:	425°C
Flash point	:	12°C
Explosion limits	:	2 % - 12.7 %
Vapor pressure	:	31.68 mm (14.7 °C)
Relative vapor density:		2.07
Density	:	0.786 g/cm ³ (20 °C)
Solubility in water	:	soluble (20 °C)

Stability

Conditions to be avoided: Strong heating.

Substances to be avoided: alkali metals, alkaline earth metals, aluminium in powder form, oxidizing agent, organic nitro compounds, aldehydes, amines, fuming sulfuric acid, phosgene.

Hazardous decomposition products: no information available.

Further information: highly inflammable; hygroscopic, explosive with air in a vapor/gas state.

Toxicology

Further toxicological information

After inhalation: Irritation symptoms in the respiratory tract Drowsiness

After skin contact: degreasing effect on the skin possibly followed by secondary inflammation.

After eye contact: Irritations.

After swallowing: after accidental swallowing the substance may pose a risk of aspiration. Passage into the lung can result in a condition resembling pneumonia

After absorption: headache, dizziness, inebriation

After uptake of large quantities: respiratory paralysis, coma.

Personal protection

Personal protective equipment: Protective clothing should be selected specifically for the working place, depending on concentration and quantity of the hazardous substances handled. The resistance of the protective clothing to chemicals should be ascertained with the respective supplier.

Industrial hygiene: Change contaminated clothing. Application of Skin-protective barrier cream recommended. Should be wash hands after working with substance.

VITA

Miss Nattaporn Jiravasavanich was born on October 14th, 1982 in Bangkok, Thailand. She finished high school from Assumption Convent School, Bangkok in 2001, and received the bachelor's degree of Chemical Engineering from Faculty of Engineering, Thammasat University in 2005. She continued her master's study at Department of Chemical Engineering, Faculty of Engineering, Chulalongkorn University in June, 2005.

