## Mathematics Course 1S4 JF Life and Earth Sciences

A mining company obtains geological material from the earth. The molar composition of copper is 21, of iron is 16, and of sulphur is 31 in a particular sample mined by the company.

The only minerals contributing to the overall copper, iron and sulphur content are Chalcopyrite ( $Cu Fe S_2$ ), Troilite (Fe S), and Bornite ( $Cu_5 Fe S_4$ ). Find the molar amounts of Chalcopyrite (x), Troilite (y), and Bornite (z), occurring in the sample.

A study of the molar amounts of copper, iron and sulphur in the three minerals indicates that the following equations must hold

The *augmented* matrix that represents the linear system of equations is

Completing the procedure of *Gauss-Jordan elimination* leads to the equivalent augmented matrix

1	0	0	6
0	1	0	7
0	0	1	3

and writing the equations explicitly with variables x, y and z yields

whence the solution set is x = 6, y = 7, z = 3. The molar amounts of Chalcopyrite ( $Cu Fe S_2$ ), Troilite (Fe S), and Bornite ( $Cu_5 Fe S_4$ ) occurring in the sample are Chalcopyrite (6), Troilite (7), and Bornite (3), a fact that may readily be checked through substitution

The mining company obtains a second sample of geological material. This time, the molar composition of copper is 13, of iron is 14, and of sulphur is 27.

The minerals contributing to the overall copper, iron and sulphur content are Covellite (CuS), Chalcopyrite (CuFeS<sub>2</sub>), and Troilite (FeS). Find the molar amounts of Covellite (x), Chalcopyrite (y), and Troilite (z) occurring in the sample.

A study of the molar amounts of copper, iron and sulphur in these particular three minerals indicates that the following equations should hold

$$x + y = 13$$
 (Cu)  
 $y + z = 14$  (Fe)  
 $x + 2y + z = 27$  (S).

The *augmented* matrix that represents the linear system of equations is

1	1	0	13
0	1	1	14
1	2	1	27

Completing the procedure of *Gauss-Jordan elimination* leads to the equivalent augmented matrix in *reduced* row-echelon form

Γ	1	1	0	13	
	0	1	1	14	
L	0	0	0	0	_

with leading *ones* in the non-zero rows and a row of *zeros* in the third row. Writing the equations explicitly with variables x, y and z yields

x	+	0y	+	-z	=	-1
0x	+	1y	+	1z	=	14
0x	+	0y	+	0z	=	0

whence the solution set is x = z - 1, y = 14 - z, where z may have any value. It is customary to set z = t and the solution is written

$$x = t - 1$$
$$y = 14 - t$$
$$z = t$$

where t is any number greater than 1 so that x is positive, and less than 14 so that y is positive.

Amounts of Covellite (CuS), Chalcopyrite (CuFeS<sub>2</sub>), and Troilite (FeS) occurring in the second sample are not uniquely determined but can be expressed in the form Covellite (t - 1), Chalcopyrite (14 - t), and Troilite (t), where 1 < t < 14, a fact that may readily be checked through substitution,

A mining company obtains a third sample from the earth. The molar composition of copper is 21, of iron is 17, and of sulphur is 33 in the sample mined by the company.

The only minerals contributing to the copper, iron and sulphur content are Isocubanite (Cu Fe<sub>2</sub>S<sub>3</sub>), Chalcopyrite (Cu FeS<sub>2</sub>), Haycockite (Cu<sub>4</sub> Fe<sub>5</sub>S<sub>8</sub>), and Bornite (Cu<sub>5</sub> FeS<sub>4</sub>). Determine the molar amounts of Isocubanite (x), Chalcopyrite (y), and Haycockite (z), in terms of the amount of Bornite (t)occurring in the sample.

A study of the molar amounts of copper, iron and sulphur in the three minerals indicates that the following equations must hold

x	+	y	+	4z	+	5t	=	21	(Cu)
2x	+	y	+	5z	+	t	=	17	(Fe)
3x	+	2y	+	8z	+	4t	=	33	(S).

The *augmented* matrix that represents the linear system of equations is

1	1	4	5	21
2	1	5	1	17
3	2	8	4	33

*Gaussian elimination* produces an augmented matrix in row-echelon form with leading *ones* (in the non-zero rows)

1	1	4	5	21	
0	1	3	9	25	
0	0	1	2	5	

The augmented matrix in *reduced* row-echelon form with *zeros* above each leading *one* is, after *Gauss-Jordan elimination*,

1	1	4	5	21
0	1	0	3	10
0	0	1	2	5

Writing the equations explicitly with variables x, y, z and t yields

x	—					6t	=	-9	(Cu)
		y	+			3t	=	10	(Fe)
				z	+	2t	=	5	(S).

whence the solution set is

$$x = 6t - 9$$
  

$$y = 10 - 3t$$
  

$$z = 5 - 2t$$
  

$$t = \text{almost any number.}$$

If all four minerals are observed to be present in the sample, positivity of the molar amounts requires that x > 0, y > 0, z > 0, t > 0, which means that

6t - 9 > 0, 10 - 3t > 0, 5 - 2t > 0, t > 0,

or equivalently, values of t are restricted to those obeying

$$t > 3/2,$$
  $t < 10/3,$   $t < 5/2,$   $t > 0.$ 

Some of these inequalities are included in others and thus the essential inequality is

1.5 < t < 2.5

If t = 2, for example, then the molar amounts of Isocubanite (Cu Fe<sub>2</sub>S<sub>3</sub>), Chalcopyrite (Cu Fe S<sub>2</sub>), Haycockite (Cu<sub>4</sub> Fe<sub>5</sub>S<sub>8</sub>), and Bornite (Cu<sub>5</sub> Fe S<sub>4</sub>) in the sample are Isocubanite (3), Chalcopyrite (4), Haycockite (1) and Bornite (2).

The extreme value t = 1.5 leads to molar amounts of Isocubanite (0), Chalcopyrite (5.5), Haycockite (2) and Bornite (1.5).

The other extreme value of t = 2.5 leads to amounts Isocubanite (6), Chalcopyrite (2.5), Haycockite (0) and Bornite (2.5).

Unless independent information exists on the molar amount of at least one of the four minerals no unique solution to the linear system of equations exists. In general, all that is known is that the molar amounts may be parametrised

Mineral	Molar amount	Bound A	Bound B
Isocubanite	6t - 9	0.0	6.0
Chalcopyrite	10 - 3t	5.5	2.5
Haycockite	5-2t	2.0	0.0
Bornite	t	1.5	2.5
Positivity	1.5 < t < 2.5	t=1.5	t=2.5

Thus the molar amounts of three of the minerals Isocubanite (Cu Fe<sub>2</sub>S<sub>3</sub>), Chalcopyrite (Cu Fe S<sub>2</sub>), Haycockite (Cu<sub>4</sub> Fe<sub>5</sub>S<sub>8</sub>), may be expressed in terms of the molar amount of Bornite (Cu<sub>5</sub> Fe S<sub>4</sub>). The amounts of the four minerals must take values that are between the two bounds exhibited in the table.

The Athena Mineralogy website provides a systematic list of many minerals

## http://un2sg4.unige.ch/athena/mineral/minppcl.html#2

where searching with 'Cu5FeS4', for example, leads to the mineral Bornite.

Karl Friedrich Gauss (1777–1855) was a German mathematician and scientist who enjoyed mineralogy and botany as hobbies. Wilhelm Jordan (1842–1899) was a German engineer whose method for solving linear systems appeared in his Handbuch der Vermessungskunde (Handbook of Geodesy), in 1888.

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