New fuels & CO_2 emissions

New Fuels (from coal, oil shale, oil sands, trash, biowaste)

$C(s) + H_2O(g) \rightarrow CO(g) + \boxed{H_2(g)}$

coke syngas/water gas

Could be any other source of “C”

Water gas shift reaction:

+1073 kJ/mol -2x803 kJ/mol

$CO(g) + H_2O(g) \rightarrow CO_2(g) + H_2(g)$=-35 kJ/mol

2x467 kJ/mol -436 kJ/mol

Steam methane reforming:

4x416 kJ/mol -2x803 kJ/mol

$CH_4(g) + 2H_2O(g) \rightarrow CO_2(g) + 4H_2(g)$ =+182 kJ/mol

4x467 kJ/mol -4x436 kJ/mol

Fischer-Tropsch process:

*n*x1073 kJ/mol (*n*-1)x356 kJ/mol (C-C)

$nCO(g) + (2n+1)H_2(g) \rightarrow C_nH_{2n+2}(g,l) + nH_2O(g)$

(2*n*+1)x436 kJ/mol (2*n*+2)x416 kJ/mol (C-H) 2*n*x467 kJ/mol

n=1->-217 kJ/mol
n=2->-394 kJ/mol
n=3->-571 kJ/mol
n=4->-748 kJ/mol

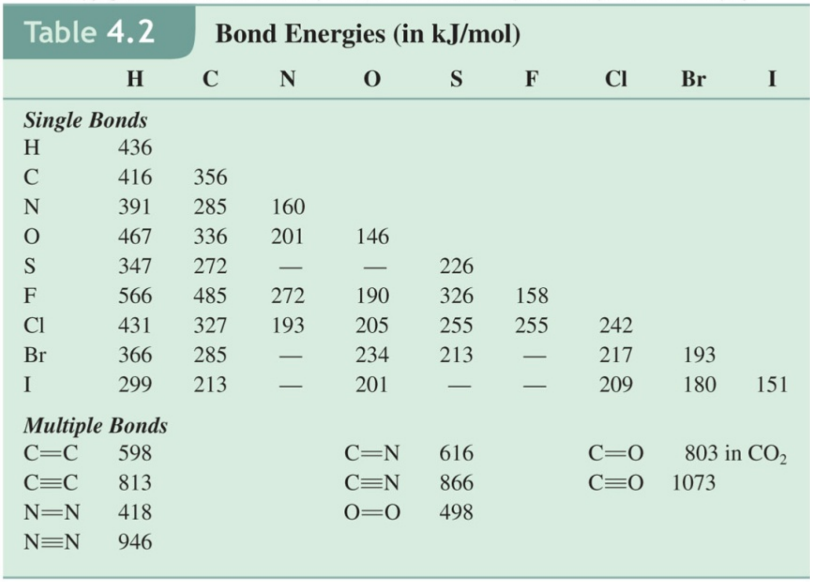


Table 4.2 Bond Energies (in kJ/mol)

	H	C	N	O	S	F	Cl	Br	I
Single Bonds									
H	436								
C	416	356							
N	391	285	160						
O	467	336	201	146					
S	347	272	—	—	226				
F	566	485	272	190	326	158			
Cl	431	327	193	205	255	255	242		
Br	366	285	—	234	213	—	217	193	
I	299	213	—	201	—	—	209	180	151

Multiple Bonds

C=C	598	C=N	616	C=O	803 in CO_2
C≡C	813	C≡N	866	C≡O	1073
N=N	418	O=O	498		
N≡N	946				

Source: Data from Darrell D. Ebbing, *General Chemistry,* Fourth Edition, 1993 Houghton Mifflin Co. Data originally from *Inorganic Chemistry: Principles of Structure and Reactivity,* Third Edition, by James E. Huheey, 1983, Addison Wesley Longman.

Comparison of CO_2 Emissions

Compare the amount of CO_2 emitted to produce 1 kJ of energy from the following fuels: coal, natural gas, gasoline

Answering the question:

kJ fuel → grams fuel → moles fuel → moles CO_2 → grams CO_2

balanced reaction (combustion)

everything else is unit conversions

“formulas”
Natural gas: CH_4
Gasoline: C_8H_{18}
Coal: $C_{135}H_{96}O_9NS$

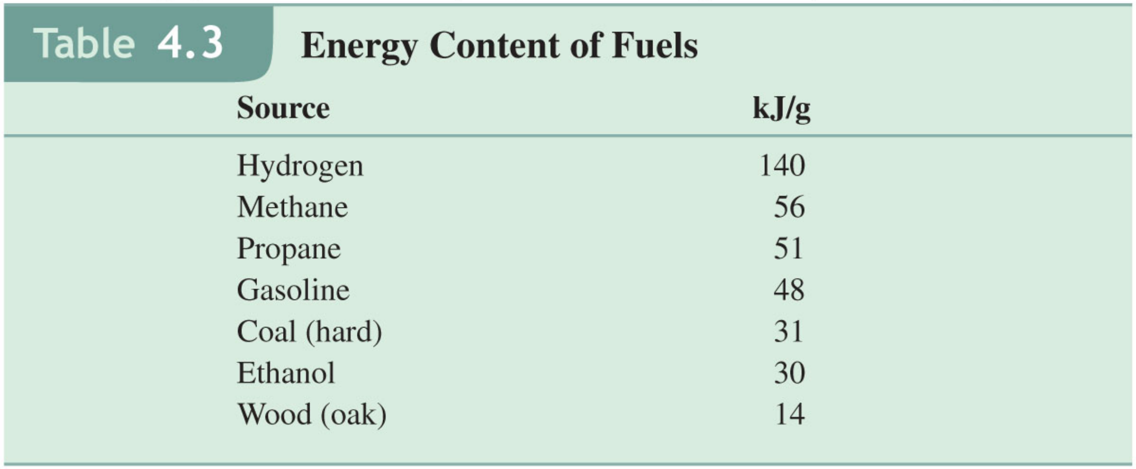


Table 4.3 Energy Content of Fuels

Source	kJ/g
Hydrogen	140
Methane	56
Propane	51
Gasoline	48
Coal (hard)	31
Ethanol	30
Wood (oak)	14

CO_2 Emissions

How much CO_2 will be produced to obtain 1kJ of energy?

Coal: $C_{135}H_{96}O_9NS$
Natural gas: CH_4
Gasoline: C_8H_{18}

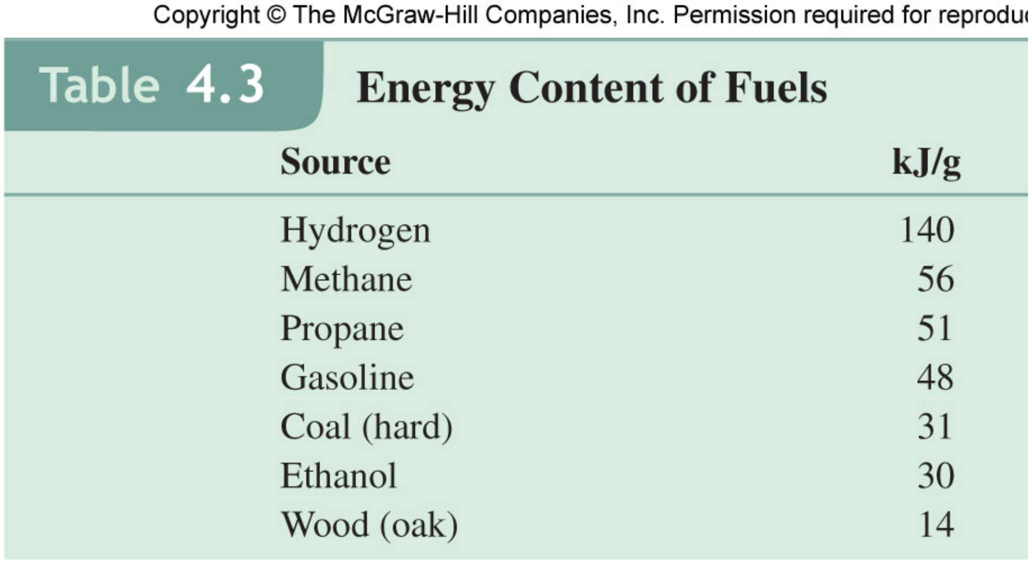


Table 4.3 Energy Content of Fuels

Source	kJ/g
Hydrogen	140
Methane	56
Propane	51
Gasoline	48
Coal (hard)	31
Ethanol	30
Wood (oak)	14

kJ fuel→Grams fuel→moles fuel→moles CO_2→grams CO_2

natural gas:

$$1\text{ kJ}\times\frac{1\text{ g }CH_4}{55.8\text{ kJ}}\times\frac{1\text{ mol }CH_4}{16.05\text{ g }CH_4}\times\frac{1\text{ mol }CO_2}{1\text{ mol }CH_4}\times\frac{44.01\text{ g }CO_2}{1\text{ mol }CO_2}=0.049\text{ g }CO_2$$

gasoline:

$$1\text{ kJ}\times\frac{1\text{ g }C_8H_{18}}{46.5\text{ kJ}}\times\frac{1\text{ mol }C_8H_{18}}{114.26\text{ g }C_8H_{18}}\times\frac{16\text{ mol }CO_2}{2\text{ mol }C_8H_{18}}\times\frac{44.01\text{ g }CO_2}{1\text{ mol }CO_2}=0.066\text{ g }CO_2$$

sub-bituminous coal:

$$1\text{ kJ}\times\frac{1\text{ g }C_{135}H_{96}O_9NS}{24.0\text{ kJ}}\times\frac{1\text{ mol }C_{135}H_{96}O_9NS}{1908\text{ g }C_{135}H_{96}O_9NS}\times\frac{270\text{ mol }CO_2}{2\text{ mol }C_{135}H_{96}O_9NS}\times\frac{44.01\text{ g }CO_2}{1\text{ mol }CO_2}=0.130\text{ g }CO_2$$

$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

$2C_8H_{18} + 25O_2 \rightarrow 16CO_2 + 18H_2O$

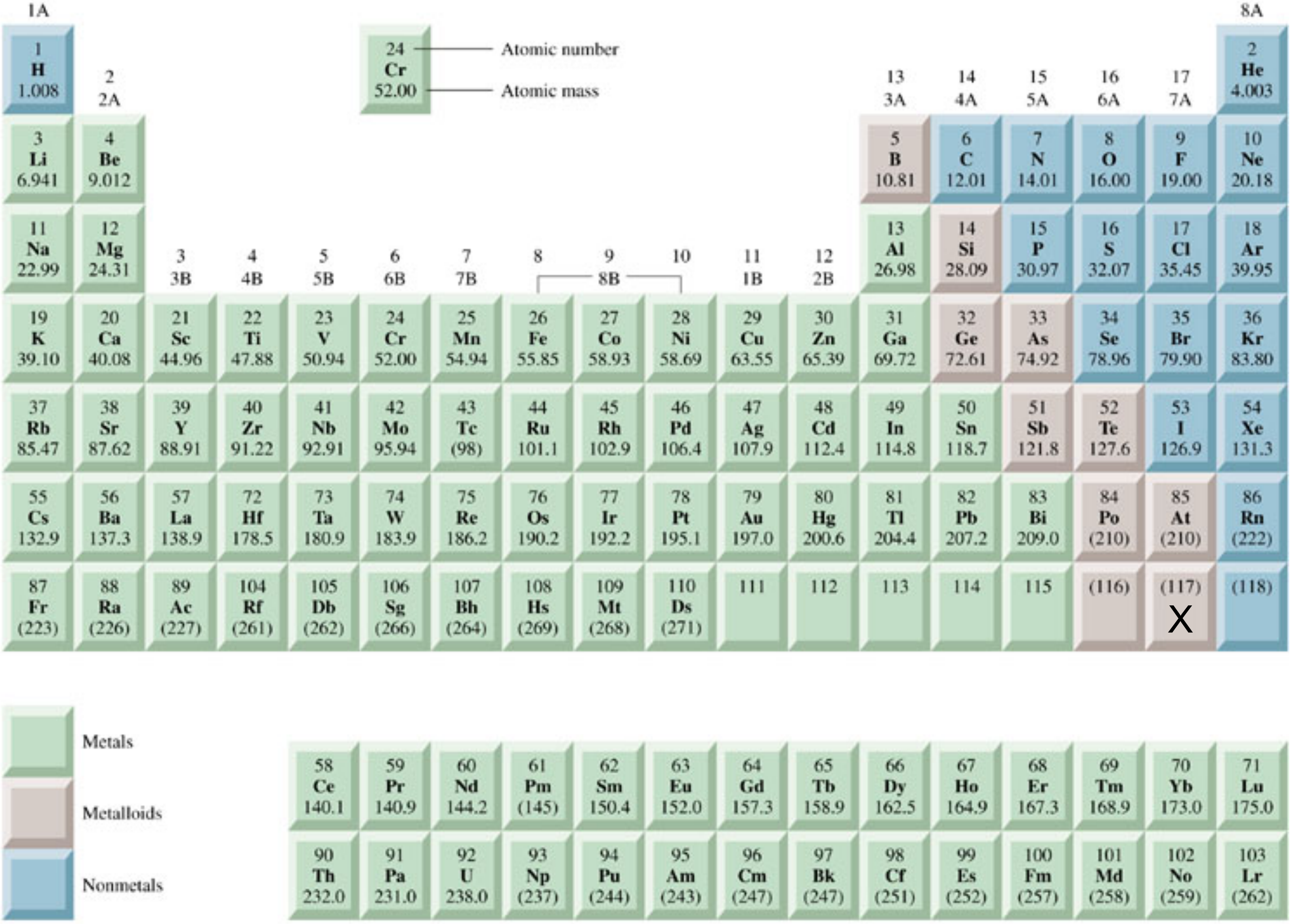
$2C_{135}H_{96}O_9NS + 313O_2 \rightarrow 270CO_2 + 96H_2O + 2NO_2 + 2SO_2$

CH_4: 12.01 +4x1.008=16.05 g/mol CO_2: 12.01 +2x16.00=44.01 g/mol

C_8H_{18}: 8x12.01 +18x1.008=114.26 g/mol

$C_{135}H_{96}O_9NS$: 135x12.01 +96x1.008+9x16.00+14.0+32.07=1908 g/mol

The Periodic Table



24 Cr 52.00
24 — Atomic number
52.00 — Atomic mass

1A																	8A
1 **H** 1.008	2 2A											13 3A	14 4A	15 5A	16 6A	17 7A	2 **He** 4.003
3 **Li** 6.941	4 **Be** 9.012											5 **B** 10.81	6 **C** 12.01	7 **N** 14.01	8 **O** 16.00	9 **F** 19.00	10 **Ne** 20.18
11 **Na** 22.99	12 **Mg** 24.31	3 3B	4 4B	5 5B	6 6B	7 7B	8	9 8B	10	11 1B	12 2B	13 **Al** 26.98	14 **Si** 28.09	15 **P** 30.97	16 **S** 32.07	17 **Cl** 35.45	18 **Ar** 39.95
19 **K** 39.10	20 **Ca** 40.08	21 **Sc** 44.96	22 **Ti** 47.88	23 **V** 50.94	24 **Cr** 52.00	25 **Mn** 54.94	26 **Fe** 55.85	27 **Co** 58.93	28 **Ni** 58.69	29 **Cu** 63.55	30 **Zn** 65.39	31 **Ga** 69.72	32 **Ge** 72.61	33 **As** 74.92	34 **Se** 78.96	35 **Br** 79.90	36 **Kr** 83.80
37 **Rb** 85.47	38 **Sr** 87.62	39 **Y** 88.91	40 **Zr** 91.22	41 **Nb** 92.91	42 **Mo** 95.94	43 **Tc** (98)	44 **Ru** 101.1	45 **Rh** 102.9	46 **Pd** 106.4	47 **Ag** 107.9	48 **Cd** 112.4	49 **In** 114.8	50 **Sn** 118.7	51 **Sb** 121.8	52 **Te** 127.6	53 **I** 126.9	54 **Xe** 131.3
55 **Cs** 132.9	56 **Ba** 137.3	57 **La** 138.9	72 **Hf** 178.5	73 **Ta** 180.9	74 **W** 183.9	75 **Re** 186.2	76 **Os** 190.2	77 **Ir** 192.2	78 **Pt** 195.1	79 **Au** 197.0	80 **Hg** 200.6	81 **Tl** 204.4	82 **Pb** 207.2	83 **Bi** 209.0	84 **Po** (210)	85 **At** (210)	86 **Rn** (222)
87 **Fr** (223)	88 **Ra** (226)	89 **Ac** (227)	104 **Rf** (261)	105 **Db** (262)	106 **Sg** (266)	107 **Bh** (264)	108 **Hs** (269)	109 **Mt** (268)	110 **Ds** (271)	111	112	113	114	115	(116)	(117) X	(118)
				58 **Ce** 140.1	59 **Pr** 140.9	60 **Nd** 144.2	61 **Pm** (145)	62 **Sm** 150.4	63 **Eu** 152.0	64 **Gd** 157.3	65 **Tb** 158.9	66 **Dy** 162.5	67 **Ho** 164.9	68 **Er** 167.3	69 **Tm** 168.9	70 **Yb** 173.0	71 **Lu** 175.0
				90 **Th** 232.0	91 **Pa** 231.0	92 **U** 238.0	93 **Np** (237)	94 **Pu** (244)	95 **Am** (243)	96 **Cm** (247)	97 **Bk** (247)	98 **Cf** (251)	99 **Es** (252)	100 **Fm** (257)	101 **Md** (258)	102 **No** (259)	103 **Lr** (262)

🟩 Metals
🟫 Metalloids
🟦 Nonmetals

CO_2 emissions, contd.

Coal: $C_{135}H_{96}O_9NS$
Wood: $C_6H_{12}O_6$

bituminous or anthracite coal:

$$1\text{ kJ}\times\frac{1\text{ g }C_{135}H_{96}O_9NS}{31.0\text{ kJ}}\times\frac{1\text{ mol }C_{135}H_{96}O_9NS}{1908\text{ g }C_{135}H_{96}O_9NS}\times\frac{270\text{ mol }CO_2}{2\text{ mol }C_{135}H_{96}O_9NS}\times\frac{44.01\text{ g }CO_2}{1\text{ mol }CO_2}=0.100\text{ g }CO_2$$

Wood:

$$1\text{ kJ}\times\frac{1\text{ g }C_6H_{12}O_6}{17\text{ kJ}}\times\frac{1\text{ mol }C_6H_{12}O_6}{180.2\text{ g }C_6H_{12}O_6}\times\frac{6\text{ mol }CO_2}{1\text{ mol }C_6H_{12}O_6}\times\frac{44.01\text{ g }CO_2}{1\text{ mol }CO_2}=0.086\text{ g }CO_2$$

$C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O$

$C_6H_{12}O_6$: 6x12.01 + 12x1.008 + 6x16.00=180.2 g/mol

Global carbon emissions

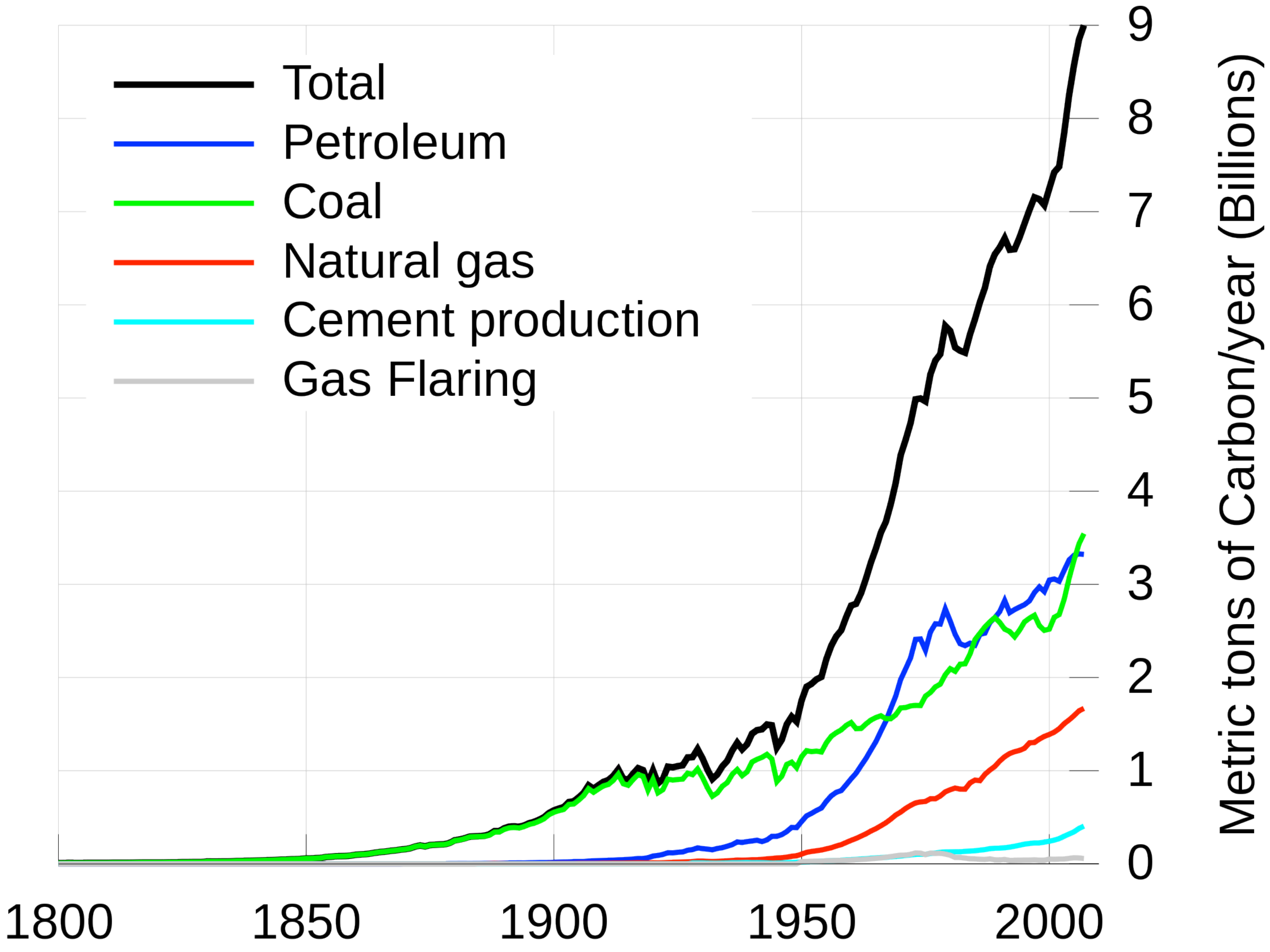


Image by Mak Thorpe, Autopilot/CC BY-SA 3.0

FIGURE 6.17 – Global carbon emissions 1800-2010

Terms and Concepts to Know (Unit 3.1)

- Energy
- Work
- Heat
- Entropy
- Bond energy
- exajoule (EJ)
- hydrocarbon
  - alkanes
- peak oil
- proved reserves
- distillation
- cracking
  - thermal
  - catalytic
- isomers
- octane rating
- oxygenated gasoline

- 1st law of thermodynamics
- 2nd law of thermodynamics
- potential vs kinetic energy
- conversion between different forms of energy (e.g. mechanical to electrical)
- efficiency (or lack thereof) in energy conversion
- exothermic versus endothermic reactions
- energy content of various fuels
- role of catalysts in making reactions go more quickly

- tradeoffs in producing and using fossil fuels