








# Major-Element Geochemistry and $\text{Fe}^{3+}/\Sigma\text{Fe}$ of Metabasites

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Metabasites (metamorphosed mafic rocks) are crucial for understanding metamorphic and tectonic processes. Their preservation in exhumed orogenic belts from throughout Earth's history and the diverse mineral assemblages they form under different pressure-temperature conditions make them valuable for studying metamorphic processes. This work compiles a database of 6186 major-element whole-rock analyses of metabasites from different metamorphic facies (low-grade, greenschist, blueschist, amphibolite, granulite, and eclogite). These are used to explore the range and variability in their composition and assess geochemical differences among metamorphic facies. To mitigate the impact of outliers, median values and median absolute deviations (MAD) are used as measures of central tendency and dispersion. Metabasites show decreased volatile content with increasing metamorphic grade and generally consistent major-element contents across facies, with subtle differences interpreted to result from sampling bias. The median worldwide metabasite is as follows (anhydrous, normalised values in wt %,  $\pm\text{MAD}$ ):  $\text{SiO}_2 = 51.36 \pm 3.40$ ,  $\text{TiO}_2 = 1.33 \pm 0.82$ ,  $\text{Al}_2\text{O}_3 = 15.47 \pm 1.97$ ,  $\text{FeO}^{\text{total}} = 11.48 \pm 2.50$ ,  $\text{MnO} = 0.20 \pm 0.06$ ,  $\text{MgO} = 6.83 \pm 2.25$ ,  $\text{CaO} = 9.84 \pm 2.34$ ,  $\text{Na}_2\text{O} = 2.82 \pm 1.05$ ,  $\text{K}_2\text{O} = 0.50 \pm 0.61$ , and  $\text{P}_2\text{O}_5 = 0.18 \pm 0.16$ . The median  $X_{\text{Mg}} = \text{MgO}/(\text{MgO} + \text{FeO}^{\text{total}})$  is  $0.51 \pm 0.09$ . The median  $\text{Fe}^{3+}/\Sigma\text{Fe}$  was measured by titration in 3153 samples and is  $0.26 \pm 0.12$ , comparable to values in altered oceanic crust or arc basalts. Future research must carefully examine the distribution of  $\text{Fe}^{3+}$  amongst minerals in metabasites, allowing for a better evaluation of the median whole-rock  $\text{Fe}^{3+}/\Sigma\text{Fe}$  and its potential susceptibility to analytical interferences.

**Key words:** Metabasites; Major-element geochemistry;  $\text{Fe}^{3+}/\Sigma\text{Fe}$ ; Metamorphic facies; Whole-rock database

## INTRODUCTION

Metabasites, a term introduced by the Finnish geologist V. Hackman (Sederholm, 1907), refer to metamorphosed mafic rocks such as basalt, dolerite, and gabbro (Miyashiro, 1973). Their mineral assemblages are sensitive to changing pressure-temperature (P-T) conditions, and since the pioneering work of Eskola (1920), they have served as the foundation for defining the metamorphic facies (Poldervaart, 1953; Fyfe et al., 1958). Due to their widespread occurrence in nearly all tectonic-magmatic settings and sensitivity to metamorphic conditions, metabasites are crucial for understanding metamorphic processes.

Barth (1959) noted in his discussion of the geochemical composition of amphibolites – a type of metabasite – that ‘among the metamorphic rocks, the amphibolites occupy a position rather similar to that of the basaltic-gabbroid rocks of the igneous suite’ but he emphasised that, unlike well-characterized basalts and gabbros, ‘no corresponding characterisation has been made of amphibolites.’ Previous studies have produced average compositions for amphibolites ( $n < 250$ ; e.g. Lapadu-Hargues, 1953; Poldervaart, 1955) and have examined compositional variations in metabasites from specific regions between metamorphic facies ( $n < 200$ , e.g. Carden, 1978;

Clough & Field, 1980). However, no comprehensive analysis has been conducted on the major-element geochemistry of metabasites across different metamorphic facies on a global scale.

With an increasing degree of recrystallisation, mafic metamorphic rocks lose traces of their original mineralogy and texture, making it difficult to determine their protolith. This poses challenges in distinguishing whether metabasites were originally basalts or gabbros, and further complicates differentiating them from hydrothermally altered mafic rocks (e.g. spilites; Vallance, 1974), metasomatically altered rocks (Adams, 1909; Orville, 1969), basic tuffs (e.g. para-amphibolites; Evans & Leake, 1960; van de Kamp, 1968, 1970), greywackes (Rivalenti & Sighinolfi, 1969), or calc-silicate sediments (Walker et al., 1959). Authors have used trace-element geochemical criteria to differentiate between the various volcanic rock protoliths (Winchester & Floyd, 1976; Floyd & Winchester, 1978) and decipher the igneous or sedimentary origin of the various types of amphibolite (Leake, 1964; Shaw & Kudo, 1965). Consequently, understanding the geochemical composition of metabasites is essential for determining their origin.

Given the numerous processes that may alter their geochemistry, the term ‘metabasite’ encompasses various rock types with

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significant compositional diversity, unlike basalts, which have a definitive compositional range (Middlemost, 1975). Even subtle variations in major-element geochemistry can affect phase equilibria, influencing the mineral assemblage and compositions formed during metamorphism (Hernández-Urbe et al., 2020; Starr et al., 2020b). Although several studies have generated phase diagrams for an average basalt composition to estimate representative  $P$ - $T$  conditions for commonly occurring metabasic mineral assemblages and to compare these conditions across different metamorphic belts (e.g. Rebay et al., 2010; Palin et al., 2016; Wei & Duan, 2019), these diagrams are limited in their ability to account for the observed geochemical variability in metabasite compositions. This paper compiles published whole-rock analyses of metabasites across a range of metamorphic grades. Our goal is to document the range of chemical compositions of metabasites, establish a median composition, and assess compositional changes amongst the metamorphic facies. This work thus complements a study of similar scope on the major-element geochemistry of metapelites (Forshaw & Pattison, 2023b).

## COMPILATION OF LITERATURE DATA

Although large databases of whole-rock data compiled from the literature are now available, they lack the comprehensive petrographic information that is required to assign metamorphic facies (e.g. Gard et al., 2019). To address this issue, we compiled a whole-rock database from studies of metabasic rocks where authors detailed metamorphic facies or metamorphic mineral assemblages. Whole-rock measurements of metabasites were collected from papers and theses identified through targeted Google Scholar and ProQuest searches using combinations of the following keywords: whole-rock, bulk-rock, metabasite, metamorphism, basalt, prehnite-pumpellyite, greenschist, blueschist, amphibolite, granulite, and eclogite. In recent publications, data could often be copied directly from the PDF or online tables, whilst older data typically required the use of optical character recognition.

Only weight percent oxide values for individual rock samples analysed using bulk techniques such as wet chemistry, X-ray fluorescence, or Fusion Inductively Coupled Plasma Optical Emission Spectroscopy were included. The following major rock-forming components were analysed in all samples:  $\text{SiO}_2$ ,  $\text{TiO}_2$ ,  $\text{Al}_2\text{O}_3$ ,  $\text{FeO}^{\text{total}}$ ,  $\text{MgO}$ , and  $\text{CaO}$ . Over 98% of the samples included values for  $\text{MnO}$ ,  $\text{Na}_2\text{O}$ , and  $\text{K}_2\text{O}$ , with the absence of these values typically due to concentrations falling below the detection limit of the analytical method. Where reported by the authors, determinations of  $\text{P}_2\text{O}_5$ ,  $\text{Fe}_2\text{O}_3$ ,  $\text{H}_2\text{O}^+$ ,  $\text{H}_2\text{O}^-$ ,  $\text{CO}_2$ ,  $\text{SO}_3$ , and loss-on-ignition (LOI) have also been included.  $\text{Fe}_2\text{O}_3$  was measured by titration,  $\text{FeO}$  was determined by difference, and volatiles were analysed by combustion (Gill, 1997). For separate determinations of volatiles, we combined  $\text{H}_2\text{O}^+$  (structurally bound water),  $\text{CO}_2$ , and  $\text{SO}_3$  together as an estimate for LOI (e.g. volatile content). We note that LOI and volatile content may not be equivalent, given the interference of ferrous-iron oxidation with LOI (Lechler & Desilets, 1987).

In this paper, we use the term metabasite in a broad sense to refer to a diverse range of metamorphosed mafic rocks, irrespective of their original protolith. Many papers and theses included whole-rock data from various metamorphosed rock types, including those that are not metabasites. Metamorphic rocks described as ultramafic, granitic, felsic, acidic, or sedimentary (e.g. banded iron formations, greywackes,  $Qz$ -bearing gneisses) were excluded based on descriptions, mineral assemblages, and chemical analyses. In high-grade, migmatitic rocks, samples

described as melanosomes, leucosomes, or selvages were excluded, whilst samples described as metatexites, diatexites, and migmatites, which incorporate a mixture of leucosome/melanosome/mesosome/palaeosome were included. Also included were samples described by metamorphic facies nomenclature, such as greenschists, blueschists, amphibolites, granulites, or eclogites, as well as those identified by their protolith, including metabasalt, metadolerite, metadiabase, metagabbro, meta-basaltic-andesite, and metamafite. Applying a compositional filter—e.g. restricting analyses to those that lie within the basalt field of the TAS diagram (Le Bas et al., 1986)—might ensure more uniform compositions. However, this approach would undermine the aim of this paper, which is to examine the variety of what is generally termed metabasites in metamorphic petrology. We acknowledge that this may introduce outliers into our database, and we address this problem by examining median values and employing median absolute deviation (MAD) and kernel density estimate (KDE) analyses.

The resulting database contains 6186 analyses from 253 studies categorised into 217 localities (Table 1). The database exhibits a significant skew, with most metabasites originating from North America (40.5%) and Europe (29.4%), and a notable proportion from Asia (15.4%). In contrast, samples from Africa (4.7%), Antarctica (1.6%), Oceania (4.7%), and South America (3.7%) are under-represented (Table 1).

## TREATMENT OF DATA

### Metamorphic facies assignment

'A metamorphic facies is a set of metamorphic mineral assemblages, repeatedly associated in space and time, such there is a constant and therefore predictable relation between mineral composition and chemical composition (Turner, 1981).' Whilst many petrologists commonly link metamorphic facies with specific  $P$ - $T$  ranges, it is crucial to note that facies are fundamentally characterized by their mineral assemblages rather than directly by  $P$ - $T$  conditions, which are interpretative. It is possible, albeit rare, to observe multiple facies within the same outcrop, which can be attributed to differences in bulk composition, kinetic factors, or variable degrees of retrogression. These instances do not imply a simultaneous  $P$ - $T$  environment but rather reflect complex histories, including both prograde and retrograde metamorphic events. Thus, in this paper, facies were classified based on some combination of the mineral assemblage and facies description given by the original authors rather than on the  $P$ - $T$  conditions recorded (Fyfe & Turner, 1966; Ghent, 2020).

Six metamorphic facies were used: low-grade (LG), greenschist (Gs), blueschist (Bs), amphibolite (A), granulite (Gr), and eclogite (E). Although we attempted to classify samples into more specific subcategories (e.g. epidote amphibolite vs amphibolite), the reported mineral assemblages were, in many cases, too ambiguous to make precise distinctions. Unmetamorphosed basaltic rocks have not been included. The low-grade category encompasses the zeolite and prehnite-pumpellyite facies. The greenschist facies includes rocks containing some combination of chlorite, epidote, actinolite, and albite, whilst blueschist facies rocks are characterised by the presence of modally abundant Na-amphibole. Amphibolite facies rocks contain hornblende and Ca-bearing plagioclase, whilst eclogite facies rocks contain omphacite and garnet, with minimal Na-amphibole and retrograde plagioclase. Granulite facies rocks include those with orthopyroxene and clinopyroxene (i.e. low-moderate- $P$ ) as well as those with clinopyroxene, garnet, and Ti-rich amphibole

**Table 1:** Geographic locations with metabasic major-element whole-rock geochemistry

Country	#L	#WR	LG	Gs	A	Gr	Bs	E	References
<b>WORLDWIDE</b>	<b>217</b>	<b>6186</b>	<b>556</b>	<b>1105</b>	<b>2017</b>	<b>1069</b>	<b>360</b>	<b>614</b>	
<b>AFRICA</b>	<b>12</b>	<b>290</b>		<b>24</b>	<b>145</b>	<b>78</b>		<b>43</b>	
Botswana	1	24		24					(Kampunzu <i>et al.</i> , 1998)
Cameroon	1	10						10	(Bouyo <i>et al.</i> , 2019)
Egypt	1	8			8				(Abdel-Karim, 2003)
Kenya	1	12			12				(Miyake, 1984)
Nigeria	2	34			34				(Olade & Elueze, 1979; Olajide-Kayode <i>et al.</i> , 2023)
Sierra Leone	1	27				2		25	(Hills & Haggerty, 1989)
South Africa	2	98			59	39			(Geringer, 1979; Zelt, 1980; Clifford <i>et al.</i> , 1981; McStay, 1991; Raith & Meisel, 2001)
Tanzania	1	47			10	37			(Coolen, 1980)
Togo	2	30			22			8	(Agbossoumondé <i>et al.</i> , 2013, 2017)
<b>ANTARCTICA</b>	<b>6</b>	<b>101</b>		<b>7</b>	<b>35</b>	<b>36</b>		<b>6</b>	(Blight & Oliver, 1977; Storey & Meneilly, 1985; Vincenzo <i>et al.</i> , 1997; Rao <i>et al.</i> , 2000; Grosch, 2005; Suda <i>et al.</i> , 2008; Palmeri <i>et al.</i> , 2018; Kim <i>et al.</i> , 2019)
<b>ASIA</b>	<b>47</b>	<b>951</b>	<b>37</b>	<b>232</b>	<b>307</b>	<b>197</b>	<b>74</b>	<b>85</b>	
China	5	105		13	19	18		55	(Zhang <i>et al.</i> , 2006; Wang <i>et al.</i> , 2014; Huang <i>et al.</i> , 2018; Lü <i>et al.</i> , 2019; Liu <i>et al.</i> , 2021; Yan <i>et al.</i> , 2022)
India	12	159		68	54	30	7		(Subramaniam, 1959; Babu, 1970; Naqvi, 1971; Sen & Ray, 1971; Subbarao, 1971; Ramaswamy & Murty, 1973; Hazarika, 1985; Honegger <i>et al.</i> , 1989; Prakash, 1994; Walia, 1996; Faak <i>et al.</i> , 2012; Srivastava, 2012; Singh, 2022)
Indonesia	1	17							(Parkinson, 1996)
Iran	1	9			9				(Fatehi & Ahmadipour, 2018)
Japan	12	244	7	106	77	14	36	4	(Seki <i>et al.</i> , 1964; Kanisawa, 1969, 1971; Ernst <i>et al.</i> , 1970; Yûjirô, 1971; Sawada, 1973; Honma, 1974; Kutsukake, 1975; Tagiri & Onuki, 1976; Hoshino, 1979; Onuki & Ishimoto, 1980; Goto & Banno, 1990; Arakawa <i>et al.</i> , 2001)
Nepal	1	4						4	(Li <i>et al.</i> , 2019)
Oman	3	99	30	11	25		23	10	(El-Shazly <i>et al.</i> , 1994; Einaudi <i>et al.</i> , 2000; Ishikawa <i>et al.</i> , 2005)
Pakistan	1	84			33	49			(Jan & Kempe, 1973; Jan, 1977, 1988)
Papua New Guinea	1	30			22		8		(Worthing & Crawford, 1996)
Russia	4	95				86		9	(Glukhovskiy & Moralev, 1993; Molina <i>et al.</i> , 2002; Turkina & Nozhkin, 2014; Turkina, 2023)
Saudi Arabia	1	5			5				(Nasseef & Gass, 1977)
South Korea	3	45			45				(So & Kim, 1975; So, 1978; Lee & Cho, 2020)
Taiwan	1	43		31	12				(Yui <i>et al.</i> , 1990)
Vietnam	1	12		3	6			3	(Zhang <i>et al.</i> , 2013)
<b>EUROPE</b>	<b>54</b>	<b>1819</b>	<b>23</b>	<b>294</b>	<b>620</b>	<b>244</b>	<b>184</b>	<b>440</b>	
Austria	1	7						7	(Miladinova <i>et al.</i> , 2022)
Croatia	1	12			12				(Pamić <i>et al.</i> , 2002)
Czechia	2	44			37	7			(Janousek <i>et al.</i> , 2006; Ilnicki <i>et al.</i> , 2020)
Finland	2	36				36			(Paavola, 1984; Nehring <i>et al.</i> , 2010)
France	4	57		8	15		17	17	(Carpenter, 1976; Triboulet, 1980; Piboule & Briand, 1985; Korh <i>et al.</i> , 2009; Pujol-Solà <i>et al.</i> , 2022)
Germany	2	79		9	28			42	(Okrusch <i>et al.</i> , 1989; Schüssler <i>et al.</i> , 1989; Massonne & Czambor, 2007)
Greece	7	435	3	55	15		131	223	(Katagas & Sapountzis, 1977; Katagas & Panagos, 1979; Schliestedt, 1986; Schliestedt & Matthews, 1987; Barr, 1989; Ganor <i>et al.</i> , 1996; Liati & Seidel, 1996; Grandy, 2000; Robson, 2000; Marschall, 2005; Bulle <i>et al.</i> , 2010; Hamelin <i>et al.</i> , 2018; Skelton <i>et al.</i> , 2019; Gyomlai <i>et al.</i> , 2021)
Ireland	2	45			45				(Ryan <i>et al.</i> , 1983; Leake, 2016)

(Continued)

Table 1: Continued

Country	#L	#WR	LG	Gs	A	Gr	Bs	E	References
Italy	9	194	10	18	28	44	30	62	(Hoffmann, 1970; Capedri <i>et al.</i> , 1977; Reinsch, 1979; Pognante <i>et al.</i> , 1982; Messiga <i>et al.</i> , 1983; Cortesogno <i>et al.</i> , 1984; Sills & Tarney, 1984; Mazzucchelli & Siena, 1986; Conti <i>et al.</i> , 1988; Bea & Montero, 1999; Giacomini <i>et al.</i> , 2005; Starr <i>et al.</i> , 2020a; Weber <i>et al.</i> , 2022)
Norway	5	275			134	125		15	(Heier, 1962; Misra & Griffin, 1972; Clough, 1977; Dekker, 1978; Clough & Field, 1980; Krogh, 1980)
Poland	2	21			21				(Puziewicz, 2006; Ilnicki <i>et al.</i> , 2013)
Russia	3	65		2	28	11		24	(Khodorevskaya, 2012; Rass <i>et al.</i> , 2014; Terentiev & Santosh, 2017)
Scotland	4	233		151	66	16			(Wilson & Leake, 1972; Graham, 1973, 1976; Skelton, 1992; Smith & Phillips, 2002; Feisel <i>et al.</i> , 2018)
Spain	6	149			122	5		19	(Bard, 1969, 1970; Suen, 1978; van der Wegen, 1978; Bard & Moine, 1979; Castro <i>et al.</i> , 1996; Molina & Montero, 2003; Lorda <i>et al.</i> , 2014; Villaseca <i>et al.</i> , 2015; Pujol-Solà <i>et al.</i> , 2022)
Switzerland	4	134		34	69			31	(Wenk <i>et al.</i> , 1974; Puschnig, 2000; Widmer, 2001; Decrausaz <i>et al.</i> , 2021)
Wales	1	33	10	17			6		(Nataraj, 1967; Bevins <i>et al.</i> , 1991)
<b>N. AMERICA</b>	<b>71</b>	<b>2504</b>	<b>393</b>	<b>496</b>	<b>680</b>	<b>441</b>	<b>93</b>	<b>4</b>	
Canada	32	1516	262	410	376	110	3		(Baragar, 1960, 1969; Jennings, 1969; Preto, 1970; Fletcher, 1971; Mummery, 1972; de Wit & Strong, 1975; Hall-Beyer, 1976; Kuniyoshi & Liou, 1976; Coish, 1977a, 1977b; Ghent <i>et al.</i> , 1977; Stamatelopoulou-Seymour & MacLean, 1977; Fryer & Jenner, 1978; Baragar <i>et al.</i> , 1979; Hynes, 1980; Jenner & Fryer, 1980; Jolly, 1980; Dostal <i>et al.</i> , 1983; Ouellet, 1988; Sevigny, 1988; Brons, 1989; Pattison, 1991; Sawyer, 1991; Lafleche <i>et al.</i> , 1992; Owen, 1993; Plint & Gordon, 1997; Hozjan, 1999; Zwanzig & Bailes, 2010; Gilbert, 2011; Syme & Whalen, 2012; Syme, 2014; Jørgensen, 2017; Starr, 2017; Jørgensen <i>et al.</i> , 2019; Starr & Pattison, 2019b; Geen, 2021; Lazzarotto <i>et al.</i> , 2023)
Greenland	8	243	8	6	109	120			(Preston, 1969; Glassley & Sørensen, 1980; Mengel, 1983; Schiøtte, 1988; Messiga <i>et al.</i> , 1990; Bevins <i>et al.</i> , 1991; Haynes, 1998; Polat <i>et al.</i> , 2003)
Mexico	1	27				27			(Culí <i>et al.</i> , 2023)
Panama	1	7			7				(Tournon <i>et al.</i> , 1989)
USA	29	711	123	80	188	184	90	4	(Buddington, 1952; Wilcox & Poldervaart, 1958; Engel & Engel, 1962; Coleman & Lee, 1963; Ernst <i>et al.</i> , 1970; Jolly, 1970; Jolly & Smith, 1972; Maxey, 1972; Ghent & Coleman, 1973; Jen, 1975; Bohman, 1976; Clark, 1976; Aleinikoff, 1977; Carden, 1978; Perfit <i>et al.</i> , 1980; Dungan <i>et al.</i> , 1983; Jayko, 1984; Weakliem, 1984; Davis & Plafker, 1985; Hollocher, 1985; Stoddard, 1985; Thurston, 1985; Schumacher, 1988; Alibert <i>et al.</i> , 1991; Harper, 1995; Walker & Murphy, 1995; Chocyk-Jaminski, 1998; Liogys & Jenkins, 2000; Chocyk-Jaminski & Dietsch, 2002; Brady <i>et al.</i> , 2004; Bruand <i>et al.</i> , 2011; Becker <i>et al.</i> , 2023)
<b>OCEANIA</b>	<b>16</b>	<b>292</b>	<b>70</b>	<b>21</b>	<b>103</b>	<b>66</b>	<b>6</b>	<b>8</b>	
Australia	12	230	50		96	66			(Binns, 1964; Bradley, 1972; Wilson, 1976; Stephenson, 1977, 1980; Stephenson & Hensel, 1982; McNaughton & Wilson, 1983; Nash, 1984; Sivell, 1986, 1988; Crawford & Keays, 1987; Sivell & Foden, 1988)
New Caledonia	1	21			7		6	8	(Spandler <i>et al.</i> , 2004)
New Zealand	3	41	20	21					(Cooper & Lovering, 1970; Sivell, 1984; Houghton, 1985)

(Continued)

**Table 1:** Continued

Country	#L	#WR	LG	Gs	A	Gr	Bs	E	References
<b>S. AMERICA</b>	<b>11</b>	<b>229</b>	<b>33</b>	<b>31</b>	<b>127</b>	<b>7</b>	<b>3</b>	<b>28</b>	
Brazil	5	132	6		119	7			(Gomes et al., 1964; Kuyumjian, 1989; de Oliveira et al., 1993; Bicalho et al., 2019; Capistrano et al., 2021)
Chile	1	9	9						(Levi, 1969)
Colombia	3	40	18	16	3			3	(Spadea et al., 1987; Spadea & Espinosa, 1996; García-Ramírez et al., 2017)
Ecuador	1	11					3	8	(John et al., 2010)
Venezuela	1	37		15	5			17	(Mottana et al., 1985)

Note: #L—number of localities, #WR—number of whole-rock analyses, LG—Low-grade facies, Gs—Greenschist facies, A—Amphibolite facies, Gr—Granulite facies, Bs—Blueschist facies, E—Eclogite facies

(i.e. higher-*P*; see Pattison, 2003). A total of 465 analyses (8%) could not be classified into specific metamorphic facies. This was either because they belong to a transitional category between two facies, or insufficient information was provided to make a clear classification. The distribution of analyses across metamorphic facies is as follows: 9.7% low-grade, 19.3% greenschist, 35.3% amphibolite, 18.7% granulite, 6.3% blueschist, and 10.7% eclogite (Table 1). A complete catalogue listing all analyses detailing sample names, metamorphic facies, literature references, and whole rock data can be found in Table S1.

## Plotting and projections

Metabasite compositions, expressed in weight percent and normalized to 100% with all iron as  $\text{FeO}^{\text{total}}$ , were plotted on a  $\text{TiO}_2$  versus  $\text{Al}_2\text{O}_3$  diagram. This approach differentiates igneous basalts from cumulates which show lower  $\text{TiO}_2$  contents and either higher  $\text{Al}_2\text{O}_3$  due to plagioclase accumulation or lower  $\text{Al}_2\text{O}_3$  due to pyroxene accumulation (Miller & Thöni, 1995). Additionally, metabasites were plotted on an igneous AFM diagram to distinguish between tholeiitic and calc-alkaline nature. This uses wt % analyses and the following formulae:  $\text{Alkali}'s = \text{K} + \text{N} = \text{K}_2\text{O} + \text{Na}_2\text{O}$ ,  $F = \text{FeO}^{\text{total}}$ , and  $M = \text{MgO}$ .

Metabasites exhibit considerable chemical variability within the 12-component system  $\text{SiO}_2$ – $\text{TiO}_2$ – $\text{Al}_2\text{O}_3$ – $\text{Fe}_2\text{O}_3$ – $\text{FeO}$ – $\text{MnO}$ – $\text{MgO}$ – $\text{CaO}$ – $\text{Na}_2\text{O}$ – $\text{K}_2\text{O}$ – $\text{P}_2\text{O}_5$ – $\text{H}_2\text{O}$  system (Spear, 1993). Visualising geochemical differences on ternary diagrams requires selecting three components, necessitating the exclusion or combination of certain components and projection from specific phases. For initial analysis, all iron was assumed to be  $\text{FeO}$  (ferrous).  $\text{MnO}$  was omitted. Whole rock analyses were then reduced to the eight-component ( $\text{SiO}_2$ – $\text{Al}_2\text{O}_3$ – $\text{FeO}^{\text{total}}$ – $\text{MgO}$ – $\text{CaO}$ – $\text{Na}_2\text{O}$ – $\text{K}_2\text{O}$ – $\text{H}_2\text{O}$ ) system using projections from apatite and ilmenite to remove  $\text{P}_2\text{O}_5$  and  $\text{TiO}_2$ , respectively. The ilmenite projection is probably not valid at higher pressures where Ti may also or instead reside in rutile. Many metabasites lack quartz, making projection from quartz less rigorous when compared to metapelites, but we assume its presence for uniformity of treatment. Additionally, we project through  $\text{H}_2\text{O}$ , assuming  $\text{H}_2\text{O}$  saturated conditions, even though this assumption may not be valid in the eclogite and granulite facies (see Spear, 1993 for a discussion of both projections).

Metamorphic ternary diagrams utilise mol % values. To plot analyses in an ACN diagram, we ignore  $\text{FeO}^{\text{total}}$ ,  $\text{MgO}$ , and  $\text{K}_2\text{O}$  and use the following formulae:  $A = \text{AlO}_{3/2}$ ,  $C = \text{CaO}$ , and  $N = \text{NaO}_{1/2}$  (after Spear, 1993). Whole-rock analyses are plotted in the ACFM tetrahedron using the following formulae:

$A' = \text{AlO}_{3/2} - \text{NaO}_{1/2} - \text{KO}_{1/2}$ ,  $C = \text{CaO}$ ,  $F = \text{FeO}^{\text{total}}$ , and  $M = \text{MgO}$ . The  $A'$  component here is calculated as in Forshaw et al. (2019), whereby the formula of Eskola (1920) is used, but with the  $A'$  coordinate expanded as in Spear (1993). Plotting the classical ACF diagram of Eskola (1920) requires  $\text{Fe}^{\text{total}}$  and  $\text{Mg}$  to be lumped together as a single component ( $F + M = \text{FeO}^{\text{total}} + \text{MgO}$ ). One major shortcoming of this lumping is obscuring variation in  $X_{\text{Mg}} = \text{MgO} / (\text{Fe}^{\text{total}} + \text{MgO})$ . Therefore, we plot a metamorphic AFM diagram in which  $A^{0.5} = \text{Al}_2\text{O}_3$  (note the difference between  $A$ ,  $A'$ , and  $A^{0.5}$ ); this requires additional projection from an average plagioclase composition ( $\text{An}_{33}$ ) and idealised epidote (Laird, 1980; Spear, 1993). Whilst epidote and plagioclase projections are only valid for upper greenschist and lower amphibolite facies rocks, all whole-rock compositions were projected the same way to allow comparison. We emphasize that the ternary diagrams presented here are designed only to show compositional variability; none of them can rigorously assess the phase relations of metabasites due to the excessive number of important components (Spear, 1993).

## Statistical analysis

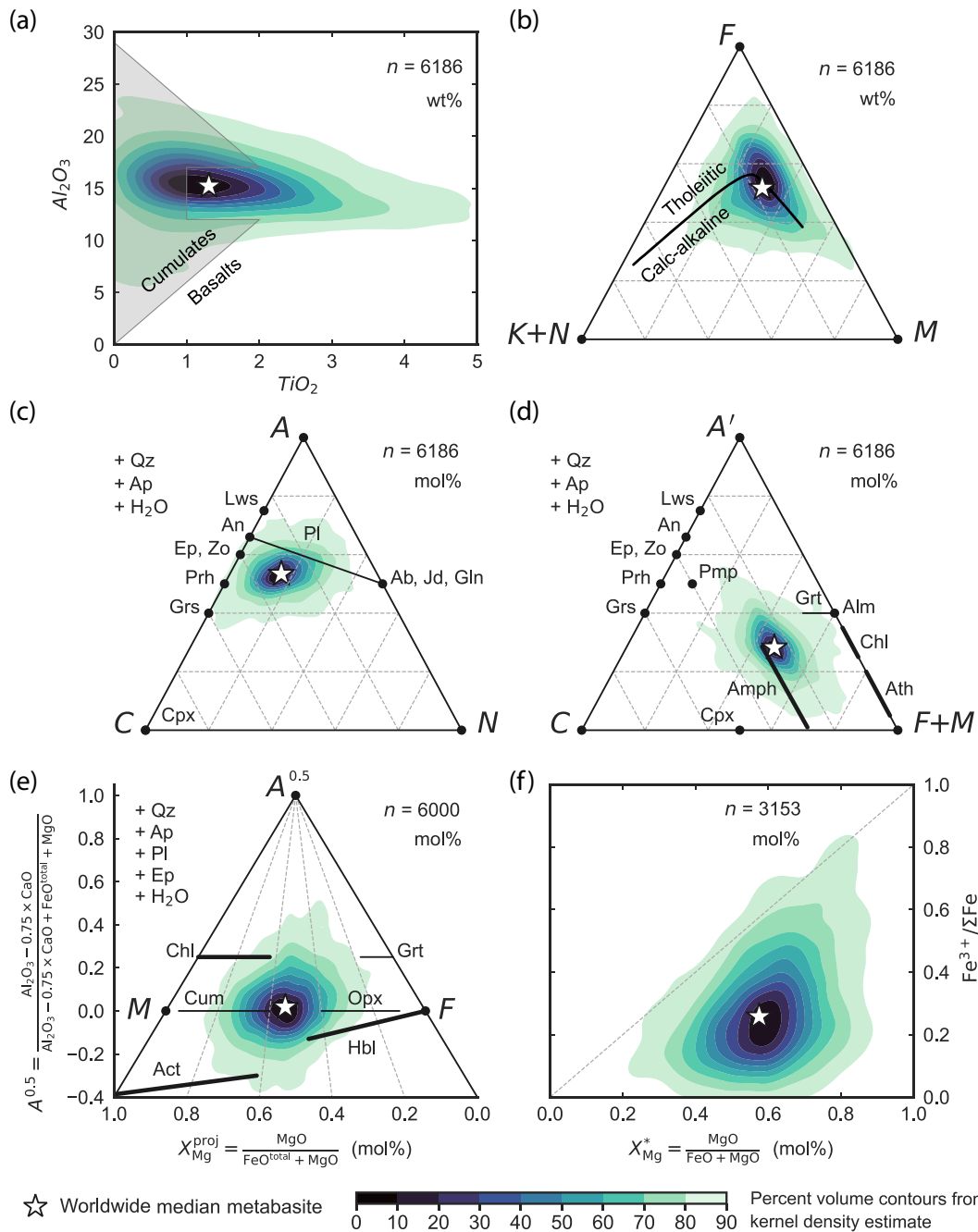
As in Forshaw & Pattison (2023b), we use median values as measures of central tendency as these are least susceptible to outliers (Rock, 1988). Histograms of each element illustrate the distribution of all analyses and verify that the median values are close to the mode (see Supplemental Material). As measures of dispersion, we use median absolute deviations (MAD), kernel density estimates (KDE), and letter-value plots. MADs are provided alongside median values in Table 2. Two-dimensional KDEs are used to show the spread between variables on ternary diagrams in Fig. 1. Letter-value plots are used to depict the spread in each element for each metamorphic facies (Fig. 2). Letter-value plots extend traditional box-and-whisker plots by showing multiple quantiles beyond the median, quartiles, and whiskers, offering a detailed depiction of data distribution at various levels of granularity (Hofmann et al., 2017). These were chosen over KDEs for this visualisation because they are less susceptible to bandwidth choice.

Compositional data are inherently multivariate, have a constant sum, and are thus constrained by the closure problem (Chayes, 1960). Compositional biplots were constructed to examine relationships in the components' covariance and distribution of the components themselves (Aitchison & Greenacre, 2002). No consistent patterns were found among the elements between different metamorphic facies (see Supplemental Material). Since interpreting log-ratio values and their associated biplots can be challenging (Rock, 1989), we use wt % oxides in our facies comparison (Forshaw & Pattison, 2023b).

Table 2: Median metabasite compositions

Facies	SiO <sub>2</sub>	TiO <sub>2</sub>	Al <sub>2</sub> O <sub>3</sub>	FeO <sup>total</sup>	MnO	MgO	CaO	Na <sub>2</sub> O	K <sub>2</sub> O	P <sub>2</sub> O <sub>5</sub>	LOI	X <sub>Mg</sub>	Fe <sup>3+</sup> /ΣFe	X <sub>Mg</sub> <sup>*</sup>
					(wt %)								(calculated from mol %)	
World-wide	MED MAD n	1.33 0.82 6186	15.47 1.97 6186	11.48 2.50 6186	0.20 0.06 6068	6.83 2.25 6186	9.84 2.34 6186	2.82 1.05 6166	0.50 0.61 6158	0.18 0.16 5698		0.51 0.09 6186	0.26 0.12 3153	0.58 0.10 3153
All-MORB Mean		1.69	14.76	10.48	0.18	7.61	11.44	2.80	0.16	0.18		0.56		
AOC Composite		1.74	12.31	12.61	0.23	6.35	13.31	2.35	0.63	0.17		0.47	0.51	0.65
Lower Cont Crust		1.40	18.10	10.44	0.18	6.87	10.11	2.85	1.22	0.23		0.54		
Continental THB		0.71	17.72	8.55	0.16	10.03	11.54	2.45	0.16	0.08		0.68		
Intra-oceanic THB		0.59	15.46	8.86	0.16	11.15	10.86	1.89	0.17	0.09		0.69		
Back-arc basin THB		1.11	16.30	8.41	0.16	9.92	11.34	2.56	0.21	0.13		0.68		
Continental CAB		1.32	16.29	8.25	0.14	9.03	9.34	3.32	1.23	0.42		0.66		
Intra-oceanic CAB		0.69	12.92	9.69	0.20	12.93	11.21	1.99	0.97	0.20		0.70		
Low-grade	MED MAD n	1.67 0.68 556	14.99 1.60 556	11.85 2.34 556	0.20 0.05 515	6.26 2.03 556	8.84 2.50 556	3.17 0.94 541	0.78 0.77 556	0.20 0.10 469	2.80 1.04 514	0.48 0.09 556	0.36 0.14 387	0.59 0.11 387
Greenschist	MED MAD n	1.20 0.75 1105	15.65 1.95 1105	10.94 2.14 1105	0.18 0.05 1059	7.00 2.54 1105	9.47 2.71 1105	3.01 1.14 1103	0.38 0.61 1094	0.18 0.18 997	3.12 1.61 1009	0.52 0.10 1105	0.24 0.12 652	0.60 0.12 652
Amphibolite	MED MAD n	1.30 0.83 2017	15.53 1.96 2017	11.61 2.30 2017	0.20 0.05 2009	6.84 2.08 2017	10.17 2.09 2017	2.58 0.83 2015	0.52 0.56 2013	0.18 0.15 1909	1.27 0.81 1627	0.51 0.09 2017	0.25 0.11 1138	0.56 0.10 1138
Granulite	MED MAD n	1.27 0.68 1069	15.52 2.10 1069	12.38 2.76 1069	0.21 0.06 1063	6.89 2.32 1069	10.12 1.90 1069	2.54 0.93 1069	0.62 0.51 1069	0.18 0.18 945	0.59 0.54 783	0.50 0.09 1069	0.21 0.09 494	0.56 0.08 494
Blueschist	MED MAD n	1.71 0.78 399	15.79 2.20 360	11.22 2.35 360	0.19 0.15 354	6.33 2.09 360	8.52 3.37 360	3.65 1.38 360	0.56 0.89 358	0.20 0.16 340	2.70 1.94 323	0.50 0.09 360	0.36 0.14 228	0.61 0.08 228
Eclogite	MED MAD n	1.44 1.48 614	15.17 2.15 614	10.95 3.19 614	0.20 0.06 607	7.05 2.46 614	9.85 2.24 614	3.46 1.54 613	0.22 0.62 605	0.13 0.24 581	1.10 0.71 539	0.52 0.11 614	0.23 0.13 174	0.60 0.11 174

Note: Median wt % oxide values did not sum to 100%, so they were normalised with all iron as FeO<sup>total</sup> and volatiles (loss-on-ignition [LOI], H<sub>2</sub>O<sup>+</sup>, CO<sub>2</sub>, and SO<sub>3</sub>) removed. Median absolute deviations (MAD) for each wt % oxide were scaled by the same factor used for normalisation of the median (e.g. if the median total was 98.4%, MAD values were scaled by 1.02 = 100/98.4). X<sub>Mg</sub>, Fe<sup>3+</sup>/ΣFe, X<sub>Mg</sub><sup>\*</sup> are defined in the text. The MAD for these variables was calculated directly from X<sub>Mg</sub>, Fe<sup>3+</sup>/ΣFe, and X<sub>Mg</sub><sup>\*</sup> without incorporating error propagation from MgO, FeO<sup>total</sup>, FeO, or Fe<sub>2</sub>O<sub>3</sub>. Therefore, the MAD for these values represents the spread of the variables themselves, rather than the propagated uncertainty from variability in the MgO, FeO<sup>total</sup>, FeO, or Fe<sub>2</sub>O<sub>3</sub>. ALL-MORB Mean (Gale et al., 2013). AOC Site 801 Super Composite (Kelley et al., 2003; Brounce et al., 2019). Lower Cont Crust (mafic end-member 45–50% composition; Hacker et al., 2015). Continental THB and CAB (Cascades), Intra-oceanic and back-arc basin THB (Izu-Bonin), Intra-oceanic CAB (Vanatu; Schmidt & Jagoutz, 2017). All literature compositions normalised to 100%. Abbreviations: MED—median, MAD—median absolute deviation, n—number of analyses, MORB—Mid-ocean ridge basalt, AOC—Altered Oceanic Crust THB—Tholeiitic basalt, CAB—Calc-alkaline basalt.



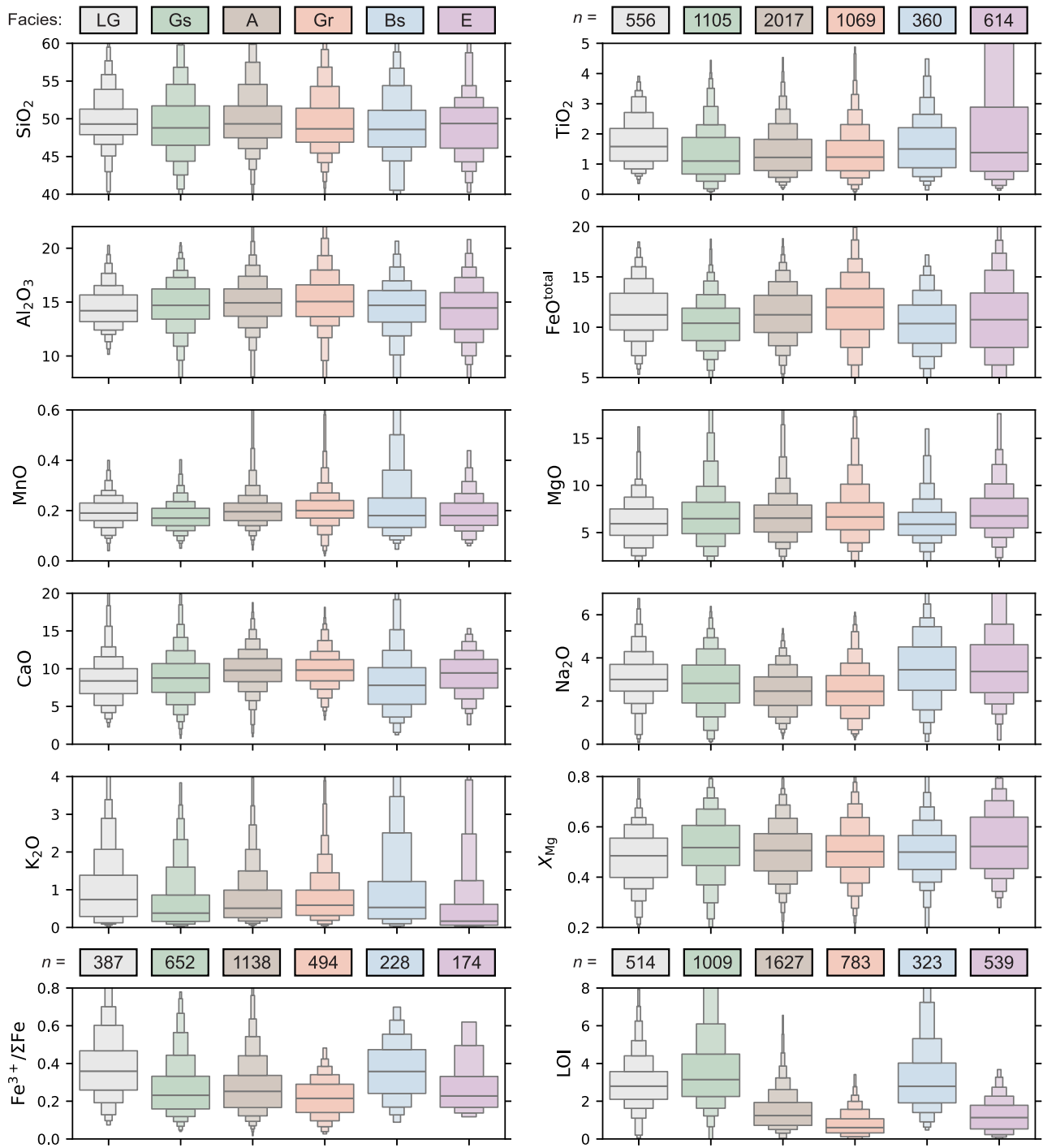
**Figure 1.** Distribution of metabasic whole-rock analyses. (a) Contoured KDE of  $Al_2O_3$  versus  $TiO_2$  (wt %). Cumulate and basalt delineation is as shown by Miller & Thöni (1995). (b) Contoured KDE of an igneous AFM (Alkali's  $K_2O+Na_2O$ ,  $FeO^{total}$ , and  $MgO$ ; wt %) diagram. Tholeiitic and calc-alkaline boundary after Rollinson & Pease (2021). (c/d) Contoured KDE of ACN and ACF diagrams after projection from apatite, ilmenite, quartz, and  $H_2O$ . (e) Contoured KDE of a metamorphic AFM diagram after projection from average plagioclase ( $An_{33}$ ), epidote, apatite, ilmenite, quartz, and  $H_2O$ . (f) Contoured KDE of  $Fe^{3+}/\Sigma Fe$  versus  $X_{Mg}^*$  for analyses where  $FeO$  was measured using titration. Median worldwide metabasite composition (star). Mineral abbreviations are after Warr (2021).

## COMPOSITIONAL VARIABILITY

### Variation diagrams

On the igneous  $TiO_2$  versus  $Al_2O_3$  diagram, metabasic whole-rock analyses span the basalt-cumulate divide, displaying the widest variation in  $TiO_2$  (Fig. 1a). On the igneous AFM diagram, the peak of the KDE intersects the boundary between calc-alkaline and tholeiitic rock series (Fig. 1b), with a greater proportion of analyses being tholeiitic. All analyses show a wide range in  $FeO^{total}$  and  $MgO$  (Fig. 1b). On the ACN diagram, metabasic whole-rock

analyses form an ellipse, showing the greatest spread in Ca and Na, with relatively less variation in Al (Fig. 1c). The 50% VPC-KDE (volume per cent contour of the kernel density estimate) covers  $A = 0.48-0.60$ ,  $C = 0.20-0.41$ , and  $N = 0.06-0.24$  (Fig. 1c). The greater variation in Na and Ca could be attributed to spilitisation, which increases Na contents, and epidotisation, which increases Ca contents (Fig. 1c). On the ACF diagram, metabasic whole-rock analyses form an ellipse with the greatest spread in Al and  $Fe^{total}+Mg$  and relatively less variation in Ca (Fig. 1d). Fifty per



**Figure 2.** Letter-value plots depicting compositional ranges for each metamorphic facies. Data include elemental oxides and loss-on-ignition (LOI) in wt %, with  $\text{Fe}^{3+}/\Sigma\text{Fe}$  and  $X_{\text{Mg}}$  calculated from mol %. The widest box shows the interquartile range (50% of the data) and the median value as a horizontal line. The second widest boxes (directly above and below the widest box) represent 25% of the data, the third widest boxes 12.5% of the data, and so forth. Metamorphic facies: Low-grade (LG), Greenschist (Gs), Amphibolite (A), Granulite (Gr), Blueschist (Bs), and Eclogite (E). The number of analyses in each category can be found in Table 2, with key differences between the number of analyses in elements or elemental ratios summarised in coloured boxes here.

cent of metabasites fall within the ranges  $A' = 0.22\text{--}0.37$ ,  $C = 0.18\text{--}0.30$ , and  $F+M = 0.37\text{--}0.56$ , as indicated by the 50% VPC-KDE (Fig. 1d). Of the 6186 analyses, 186 plotted at anomalously low or high  $A^{0.5}$  values ( $>1.0$  or  $<0.4$ ) after projection from average plagioclase and epidote, which are not shown in Fig. 1e. On the metamorphic AFM diagram, metabasic whole-rock analyses show similar variations in Al,  $\text{Fe}^{\text{total}}$ , and Mg, with the 50% VPC-KDE covering  $A^{0.5} = -0.13\text{--}0.17$  and  $X_{\text{Mg}}^{\text{proj}} = 0.34\text{--}0.64$  (Fig. 1e).

### $\text{Fe}^{3+}/\Sigma\text{Fe}$

3153 analyses in the database had FeO measured by titration, permitting an estimate of the whole-rock  $\text{Fe}^{3+}/\Sigma\text{Fe}$  and in turn  $X_{\text{Mg}}^* = \text{Mg}/(\text{Fe}^{2+} + \text{Mg})$ . We note that  $\text{Fe}^{3+}/\Sigma\text{Fe}$  is defined using molar quantities and is equivalent to the following variables used to describe the oxidation state of metamorphic rocks:  $X_{\text{Fe}^{3+}} = \text{Fe}^{3+}/(\text{Fe}^{2+} + \text{Fe}^{3+}) = 2x\text{Fe}_2\text{O}_3/(2x\text{Fe}_2\text{O}_3 + \text{FeO}) = \text{Oxidation Ratio}/100$  (Chinner, 1960; Diener & Powell, 2010; Forshaw & Pattison, 2023a).



The 50% VPC-KDE covers a wide range of  $\text{Fe}^{3+}/\Sigma\text{Fe}=0.08\text{--}0.43$  and  $X_{\text{Mg}}^*=0.42\text{--}0.72$  (Fig. 1f). The median worldwide metabasite has  $\text{Fe}^{3+}/\Sigma\text{Fe}=0.26\pm 0.12$  and  $X_{\text{Mg}}^*=0.56\pm 0.10$ , compared to  $X_{\text{Mg}}=0.51\pm 0.09$  for all 6186 samples assuming all iron is FeO (Table 2).

## Metamorphic facies

Fig. 2 shows compositional ranges for each metamorphic facies. A decrease in volatile content with increasing metamorphic grade is well-documented in metamorphic rocks (Fyfe et al., 1978). Mafic rocks are predominantly anhydrous when crystallised and become variably hydrated at low temperatures before undergoing metamorphism. The extent of pre-metamorphic alteration in the protolith influences LOI content, accounting for the wide range of LOI values observed in rocks from lower-temperature facies (Fig. 2). The median and distribution of LOI are comparable for low-grade, greenschist, and blueschist facies rocks, all of which exhibit higher LOI than the other facies. A progressive decrease is observed from the greenschist to amphibolite and then granulite facies, similar to the trend found in pelitic rocks (Forshaw & Pattison, 2023b). Median LOI contents for blueschist and eclogite facies metabasites in this study ( $B_s=2.7$  and  $E=1.1$ ) are lower than the average LOI contents of lawsonite-bearing blueschists and eclogites ( $Lws\text{-}B_s\sim 5.0$  and  $Lws\text{-}E\sim 3.0$ ; Whitney et al., 2020). Median  $\text{Fe}^{3+}/\Sigma\text{Fe}$  is higher in the low-grade and blueschist facies, but comparable across the other facies (Fig. 2). A similar trend in median  $\text{Fe}^{3+}/\Sigma\text{Fe}$  was found for the pelites, in which  $\text{Fe}^{3+}/\Sigma\text{Fe}$  decreased from diagenetic shales up to the biotite zone in pelites (roughly greenschist facies in metabasites) and remained constant in higher grade zones (Forshaw & Pattison, 2023b). To evaluate variations in other major elements between facies, analyses were normalised to 100% on a volatile-free basis, with iron as  $\text{FeO}^{\text{total}}$ .

Median values and distribution patterns show no significant variation as a function of metamorphic facies for several major elements, including  $\text{SiO}_2$ ,  $\text{Al}_2\text{O}_3$ ,  $\text{MnO}$ ,  $\text{MgO}$ , and  $\text{K}_2\text{O}$  (Fig. 2). Median  $\text{TiO}_2$  is relatively higher in low-grade and blueschist facies rocks, and  $\text{TiO}_2$  shows greater variability in eclogite facies samples. Median  $\text{Na}_2\text{O}$  is elevated in blueschist and eclogite facies rocks, whilst median  $\text{CaO}$  is lower in blueschist facies samples. Median  $\text{FeO}^{\text{total}}$  is slightly higher for the granulite facies than other metamorphic facies. The elevated  $\text{Na}_2\text{O}$  and lower  $\text{CaO}$  contents suggest increased spilitisation in blueschist facies rocks compared to other metamorphic facies (Vallance, 1974). This likely reflects sampling bias, where geologists tend to collect and analyse blueschist facies rocks rich in Na-amphiboles, which are prevalent in metaspilites. The greater variation in  $\text{TiO}_2$  contents for eclogite facies rocks reflects the many Ti-rich, Fe-Ti gabbro samples included from Robson (2000); Fe-Ti gabbros and basalts typically contain zircon and, therefore, may be oversampled. Additionally, granulite facies metabasites show increased  $\text{FeO}^{\text{total}}$ , possibly due to the preferential analysis of garnet-bearing samples, an  $\text{Fe}^{2+}$ -rich mineral useful for thermobarometry.

## DISCUSSION

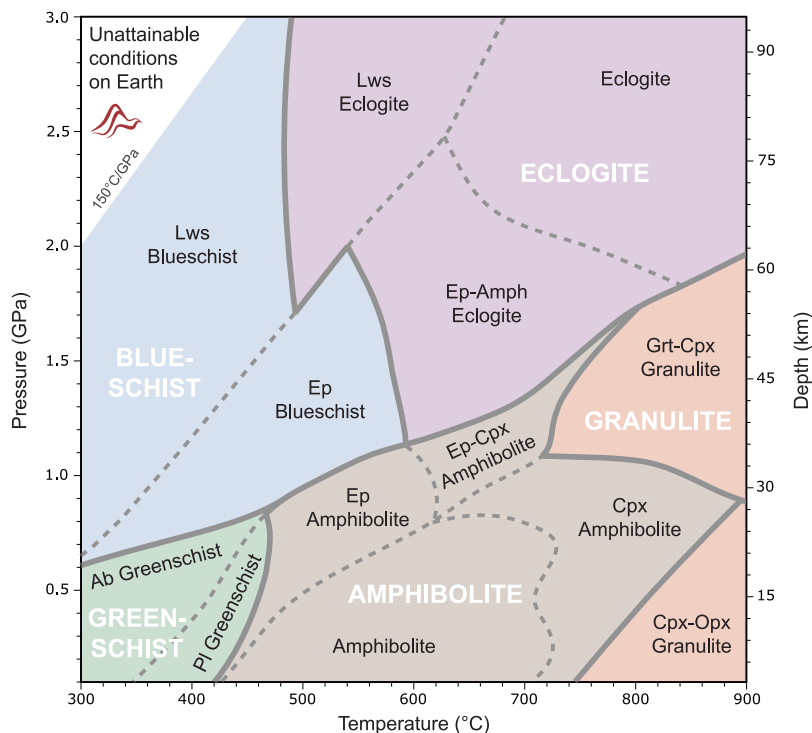
Our comparison revealed only subtle compositional differences between metamorphic facies, apart from LOI and  $\text{Fe}^{3+}/\Sigma\text{Fe}$ . Therefore, we calculated a worldwide median metabasite with volatiles removed and all iron as  $\text{FeO}^{\text{total}}$  (Table 2; Fig. 1). This median gives equal weight to all analyses, which biases it towards amphibolite and granulite facies rocks, the most abundant in the database. Table 2 compares the worldwide median metabasite, and median

metabasites for each metamorphic facies, with several mean and representative mafic igneous compositions from the literature. Literature compositions are within one MAD of the worldwide median metabasite for most elements. Notable exceptions include the low  $\text{Al}_2\text{O}_3$  of altered oceanic crust and intra-oceanic calc-alkaline basalts, high  $\text{K}_2\text{O}$  of mafic lower continental crust and continental calc-alkaline basalts, and high  $X_{\text{Mg}}$  (i.e. low FeO and high MgO) of continental arc, intra-oceanic arc, and back-arc basin basalts (Table 2). Future work may benefit from compiling trace-element data where available to further distinguish compositional trends in metabasites across tectonic settings, though this would require careful consideration of data quality and analytical consistency given the variability in techniques over recent decades.

Iron, as the most abundant element with a variable valence state, plays a crucial role in controlling the redox budget of global rock cycles and the fluid-buffering capacity of rocks during metamorphism (Evans, 2006, 2012). Most of the literature compositions in Table 2 do not include measurements of  $\text{Fe}^{3+}/\Sigma\text{Fe}$ . Bézous et al. (2021) highlighted that 'the accurate and precise determination of the iron oxidation state ratio of MORB glasses has been a matter of controversy for the last three decades. None of the wet chemical methods used in the literature to measure this ratio converge toward a consensus value. The same difficulties have been observed for the most recent data obtained by XANES spectroscopy.' Bézous et al. (2021) found that colorimetric measurements tend to overestimate ferrous iron in sulfide-bearing samples. By recalculating  $\text{Fe}^{3+}/\Sigma\text{Fe}$  for 49 MORB glasses, they determined an average of  $0.10\pm 0.02$ , which aligns with corrected colorimetric data ( $0.07\pm 0.03$ ,  $n=78$ , Christie et al., 1986), previous titration results ( $0.12\pm 0.02$ ,  $n=104$ , Bézous & Humler, 2005), and some XANES measurements ( $0.10\pm 0.02$ ,  $n=42$ , Berry et al., 2018), but not others ( $0.16\pm 0.01$ ,  $n=103$ , Cottrell & Kelley, 2011;  $0.14\pm 0.01$ ,  $n=103$ , Zhang et al., 2018). Discrepancies are attributed to differences in the XANES spectra calibration, particularly the use of Mössbauer spectroscopy, which is subject to ongoing debate regarding acquisition conditions and data interpretation (Berry & O'Neill, 2021; Bézous et al., 2021).

Given that most metabasites in the database likely did not develop at mid-ocean ridges, and that they have been variably hydrated and hydrothermally altered, it is important to compare them to basalts other than MORB. Rutter (2015), based on over 3000 titrations of variably altered ODP samples, estimated the average  $\text{Fe}^{3+}/\Sigma\text{Fe}$  of young and old ocean crust to be  $0.21\pm 0.04$  and  $0.23\pm 0.04$ , respectively. Brounce et al. (2019) determined by colorimetry a considerably higher average  $\text{Fe}^{3+}/\Sigma\text{Fe}$  of 0.51 for altered oceanic crust at ODP site 801 (Table 2). These differences are likely due to Rutter's (2015) inclusion of both fresh and a range of altered samples, whilst Brounce et al. (2019) focused explicitly on altered oceanic crust. Using  $\mu\text{-XANES}$ , several studies have shown that the  $\text{Fe}^{3+}/\Sigma\text{Fe}$  of olivine-hosted melt inclusions representative of arc basalt magmas are more oxidised than MORB (reported  $\text{Fe}^{3+}/\Sigma\text{Fe}$  values are not given here due to their sensitivity to the choice of XANES spectra calibration; Kelley & Cottrell, 2012; Gaborieau et al., 2020; Cottrell et al., 2021).

The observed median  $\text{Fe}^{3+}/\Sigma\text{Fe}$  in our database is greater than that of MORB glass, lower than that of altered oceanic crust, and similar to that of arc basalts and the average of variably altered young and old ocean crust. However, the reliability of titration  $\text{Fe}^{3+}/\Sigma\text{Fe}$  analyses, which make up the majority of our database, is also questionable due to several potential interferences (Flanagan, 1986; Potts, 1992). These include oxidation during modern surface weathering, the introduction of 'tramp' iron from steel crushing equipment, the oxidation of  $\text{Fe}^{2+}$ -bearing



**Figure 3.** Predicted distribution of the metamorphic facies and their constituent subfacies as a function of pressure and temperature for the worldwide median metabasite ( $\text{Fe}^{3+}/\Sigma\text{Fe} = 0.26$ ). Fields were delineated using the Gibbs-free energy minimiser MAGEMin (Riel *et al.*, 2022), an internally consistent thermodynamic dataset (Holland & Powell, 2011) and solution models (Green *et al.*, 2016). See Supplemental Material for further details.

minerals during grinding, the reduction of  $\text{Fe}^{3+}$  during solution if  $\text{S}^{2-}$  is present in soluble sulphide minerals, and the incomplete dissolution of  $\text{Fe}^{2+}$ -bearing porphyroblasts (Stokes, 1901; Mauzelius, 1907; Hillebrand, 1908; Schafer, 1966; Ritchie, 1968; Fitton & Gill, 1970; French & Adams, 1972; Atkin, 1977; Reay, 1981; Whipple *et al.*, 1984; O'Neill *et al.*, 1993; Saikkonen & Rautiainen, 1993; Canil *et al.*, 1994). The impact of each of these interferences, and consequently whether  $\text{Fe}^{3+}/\Sigma\text{Fe}$  is overestimated or underestimated, largely depends on specific sample characteristics, processing procedures, and analytical methods.

If the median  $\text{Fe}^{3+}/\Sigma\text{Fe}$  of  $0.26 \pm 0.12$  determined here is not an analytical artefact, there must be a modally abundant and commonly occurring mineral with moderate to high  $\text{Fe}^{\text{total}}$  and moderate to high  $\text{Fe}^{3+}/\Sigma\text{Fe}$  in each facies. In the low-grade and blueschist facies, pumpellyite, chlorite, epidote, and Na-amphiboles are possible candidates (Borg, 1956; Manganjuola & Howie, 1972; Zen, 1974). In the greenschist and amphibolite facies, epidote, actinolite, and hornblende are abundant and may contain substantial  $\text{Fe}^{3+}$  (Tilley, 1938; Buddington, 1952; Engel & Engel, 1962; Bard, 1970; Cooper, 1972; Wenk *et al.*, 1974; Starr & Pattison, 2019a). In the eclogite facies, omphacite is the only mineral with moderate  $\text{Fe}^{3+}/\Sigma\text{Fe}$ , but it has low to moderate  $\text{Fe}^{\text{total}}$  (Alderman, 1936; Switzer, 1945; Coleman *et al.*, 1965; Binns, 1967; Walters *et al.*, 2020). In the granulite facies, hornblende, if present, is modally minor, whilst orthopyroxene, clinopyroxene, and garnet only contain small amounts of  $\text{Fe}^{3+}$  (Binns, 1962, 1965a, 1965b; Engel *et al.*, 1964; Davidson, 1968, 1971; Ray & Sen, 1970; Sen & Ray, 1971; Jen & Kretz, 1981; Forshaw *et al.*, 2019). This uncertainty regarding which minerals host  $\text{Fe}^{3+}$  and the quantity present in each highlights the need for further study of the distribution of iron in metabasic minerals and rocks across all metamorphic facies. A similar disparity between  $\text{Fe}^{3+}/\Sigma\text{Fe}$  from titration and that obtained by combining mineral modes with their estimated

$\text{Fe}^{3+}/\Sigma\text{Fe}$  exists in metapelites (Forshaw & Pattison, 2023a, 2023b), suggesting that this is a universal problem. Insights may come from new in-situ synchrotron analyses (e.g. Dyar *et al.*, 2002; Masci *et al.*, 2019; Aulbach *et al.*, 2022; Marras *et al.*, 2024) or compilations of older wet chemical data (e.g. Forshaw & Pattison, 2021; Dubacq & Forshaw, 2024).

$\text{Fe}^{3+}$  plays a critical role in the phase equilibria of metabasites, with many previous studies exploring this topic in detail (Diener & Powell, 2010; Rebay *et al.*, 2010; Palin *et al.*, 2016). Therefore, we do not extensively discuss this here; instead, we calculated equilibrium assemblage diagrams for the worldwide median metabasite using  $\text{Fe}^{3+}/\Sigma\text{Fe} = 0$  and  $\text{Fe}^{3+}/\Sigma\text{Fe} = 0.26$ , providing a reference point for the predicted phase equilibria of this composition (Fig. S4–7). Figure 3 shows the predicted distribution of the metamorphic facies and their constituent subfacies as a function of pressure and temperature for the worldwide median metabasite ( $\text{Fe}^{3+}/\Sigma\text{Fe} = 0.26$ ).

## CONCLUSIONS

Major-element metabasite compositions vary due to differences in igneous crystallisation conditions, the extent of hydrothermal or metasomatic alteration, and whether they originate from mafic igneous rocks or certain calcareous sediments. This study compiled a database of 6186 major-element whole-rock analyses of metabasites from different metamorphic facies. It complements an earlier study of similar aims and scope concerned with metapelites (Forshaw & Pattison, 2023b).  $\text{SiO}_2$ ,  $\text{Al}_2\text{O}_3$ , MnO, MgO, and  $\text{K}_2\text{O}$  show no significant variation as a function of metamorphic facies. Small variations in  $\text{TiO}_2$ , FeO, CaO, and  $\text{Na}_2\text{O}$  amongst facies are interpreted to represent sampling bias. Titration measurements indicate that  $\text{Fe}^{3+}$  is a significant component of the total Fe in metabasites. Further work is needed to

ascertain the distribution of  $\text{Fe}^{3+}$  amongst minerals in metabasic rocks and whether the median  $\text{Fe}^{3+}/\Sigma\text{Fe}$  of  $0.26\pm 0.12$  is reliable or affected by analytical interferences. Changes in the proportions of major elements, particularly  $\text{Fe}^{3+}/\Sigma\text{Fe}$ , affect calculated phase equilibria significantly and, consequently, estimates of P–T conditions.

## CONFLICTS OF INTEREST/COMPETING INTERESTS

Not applicable.

## AVAILABILITY OF DATA AND MATERIAL

Not applicable.

## CODE AVAILABILITY

Not applicable.

## SUPPLEMENTARY DATA

Supplementary data are available at *Journal of Petrology* online.

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