

## Supplementary information

Table 4. *Model compounds and local-atomic site symmetry used in invariom modeling of*

Atom	Invariom	site-symmetry	L-homoserine model compound
O(1)	O1.5c[1.5o1c]	<i>mz</i>	acetic acid anion
O(2)	O1.5c[1.5o1c]	<i>mz</i>	acetic acid anion
O(3)	O1c1h	<i>mz</i>	methanol
N(1)	N1c1h1h1h	3	methylammonium
C(1)	C1.5o1.5o1c	<i>mz</i>	acetic acid anion
C(2)	C1n1c1c1h	<i>mz</i>	2-aminopropane
C(3)	C1c1c1h1h	<i>mm2</i>	propane
C(4)	C1o1c1h1h	<i>mz</i>	ethanol
H(9)	H1o[1c]	6	methanol
H(6)	H1n[1c1h1h]	6	methylammonium
H(7)	H1n[1c1h1h]	6	methylammonium
H(8)	H1n[1c1h1h]	6	methylammonium
H(1)	H1c[1n1c1c]	6	2-aminopropane
H(2)	H1c[1c1c1h]	6	propane
H(3)	H1c[1c1c1h]	6	propane
H(4)	H1c[1o1c1h]	6	ethanol
H(5)	H1c[1o1c1h]	6	ethanol