

**Table 2. Rate coefficients**

<b>Carbon monoxide</b>		Henry <i>et al.</i> (1)*	Simulations <sup>†</sup>
$k_{gem}(t)$	$s^{-1}$	$8 \times 10^3$	$3.3 \times 10^4$
$k_{gem}(r)$	$s^{-1}$	$6 \times 10^6$	$5 \times 10^6$
$k_{diss}(t)$	$s^{-1}$	0.07	0.2
$k_{diss}(r)$	$s^{-1}$	0.02	0.022
$k(t,r)_{out}$	$s^{-1}$	$7 \times 10^6$	$6 \times 10^6$
$k(t,r)_{in}$	$M^{-1} \cdot s^{-1}$	$7 \times 10^6$	$2.2 \times 10^7$
$k_T(r \rightarrow t)$ <sup>§</sup>	$s^{-1}$	$1 \times 10^8 / \sigma$	$1 \times 10^8 / \sigma$
$k_T(t \rightarrow r)$	$s^{-1}$	$3 \times 10^5 / \sigma$	$1.5 \times 10^5 / \sigma$
$k_T(rx \rightarrow tx)$	$s^{-1}$	$90 / \sigma$	$200 / \sigma$
$k_T(tx \rightarrow rx)$	$s^{-1}$	$900 / \sigma$	$400 / \sigma$
<b>Carbon monoxide</b>		Unzai <i>et al.</i> (2) <sup>‡</sup>	
$k_{on}(t)$	$M^{-1} \cdot s^{-1}$	$8 \times 10^4$	$1.2 \times 10^5$
$k_{off}(t)$	$s^{-1}$	0.2	0.2
$k_{on}(r)$	$M^{-1} \cdot s^{-1}$	$1 \times 10^7$	$1 \times 10^7$
$k_{off}(r)$	$s^{-1}$	0.01	0.012
<b>Oxygen</b>			
$k_{on}(t)$	$M^{-1} \cdot s^{-1}$	$8 \times 10^6$	$6.8 \times 10^6$
$k_{off}(t)$	$s^{-1}$	$3 \times 10^3$	$1.1 \times 10^3$
$k_{on}(r)$	$M^{-1} \cdot s^{-1}$	$1 \times 10^8$	$1 \times 10^8$
$k_{off}(r)$	$s^{-1}$	20	12

\*0.1 M potassium phosphate, pH 7, 20°C.

<sup>†</sup>Gel conditions, 15°C (see *Methods*).

<sup>‡</sup>pH 7.4, 25°C (plus 0.1 mM IHP for the quaternary *T*-state, which corresponds to the *t* state of the TTS model). The overall binding and dissociation rate coefficients [ $k_{on}(t,r)$  and  $k_{off}(t,r)$ ] are related to the rate coefficients of the TTS model by:

$$k_{on}(t,r) = k_{in} \frac{k_{gem}(t,r)}{k_{gem}(t,r) + k_{out}} \quad \text{and} \quad k_{off}(t,r) = k_{out} \frac{k_{diss}(t,r)}{k_{gem}(t,r) + k_{out}}.$$

<sup>§</sup> $\sigma$  is the slowing factor due to the constraints of encapsulation by the gel.

1. Henry, E. R., Bettati, S., Hofrichter, J. & Eaton, W. A. (2002) *Biophys. Chem.* **98**, 149-164.
2. Unzai, S., Eich, R., Shibayama, N., Olson, J. S. & Morimoto, H. (1998) *J. Biol. Chem.* **273**, 23150-23159.