

TABLE I: The STO exponents.

	Cl	H
1s	18.0505, 13.3358	1s 1.0
2s	7.32724, 5.75219	2s, 2p 0.5
2p	10.2877, 5.61299	
3s	2.92737, 1.85365	
3p, 3d	2.62421, 1.47458	
4s, 4p, 4d, 4f	1.9775	
5s, 5p, 5d, 5f, 5g	1.5820	
6s, 6p, 6d, 6f, 6g	1.318337	
7s, 7p, 7d, 7f, 7g	1.130000	
8s, 8p, 8d, 8f, 8g	1.108750	

TABLE II: Comparison of asymptotic separated-atom energies (in eV) between the ALCHEMY calculations and experiment for  $\text{ClH}^{7+}$ . The 38 molecular states are of symmetries  ${}^2\Sigma^+$  and  ${}^2\Pi$ .

Asymptotic atomic state	Mol. state	This work	Expt. <sup>a</sup>
$\text{Cl}^{6+}(2p^6 3s {}^2S) + \text{H}^+$	1 ${}^2\Sigma^+$	-99.7719	-100.6026
$\text{Cl}^{6+}(2p^6 3p {}^2P^o) + \text{H}^+$	2 ${}^2\Sigma^+$	-84.6436	-85.1952
	1 ${}^2\Pi$	-84.6422	
$\text{Cl}^{6+}(2p^6 3d {}^2D) + \text{H}^+$	3 ${}^2\Sigma^+$	-64.0412	-64.6201
	2 ${}^2\Pi$	-64.0408	
$\text{Cl}^{6+}(2p^6 4s {}^2S) + \text{H}^+$	4 ${}^2\Sigma^+$	-42.7737	-43.0736
$\text{Cl}^{6+}(2p^6 4p {}^2P^o) + \text{H}^+$	5 ${}^2\Sigma^+$	-37.2018	-37.4133
	3 ${}^2\Pi$	-37.1967	
$\text{Cl}^{6+}(2p^6 4d {}^2D) + \text{H}^+$	6 ${}^2\Sigma^+$	-29.7875	-30.0350
	4 ${}^2\Pi$	-29.7859	
$\text{Cl}^{6+}(2p^6 4f {}^2F^o) + \text{H}^+$	7 ${}^2\Sigma^+$	-28.1147	-28.1843
	5 ${}^2\Pi$	-28.1142	
$\text{Cl}^{6+}(2p^6 5s {}^2S) + \text{H}^+$	8 ${}^2\Sigma^+$	-20.1624	-20.3009
$\text{Cl}^{6+}(2p^6 5p {}^2P^o) + \text{H}^+$	9 ${}^2\Sigma^+$	-17.5044	-17.6088
	6 ${}^2\Pi$	-17.4910	
$\text{Cl}^{6+}(2p^6 5d {}^2D) + \text{H}^+$	10 ${}^2\Sigma^+$	-13.9801	-14.1099
	7 ${}^2\Pi$	-13.9750	
$\text{Cl}^{6+}(2p^6 5f {}^2F^o) + \text{H}^+$	11 ${}^2\Sigma^+$	-13.1355	-13.1436
	8 ${}^2\Pi$	-13.1328	
$\text{Cl}^{6+}(2p^6 5g {}^2G) + \text{H}^+$	12 ${}^2\Sigma^+$	-13.0266	-13.0768
	9 ${}^2\Pi$	-13.0274	
$\text{Cl}^{6+}(2p^6 6s {}^2S) + \text{H}^+$	13 ${}^2\Sigma^+$	-8.8827	-8.8915
$\text{Cl}^{6+}(2p^6 6p {}^2P^o) + \text{H}^+$	14 ${}^2\Sigma^+$	-7.4038	-7.4582
	10 ${}^2\Pi$	-7.3766	
$\text{Cl}^{7+}(2p^6 {}^1S) + \text{H}$	15 ${}^2\Sigma^+$	0.0000	0.0000
$\text{Cl}^{6+}(2p^6 6d {}^2D) + \text{H}^+$	16 ${}^2\Sigma^+$	-5.4825	-5.5278
	11 ${}^2\Pi$	-5.4688	
$\text{Cl}^{6+}(2p^6 6f {}^2F^o) + \text{H}^+$	17 ${}^2\Sigma^+$	-5.0138	-4.9679
	12 ${}^2\Pi$	-5.0091	
$\text{Cl}^{6+}(2p^6 6g {}^2G) + \text{H}^+$	18 ${}^2\Sigma^+$	-4.8323	-4.9278
	13 ${}^2\Pi$	-4.8338	
$\text{Cl}^{6+}(2p^6 7s {}^2S) + \text{H}^+$	19 ${}^2\Sigma^+$	-2.4611	
$\text{Cl}^{6+}(2p^6 7p {}^2P^o) + \text{H}^+$	20 ${}^2\Sigma^+$	-1.5711	
	14 ${}^2\Pi$	-1.5265	
$\text{Cl}^{6+}(2p^6 7d {}^2D) + \text{H}^+$	21 ${}^2\Sigma^+$	-0.4246	
	15 ${}^2\Pi$	-0.3979	
$\text{Cl}^{6+}(2p^6 7f {}^2F^o) + \text{H}^+$	22 ${}^2\Sigma^+$	-0.0896	
	16 ${}^2\Pi$	-0.0849	

<sup>a</sup>Ref. [19]

TABLE III: Rate coefficients for electron capture into the  $\text{Cl}^{6+}(2p^6nl\ ^2\text{S},\ ^2\text{P}^o,\ ^2\text{D},\ ^2\text{F}^o,\ ^2\text{G}) + \text{H}^+$  channels due to  $\text{Cl}^{7+}(2p^6\ ^1\text{S}) + \text{H}$  collisions.  $T$  is in K and the rate coefficients are in  $\text{cm}^3/\text{s}$ . *Total* represents the rate coefficients summed over all the exit channels.

$T$	$5s\ ^2\text{S}$	$5p\ ^2\text{P}^o$	$5d\ ^2\text{D}$	$5f\ ^2\text{F}^o$	$5g\ ^2\text{G}$	$6s\ ^2\text{S}$	$6p\ ^2\text{P}^o$	Total
10	2.18(-14) <sup>a</sup>	2.20(-12)	2.08(-09)	7.65(-10)	7.73(-10)	4.32(-10)	2.79(-09)	6.85(-09)
20	3.80(-14)	2.04(-12)	2.02(-09)	9.03(-10)	7.02(-10)	4.28(-10)	2.94(-09)	6.99(-09)
30	5.24(-14)	1.92(-12)	1.93(-09)	9.78(-10)	6.52(-10)	4.23(-10)	2.99(-09)	6.98(-09)
40	6.38(-14)	1.85(-12)	1.86(-09)	1.04(-09)	6.18(-10)	4.21(-10)	3.04(-09)	6.98(-09)
50	7.30(-14)	1.80(-12)	1.79(-09)	1.10(-09)	5.95(-10)	4.21(-10)	3.09(-09)	7.00(-09)
60	8.07(-14)	1.77(-12)	1.74(-09)	1.15(-09)	5.78(-10)	4.21(-10)	3.13(-09)	7.02(-09)
70	8.75(-14)	1.75(-12)	1.70(-09)	1.20(-09)	5.66(-10)	4.22(-10)	3.17(-09)	7.06(-09)
80	9.38(-14)	1.73(-12)	1.66(-09)	1.25(-09)	5.57(-10)	4.23(-10)	3.21(-09)	7.09(-09)
90	9.95(-14)	1.73(-12)	1.62(-09)	1.29(-09)	5.51(-10)	4.25(-10)	3.24(-09)	7.12(-09)
100	1.05(-13)	1.72(-12)	1.59(-09)	1.33(-09)	5.47(-10)	4.26(-10)	3.26(-09)	7.15(-09)
200	1.42(-13)	1.85(-12)	1.37(-09)	1.58(-09)	5.45(-10)	4.42(-10)	3.46(-09)	7.39(-09)
300	1.62(-13)	2.19(-12)	1.28(-09)	1.68(-09)	5.50(-10)	4.55(-10)	3.60(-09)	7.57(-09)
400	1.75(-13)	2.67(-12)	1.25(-09)	1.74(-09)	5.51(-10)	4.66(-10)	3.74(-09)	7.74(-09)
500	1.83(-13)	3.21(-12)	1.25(-09)	1.77(-09)	5.49(-10)	4.76(-10)	3.86(-09)	7.91(-09)
600	1.87(-13)	3.78(-12)	1.28(-09)	1.78(-09)	5.46(-10)	4.86(-10)	3.99(-09)	8.09(-09)
700	1.88(-13)	4.36(-12)	1.32(-09)	1.79(-09)	5.42(-10)	4.96(-10)	4.12(-09)	8.27(-09)
800	1.88(-13)	4.95(-12)	1.36(-09)	1.80(-09)	5.38(-10)	5.05(-10)	4.25(-09)	8.46(-09)
900	1.87(-13)	5.56(-12)	1.41(-09)	1.80(-09)	5.34(-10)	5.14(-10)	4.38(-09)	8.64(-09)
1000	1.86(-13)	6.19(-12)	1.46(-09)	1.79(-09)	5.30(-10)	5.23(-10)	4.51(-09)	8.83(-09)
2000	1.77(-13)	1.57(-11)	2.08(-09)	1.72(-09)	5.03(-10)	5.95(-10)	5.70(-09)	1.06(-08)
3000	2.03(-13)	3.29(-11)	2.73(-09)	1.64(-09)	4.92(-10)	6.50(-10)	6.67(-09)	1.22(-08)
4000	2.70(-13)	5.80(-11)	3.37(-09)	1.57(-09)	4.88(-10)	6.97(-10)	7.49(-09)	1.37(-08)
5000	3.89(-13)	9.17(-11)	3.98(-09)	1.52(-09)	4.88(-10)	7.38(-10)	8.19(-09)	1.50(-08)
6000	5.71(-13)	1.34(-10)	4.56(-09)	1.48(-09)	4.90(-10)	7.76(-10)	8.82(-09)	1.62(-08)
7000	8.29(-13)	1.84(-10)	5.10(-09)	1.44(-09)	4.93(-10)	8.11(-10)	9.37(-09)	1.74(-08)
8000	1.18(-12)	2.42(-10)	5.61(-09)	1.41(-09)	4.96(-10)	8.43(-10)	9.88(-09)	1.85(-08)
9000	1.63(-12)	3.06(-10)	6.10(-09)	1.39(-09)	4.99(-10)	8.74(-10)	1.03(-08)	1.95(-08)
10000	2.21(-12)	3.77(-10)	6.56(-09)	1.37(-09)	5.03(-10)	9.02(-10)	1.08(-08)	2.05(-08)
20000	1.71(-11)	1.30(-09)	1.03(-08)	1.25(-09)	5.43(-10)	1.13(-09)	1.40(-08)	2.85(-08)
30000	5.32(-11)	2.42(-09)	1.30(-08)	1.20(-09)	5.81(-10)	1.29(-09)	1.62(-08)	3.47(-08)
40000	1.12(-10)	3.59(-09)	1.51(-08)	1.20(-09)	6.16(-10)	1.41(-09)	1.79(-08)	4.00(-08)
50000	1.91(-10)	4.74(-09)	1.68(-08)	1.21(-09)	6.53(-10)	1.51(-09)	1.95(-08)	4.46(-08)
60000	2.89(-10)	5.87(-09)	1.82(-08)	1.24(-09)	6.93(-10)	1.60(-09)	2.09(-08)	4.88(-08)
70000	4.01(-10)	6.95(-09)	1.94(-08)	1.28(-09)	7.37(-10)	1.68(-09)	2.22(-08)	5.26(-08)
80000	5.26(-10)	7.99(-09)	2.04(-08)	1.31(-09)	7.85(-10)	1.75(-09)	2.34(-08)	5.62(-08)
90000	6.61(-10)	8.98(-09)	2.13(-08)	1.35(-09)	8.37(-10)	1.83(-09)	2.46(-08)	5.96(-08)
100000	8.06(-10)	9.94(-09)	2.21(-08)	1.38(-09)	8.92(-10)	1.90(-09)	2.57(-08)	6.27(-08)
200000	2.71(-09)	1.75(-08)	2.75(-08)	1.63(-09)	1.48(-09)	2.60(-09)	3.52(-08)	8.86(-08)

$${}^a A(-B) = A \times 10^{-B}$$

TABLE IV: Fitting parameters of rate coefficients for capture into  $\text{Cl}^{6+}(2p^6nl\ ^2\text{S},\ ^2\text{P}^o,\ ^2\text{D},\ ^2\text{F}^o,\ ^2\text{G}) + \text{H}^+$  channels, and the summed exit channels (Total) due to  $\text{Cl}^{7+}(2p^6\ ^1\text{S}) + \text{H}$  collisions.  $T$  is in K;  $a_i$  and  $c_i$  are in units of  $\text{cm}^3/\text{s}$  and K, respectively.

Param.	$5s\ ^2\text{S}$	$5p\ ^2\text{P}^o$	$5d\ ^2\text{D}$	$5f\ ^2\text{F}^o$	$5g\ ^2\text{G}$	$6s\ ^2\text{S}$	$6p\ ^2\text{P}^o$	Total
$a_1$	2.5997(-12) <sup>a</sup>	3.9231(-10)	6.5199(-09)	1.0037(-09)	3.4663(-10)	6.3211(-10)	8.4735(-09)	1.4656(-08)
$b_1$	2.9165(+00)	1.9538(+00)	9.6442(-01)	1.3737(-01)	7.8431(-02)	4.7284(-01)	5.9359(-01)	7.0547(-01)
$c_1$	1.0987(+05)	7.7302(+04)	8.3387(+04)	-9.3204(+06)	-2.0014(+05)	2.8849(+05)	1.6200(+05)	2.1728(+05)
$a_2$	1.4413(-12)	1.5820(-12)	4.7009(-10)	2.4833(-09)	1.3895(-10)	2.6759(-10)	2.3249(-09)	5.6402(-09)
$b_2$	5.7480(-01)	-2.7907(-02)	-2.3686(-01)	2.5637(-01)	-1.9133(-01)	-6.1187(-02)	-2.6475(-02)	-3.0024(-02)
$c_2$	1.5419(+03)	-2.3482(+04)	-4.6553(+04)	4.4044(+03)	-1.3881(+05)	-1.1338(+05)	-8.8121(+04)	-9.7076(+04)

$${}^a A(-B) = A \times 10^{-B}$$