Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supporting Information for

Vibrational relaxation rate coefficients in CS-He collisions up to the dissociation limit: mixed quantum-classical calculations and neural network predictions

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Table S1: MQC and VCC-IOS rate coefficients for selected CS(v_i,j_i) + He → CS(v_f,$\sum_0^{37} j_f$) + He processes.

Temp (K)	k_{07LiSp}	k_{MQC}	Ratio
$v_i \rightarrow v_f = 0$			
$j_i = 0$			
300	5.57786×10^{-16}	5.98×10^{-16}	1.0721
400	1.73868×10^{-15}	1.83×10^{-15}	1.0525
500	4.14831×10^{-15}	4.23×10^{-15}	1.0197
700	1.48204×10^{-14}	1.43×10^{-14}	0.9649
900	3.68209×10^{-14}	3.38×10^{-14}	0.9180
1200	9.82165×10^{-14}	8.55×10^{-14}	0.8705
1500	1.96454×10^{-13}	1.66×10^{-13}	0.8450
$j_i = 1$			
300	5.5752×10^{-16}	6.85×10^{-16}	1.2287
400	1.737676×10^{-15}	2.08×10^{-15}	1.1970
500	4.1463×10^{-15}	4.77×10^{-15}	1.1504
700	1.481403×10^{-14}	1.57×10^{-14}	1.0598
900	3.680749×10^{-14}	3.69×10^{-14}	1.0025
1200	9.81802×10^{-14}	9.35×10^{-14}	0.9523
1500	1.963904×10^{-13}	1.82×10^{-13}	0.9267
$j_i = 2$			
300	5.57012×10^{-16}	7.40×10^{-16}	1.3285
400	1.736231×10^{-15}	2.25×10^{-15}	1.2959
500	4.14302×10^{-15}	5.19×10^{-15}	1.2527
700	1.480396×10^{-14}	1.74×10^{-14}	1.1754
900	3.67846×10^{-14}	4.11×10^{-14}	1.1173
1200	9.81285×10^{-14}	1.03×10^{-13}	1.0496
1500	1.962964×10^{-13}	1.98×10^{-13}	1.0087
$j_i = 5$			
300	5.54016×10^{-16}	8.08×10^{-16}	1.4584
400	1.726439×10^{-15}	2.41×10^{-15}	1.3959
500	4.12139×10^{-15}	5.49×10^{-15}	1.3321
700	1.473705×10^{-14}	1.81×10^{-14}	1.2282
900	3.663669×10^{-14}	4.25×10^{-14}	1.1600
1200	9.77734×10^{-14}	1.07×10^{-13}	1.0944
1500	1.956211×10^{-13}	2.09×10^{-13}	1.0684
$j_i = 10$			
300	5.4429×10^{-16}	1.08×10^{-15}	1.9842
400	1.695671×10^{-15}	2.99×10^{-15}	1.7633
500	4.05123×10^{-15}	6.55×10^{-15}	1.6168
700	1.451298×10^{-14}	2.08×10^{-14}	1.4332
900	3.612554×10^{-14}	4.77×10^{-14}	1.3204
1200	9.6512×10^{-14}	1.18×10^{-13}	1.2226
1500	1.93195×10^{-13}	2.24×10^{-13}	1.1595
$j_i = 30$			
300	4.141815×10^{-16}	7.33×10^{-15}	17.6976
400	1.265255×10^{-15}	1.31×10^{-14}	10.3536
500	2.990933×10^{-15}	2.19×10^{-14}	7.3221
700	1.06102×10^{-14}	5.04×10^{-14}	4.7501
900	2.628532×10^{-14}	9.47×10^{-14}	3.6028
1200	6.989291×10^{-14}	1.93×10^{-13}	2.7614
1500	1.39397×10^{-13}	3.25×10^{-13}	2.3315
$v_i = 2 \rightarrow v_f = 1$			

Temp (K)	k_{07LiSp}	k_{MQC}	Ratio
$j_i = 0$			
300	1.24×10^{-15}	1.27×10^{-15}	1.0279
400	3.81×10^{-15}	3.93×10^{-15}	1.0305
500	9.02×10^{-15}	9.04×10^{-15}	1.0023
700	3.17×10^{-14}	2.96×10^{-14}	0.9337
900	7.74×10^{-14}	6.78×10^{-14}	0.8758
1200	1.99×10^{-13}	1.66×10^{-13}	0.8329
1500	3.81×10^{-13}	3.16×10^{-13}	0.8302
$j_i = 5$			
300	1.23×10^{-15}	1.75×10^{-15}	1.4262
400	3.79×10^{-15}	5.19×10^{-15}	1.3705
500	8.96×10^{-15}	1.17×10^{-14}	1.3056
700	3.15×10^{-14}	3.78×10^{-14}	1.1989
900	7.70×10^{-14}	8.63×10^{-14}	1.1202
1200	1.98×10^{-13}	2.09×10^{-13}	1.0531
1500	3.79×10^{-13}	3.92×10^{-13}	1.0340
$j_i = 10$			
300	1.21×10^{-15}	2.31×10^{-15}	1.9091
400	3.72×10^{-15}	6.47×10^{-15}	1.7392
500	8.81×10^{-15}	1.41×10^{-14}	1.6005
700	3.11×10^{-14}	4.32×10^{-14}	1.3891
900	7.60×10^{-14}	9.50×10^{-14}	1.2500
1200	1.96×10^{-13}	2.23×10^{-13}	1.1378
1500	3.75×10^{-13}	4.12×10^{-13}	1.0987
$j_i = 30$			
300	9.18×10^{-16}	1.64×10^{-14}	17.8649
400	2.78×10^{-15}	2.83×10^{-14}	10.1798
500	6.52×10^{-15}	4.60×10^{-14}	7.0552
700	2.28×10^{-14}	1.01×10^{-13}	4.4298
900	5.55×10^{-14}	1.85×10^{-13}	3.3333
1200	1.43×10^{-13}	3.63×10^{-13}	2.5385
1500	2.72×10^{-13}	5.94×10^{-13}	2.1838
$v_i = 2 \rightarrow v_f = 0$			
$j_i = 0$			
300	5.81×10^{-19}	3.19×10^{-19}	0.5491
400	3.02×10^{-18}	1.38×10^{-18}	0.4557
500	1.08×10^{-17}	4.25×10^{-18}	0.3930
700	6.69×10^{-17}	2.26×10^{-17}	0.3235
900	2.59×10^{-16}	7.66×10^{-17}	0.2949
1200	9.98×10^{-16}	2.86×10^{-16}	0.2864
1500	2.41×10^{-15}	7.06×10^{-16}	0.2933
$j_i = 5$			
300	5.74×10^{-19}	4.89×10^{-19}	0.8507
400	3.00×10^{-18}	2.10×10^{-18}	0.7011
500	1.07×10^{-17}	6.40×10^{-18}	0.5983
700	6.91×10^{-17}	3.27×10^{-17}	0.4729
900	2.57×10^{-16}	1.05×10^{-16}	0.4082
1200	9.90×10^{-16}	3.74×10^{-16}	0.3779
1500	2.39×10^{-15}	9.09×10^{-16}	0.3808
$j_i = 10$			
300	5.58×10^{-19}	7.80×10^{-19}	1.3978
400	2.91×10^{-18}	3.06×10^{-18}	1.0515
500	1.04×10^{-17}	8.70×10^{-18}	0.8365
700	6.73×10^{-17}	4.11×10^{-17}	0.6107

Temp (K)	$k_{07\mathrm{LiSp}}$	k_{MQC}	Ratio
900	2.51×10^{-16}	1.28×10^{-16}	0.5100
1200	9.67×10^{-16}	4.33×10^{-16}	0.4478
1500	2.33×10^{-15}	1.02×10^{-15}	0.4378
$j_{\mathrm{i}} = 30$			
300	3.81×10^{-19}	1.17×10^{-17}	30.7086
400	1.98×10^{-18}	2.65×10^{-17}	13.3838
500	7.13×10^{-18}	5.59×10^{-17}	7.8401
700	4.70×10^{-17}	1.86×10^{-16}	3.9574
900	1.78×10^{-16}	4.46×10^{-16}	2.5056
1200	6.99×10^{-16}	1.18×10^{-15}	1.6881
1500	1.70×10^{-15}	2.39×10^{-15}	1.7000

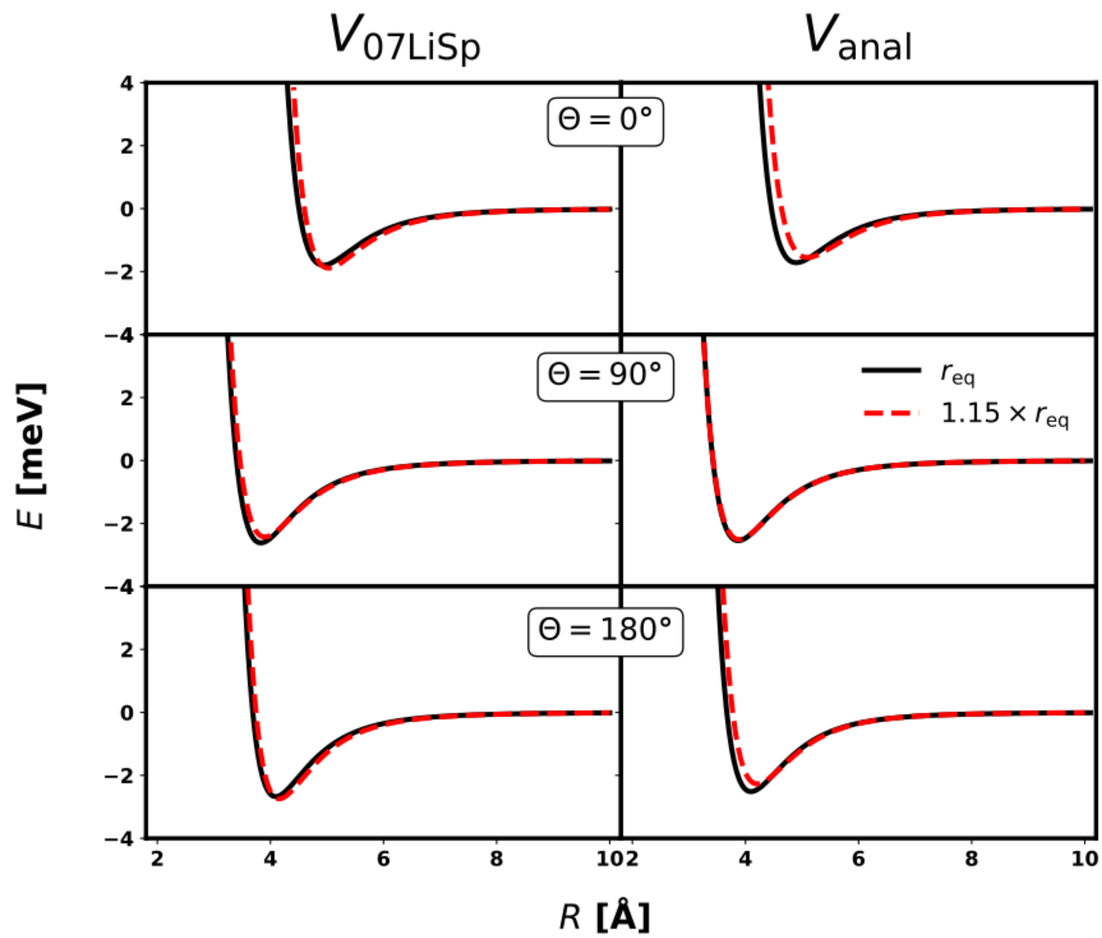

Figure S1: Different energy cuts of the Lique and Spielfiedel [1] (V_{07LiSp}) and the new potential (V_{anal}) for CS bond lengths $r = r_{eq}$ (black lines) and $r = 1.15 \times r_{eq}^{CS}$ (red dashed lines).

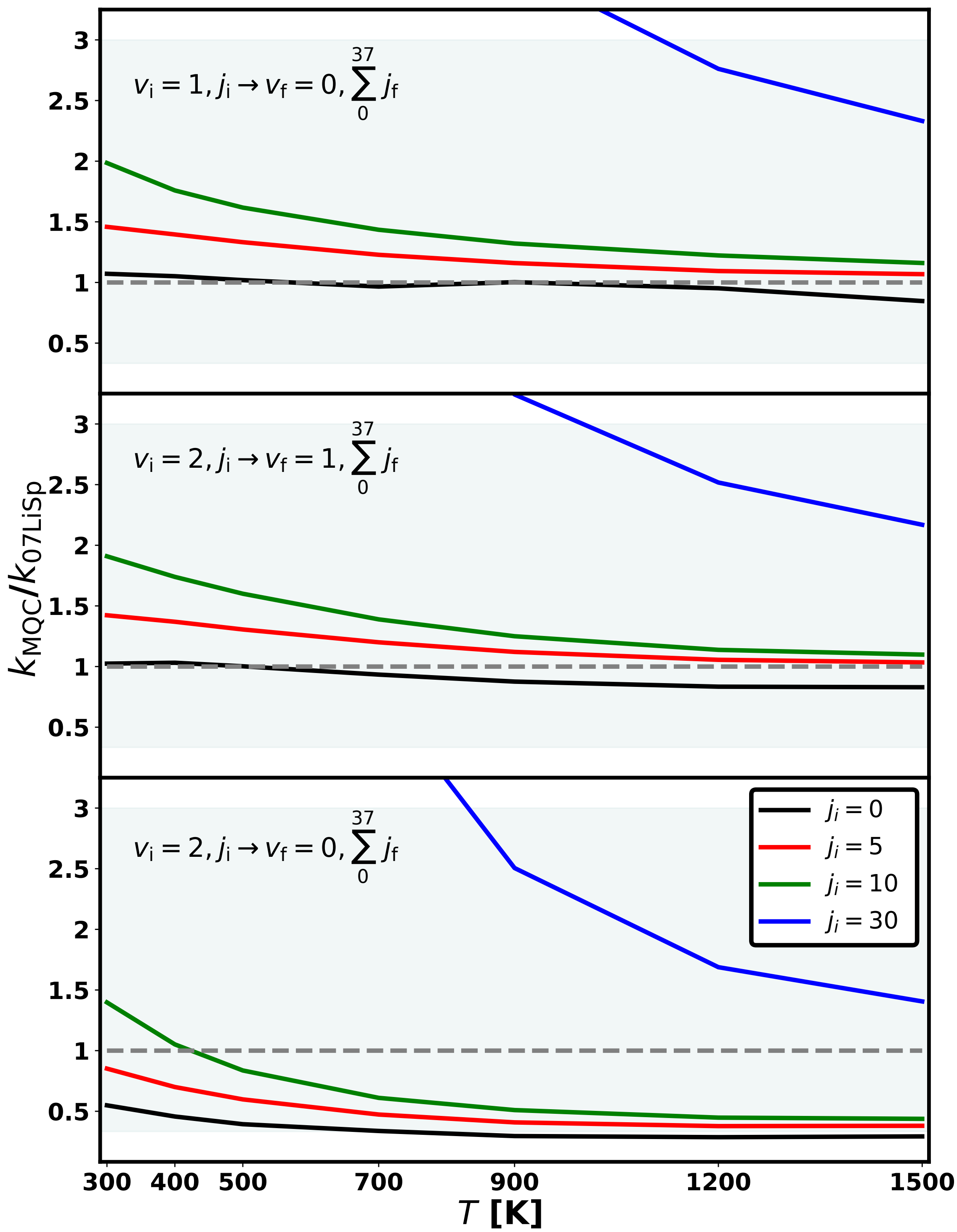

Figure S2: Ratio between MQC and VCC-IOS[1] collisional relaxation rate coefficients. The colored area represents the estimated accuracy of VCC-IOS values

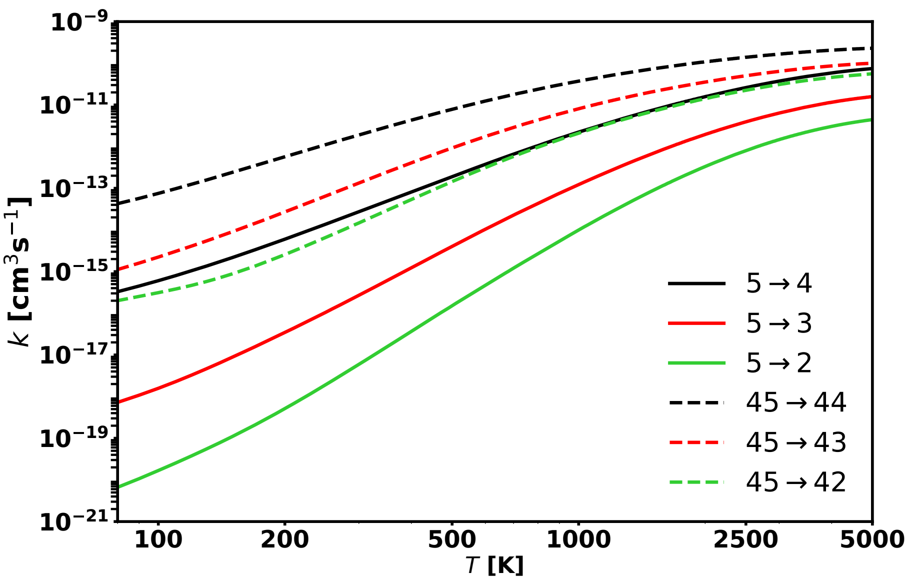

Figure S3: MQC rate coefficients for CS(v) + He $\rightarrow$ CS($v - \Delta v$) + He for $v_{\mathrm{i}} = 5$ (solid line) and $v_{\mathrm{i}} = 45$ (dashed line) as a function of temperature.

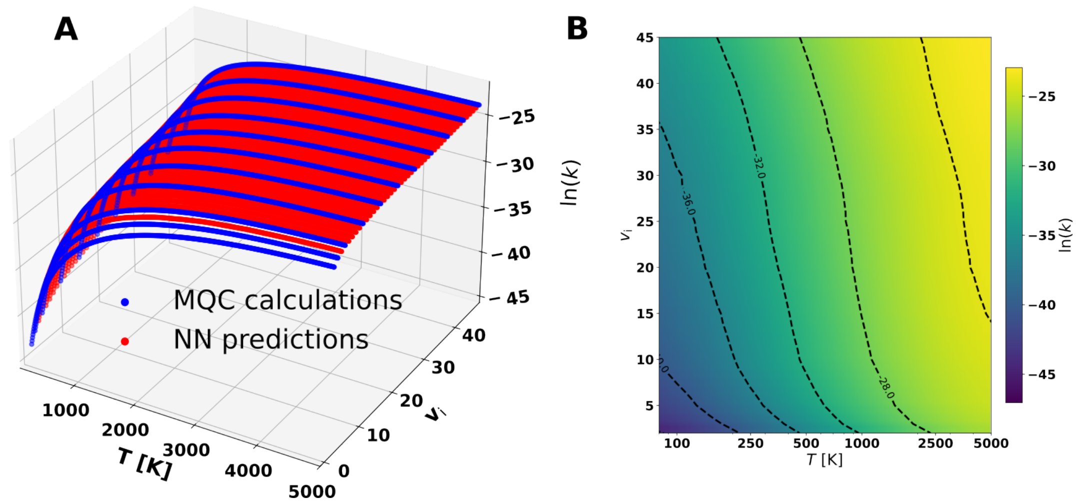

Figure S4: MQC calculated and NN predicted rate coefficients for CS(v) + He → CS($v-2$) + He. Panel A shows calculated values (in blue) and the predicted values (in red) as a function of the initial vibrational number and temperature. Panel B shows the contour plot of both calculated and predicted rate coefficients.

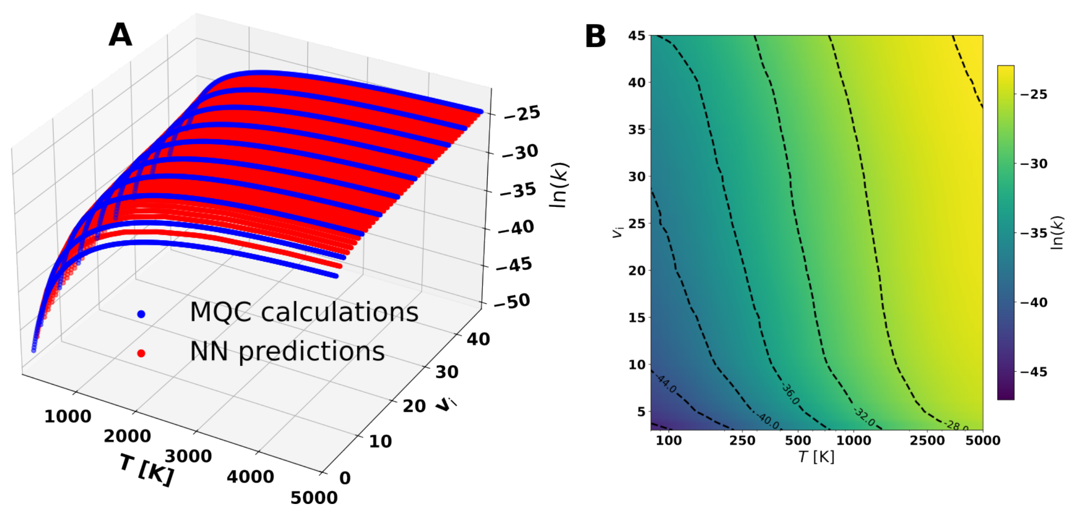

Figure S5: MQC calculated and NN predicted rate coefficients for CS(v) + He → CS($v-3$) + He. Panel A shows calculated values (in blue) and the predicted values (in red) as a function of the initial vibrational number and temperature. Panel B shows the contour plot of both calculated and predicted rate coefficients.

References

1 F. Lique and A. Spielfiedel, Astronomy and Astrophysics, 2007, **462**, 1179–1185.