

## Physical Chemistry Chemical Physics

### Supplementary Information

*Ab initio* Potential Energy Surface of NC<sub>4</sub>N–He:  
Rotationally Inelastic Collisions and Rate Coefficients

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**Table S1:** Data of interaction energy (Hartree) for potential energy surface of NC<sub>4</sub>N - He complex as a function of  $R$  and  $\theta$ .  $\theta$  varies from 0° to 90°.

|     |   |                   |
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| 3.3 | 0 | -240.656444970105 |
| 3.4 | 0 | -254.56729932104  |
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| 5   | 0 | -264.256368808865 |

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| 9.6  | 90 | -264.281508364323 |
| 9.7  | 90 | -264.281508313185 |
| 9.8  | 90 | -264.281508265515 |
| 9.9  | 90 | -264.281508221054 |
| 10   | 90 | -264.281508179538 |
| 10.1 | 90 | -264.281508140762 |
| 10.2 | 90 | -264.28150810453  |
| 10.4 | 90 | -264.281508038913 |
| 10.6 | 90 | -264.281507981382 |
| 10.8 | 90 | -264.281507930809 |
| 11   | 90 | -264.281507886246 |
| 11.2 | 90 | -264.281507846902 |
| 11.4 | 90 | -264.281507812091 |
| 11.6 | 90 | -264.281507781218 |
| 11.8 | 90 | -264.281507753786 |
| 12   | 90 | -264.28150772937  |
| 12.2 | 90 | -264.281507707591 |
| 12.4 | 90 | -264.28150768813  |
| 12.6 | 90 | -264.281507670723 |
| 12.8 | 90 | -264.281507655104 |
| 13   | 90 | -264.28150764108  |
| 13.2 | 90 | -264.281507628466 |
| 13.4 | 90 | -264.281507617099 |
| 13.6 | 90 | -264.281507606842 |
| 13.8 | 90 | -264.281507597578 |
| 14   | 90 | -264.28150758919  |
| 14.2 | 90 | -264.281507581585 |
| 14.4 | 90 | -264.2815075747   |
| 14.6 | 90 | -264.281507568431 |
| 14.8 | 90 | -264.28150756273  |
| 15   | 90 | -264.281507557541 |
| 20   | 90 | -264.281507506192 |
| 50   | 90 | -264.281507494911 |

**Table S2:** Data of rotational excitation rate coefficients (in  $10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ) of  $\text{NC}_4\text{N-He}$  complex for various transitions with temperature ranging from 1-100 K

| T(K) | 0→2               | 2→4               | 4→6               | 6→8               |
|------|-------------------|-------------------|-------------------|-------------------|
| 1    | 0.676196513660929 | 0.463202770155807 | 0.242513114814789 | 0.116588749728627 |
| 2    | 0.894748567200679 | 0.72262697244217  | 0.500303795619961 | 0.332892613905699 |
| 3    | 1.01784938892283  | 0.847799842104206 | 0.645698991178162 | 0.487457283297436 |
| 4    | 1.10220505378327  | 0.928129099192806 | 0.742407093854749 | 0.59815580661108  |
| 5    | 1.1668667206578   | 0.98748607317359  | 0.813919919717304 | 0.681087999856726 |
| 6    | 1.21987016053527  | 1.03431749536944  | 0.869887554329317 | 0.745602535205596 |
| 7    | 1.26504686502777  | 1.07246555275083  | 0.915098735490408 | 0.797277657744462 |
| 8    | 1.30440175019986  | 1.10409555498834  | 0.952339366252908 | 0.839621687356916 |
| 9    | 1.33909528432306  | 1.13061647503704  | 0.983424472972758 | 0.87494585085562  |
| 10   | 1.36987273360889  | 1.15302561329681  | 1.00962463460454  | 0.904832003533655 |
| 11   | 1.39725857378803  | 1.1720629959681   | 1.03186889790017  | 0.930397384940985 |
| 12   | 1.42164836191937  | 1.18829252464304  | 1.05085511601618  | 0.952451922479606 |
| 13   | 1.44335486076207  | 1.20215058157011  | 1.06711687239581  | 0.971595657913409 |
| 14   | 1.46263317706723  | 1.21397818746597  | 1.0810674432284   | 0.988281367744415 |
| 15   | 1.47969586539056  | 1.22404382239377  | 1.09303031451552  | 1.00285621133825  |
| 16   | 1.49472292674048  | 1.23256037241351  | 1.10326117917698  | 1.0155903091006   |
| 17   | 1.50786897166936  | 1.23969805170558  | 1.11196420152676  | 1.02669689194503  |
| 18   | 1.51926862831474  | 1.2455943849677   | 1.11930424276308  | 1.03634682219401  |
| 19   | 1.52904073985876  | 1.25036194879066  | 1.12541613922258  | 1.04467922732525  |
| 20   | 1.5372916532234   | 1.25409436233262  | 1.13041177473738  | 1.05180936845005  |
| 21   | 1.54411779000515  | 1.25687089540998  | 1.13438547403989  | 1.05783449468103  |
| 22   | 1.54960763807864  | 1.25875998294063  | 1.13741810611909  | 1.06283820575345  |
| 23   | 1.55384327450818  | 1.25982187793392  | 1.139580192648    | 1.06689369840387  |
| 24   | 1.55690151260178  | 1.26011063118368  | 1.14093424949761  | 1.07006617347299  |
| 25   | 1.5588547519887   | 1.25967554993676  | 1.14153653919863  | 1.07241461164954  |
| 26   | 1.55977159827034  | 1.25856225793488  | 1.14143837352966  | 1.07399307555441  |
| 27   | 1.55971730749615  | 1.25681345426741  | 1.14068707499747  | 1.07485165831264  |
| 28   | 1.55875410044769  | 1.25446944774709  | 1.13932668184688  | 1.07503717016659  |
| 29   | 1.55694138260604  | 1.25156852649841  | 1.13739846205717  | 1.07459363269131  |
| 30   | 1.55433589781841  | 1.24814720864129  | 1.13494128657472  | 1.0735626331932   |
| 31   | 1.55099183707656  | 1.24424040889862  | 1.13199190003789  | 1.07198357876802  |
| 32   | 1.54696091840596  | 1.23988154721677  | 1.128585117856    | 1.06989387941242  |
| 33   | 1.5422924495239   | 1.23510261866346  | 1.12475397120149  | 1.06732908186596  |
| 34   | 1.53703338151728  | 1.22993423860059  | 1.12052981584426  | 1.06432296999065  |
| 35   | 1.53122835916796  | 1.22440567311265  | 1.11594241645184  | 1.06090764306262  |
| 36   | 1.52491977157665  | 1.21854486164456  | 1.11102001471697  | 1.05711358003066  |
| 37   | 1.51814780527691  | 1.2123784365501   | 1.10578938722432  | 1.0529696953326   |
| 38   | 1.51095050097948  | 1.20593174259883  | 1.10027589714691  | 1.04850339005023  |
| 39   | 1.50336381435203  | 1.19922885829485  | 1.09450354252437  | 1.04374060086993  |
| 40   | 1.49542168074358  | 1.19229262001358  | 1.08849500290336  | 1.0387058483757   |
| 41   | 1.4871560834465   | 1.18514464937615  | 1.08227168542568  | 1.03342228553996  |
| 42   | 1.47859712490401  | 1.17780538388713  | 1.07585377096231  | 1.02791174682273  |
| 43   | 1.46977310017938  | 1.17029411060857  | 1.06926026055756  | 1.02219479798606  |
| 44   | 1.46071057197763  | 1.16262900249259  | 1.06250902222624  | 1.01629078653663  |
| 45   | 1.451434444652826 | 1.15482715691529  | 1.05561683800672  | 1.01021789259353  |
| 46   | 1.44196804968432  | 1.14690463592625  | 1.04859945109149  | 1.00399317991747  |
| 47   | 1.43233320265521  | 1.13887650773157  | 1.04147161281529  | 0.997632646814131 |
| 48   | 1.42255029686241  | 1.13075688895471  | 1.03424712926855  | 0.991151276626322 |

|     |                   |                   |                   |                   |
|-----|-------------------|-------------------|-------------------|-------------------|
| 49  | 1.41263836747994  | 1.12255898725797  | 1.02693890730835  | 0.984563087547295 |
| 50  | 1.40261516529414  | 1.11429514395296  | 1.01955899975682  | 0.977881181514475 |
| 51  | 1.39249722658469  | 1.10597687627658  | 1.01211864959976  | 0.97111779197493  |
| 52  | 1.38229994079202  | 1.09761491905699  | 1.00462833302565  | 0.964284330347387 |
| 53  | 1.37203761579224  | 1.08921926553927  | 0.997097801172538 | 0.95739143103879  |
| 54  | 1.36172354065077  | 1.08079920718352  | 0.989536120477671 | 0.95044899490481  |
| 55  | 1.35137004576945  | 1.07236337228598  | 0.981951711550194 | 0.943466231072571 |
| 56  | 1.34098856037909  | 1.06391976330872  | 0.974352386510417 | 0.936451697069775 |
| 57  | 1.33058966736125  | 1.05547579283318  | 0.966745384760088 | 0.929413337227215 |
| 58  | 1.32018315540943  | 1.04703831807948  | 0.959137407166291 | 0.922358519341396 |
| 59  | 1.30977806856176  | 1.03861367395551  | 0.95153464865733  | 0.915294069600759 |
| 60  | 1.29938275315489  | 1.03020770461931  | 0.943942829242239 | 0.908226305793087 |
| 61  | 1.28900490226282  | 1.02182579355382  | 0.936367223476683 | 0.901161068823236 |
| 62  | 1.27865159769556  | 1.01347289216637  | 0.92881268840706  | 0.8941037525797   |
| 63  | 1.26832934964039  | 1.00515354693613  | 0.921283690031892 | 0.887059332195898 |
| 64  | 1.25804413403474  | 0.996871925141263 | 0.913784328325289 | 0.880032390757776 |
| 65  | 1.24780142776343  | 0.988631839204136 | 0.906318360871537 | 0.873027144513485 |
| 66  | 1.23760624177564  | 0.980436769698361 | 0.898889225162984 | 0.866047466643874 |
| 67  | 1.22746315221777  | 0.972289887065077 | 0.891500059615483 | 0.859096909654359 |
| 68  | 1.21737632967833  | 0.96419407208859  | 0.884153723356841 | 0.85217872644973  |
| 69  | 1.20734956664004  | 0.956151935183221 | 0.876852814844277 | 0.845295890153682 |
| 70  | 1.19738630323266  | 0.948165834544085 | 0.869599689366735 | 0.83845111273444  |
| 71  | 1.18748965137768  | 0.940237893214798 | 0.862396475487366 | 0.831646862497024 |
| 72  | 1.17766241741339  | 0.932370015124815 | 0.855245090480489 | 0.824885380501378 |
| 73  | 1.16790712328583  | 0.92456390014836  | 0.848147254816074 | 0.818168695964034 |
| 74  | 1.15822602638793  | 0.916821058235883 | 0.841104505743238 | 0.811498640699187 |
| 75  | 1.14862113812552  | 0.909142822667607 | 0.834118210022577 | 0.804876862653032 |
| 76  | 1.13909424128574  | 0.901530362477213 | 0.827189575855275 | 0.798304838583143 |
| 77  | 1.12964690627966  | 0.893984694092025 | 0.820319664055044 | 0.791783885932505 |
| 78  | 1.12028050632725  | 0.886506692234239 | 0.813509398506924 | 0.78531517394553  |
| 79  | 1.11099623164979  | 0.879097100125926 | 0.806759575955021 | 0.778899734071236 |
| 80  | 1.10179510273097  | 0.871756539038589 | 0.800070875159188 | 0.772538469696481 |
| 81  | 1.09267798270479  | 0.864485517226189 | 0.793443865458731 | 0.766232165249978 |
| 82  | 1.08364558892516  | 0.857284438278634 | 0.786879014779206 | 0.759981494715695 |
| 83  | 1.07469850376886  | 0.850153608930856 | 0.780376697116513 | 0.753787029592102 |
| 84  | 1.06583718472069  | 0.843093246360764 | 0.773937199530589 | 0.747649246331766 |
| 85  | 1.05706197378667  | 0.836103485007584 | 0.767560728679252 | 0.741568533293809 |
| 86  | 1.04837310627833  | 0.829184382940341 | 0.761247416920988 | 0.735545197239879 |
| 87  | 1.0397707190087   | 0.822335927804607 | 0.754997328013824 | 0.729579469402506 |
| 88  | 1.03125485793812  | 0.815558042373982 | 0.748810462435848 | 0.723671511152995 |
| 89  | 1.02282548530538  | 0.808850589731295 | 0.742686762351414 | 0.717821419294375 |
| 90  | 1.0144824862778   | 0.802213378102994 | 0.73662611624565  | 0.71202923100339  |
| 91  | 1.0062256751516   | 0.795646165368827 | 0.73062836324847  | 0.706294928444039 |
| 92  | 0.998054801131963 | 0.789148663267569 | 0.724693297168072 | 0.700618443073787 |
| 93  | 0.989969553720224 | 0.782720541318302 | 0.718820670252582 | 0.694999659662262 |
| 94  | 0.981969567734075 | 0.776361430475545 | 0.713010196697432 | 0.689438420040997 |
| 95  | 0.974054427984794 | 0.7700709265354   | 0.707261555914894 | 0.683934526601633 |
| 96  | 0.966223673634099 | 0.76384859330884  | 0.701574395581201 | 0.678487745558873 |
| 97  | 0.958476802251706 | 0.757693965577212 | 0.695948334475701 | 0.673097809993457 |
| 98  | 0.950813273593312 | 0.75160655184412  | 0.690382965125562 | 0.667764422689455 |
| 99  | 0.94323251311746  | 0.745585836896929 | 0.684877856268705 | 0.662487258779243 |
| 100 | 0.935733915258493 | 0.739631284190315 | 0.679432555146824 | 0.657265968208692 |