**Atmospheric Chlorine Reaction with N-methyl-2-pyrrolidinone (NMP)**

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| 1-Geometries Gaussian files in Cartesian Coordinates |

**Complex reactant CR1**

0 2

 C 0.78643800 0.85023700 0.30368200

 C 2.15861300 0.95762600 -0.34260800

 C 2.43097000 -0.45543800 -0.88213000

 C 1.53058200 -1.37602600 -0.03073000

 H 2.87439100 1.25479100 0.42942500

 H 2.15900000 1.73445400 -1.10519000

 H 2.12983600 -0.51794700 -1.92871100

 H 3.47867400 -0.74603900 -0.82073100

 H 1.07160400 -2.17080700 -0.62221300

 H 2.08128800 -1.84550800 0.79188600

 O 0.03599300 1.76114700 0.61494400

 N 0.51012600 -0.47400700 0.49547800

 C -0.71043700 -0.89883700 1.10133900

 H -1.63954300 -0.53912100 0.43248400

 H -0.75490600 -1.98369200 1.16873500

 H -0.87173000 -0.43032400 2.07266400

 Cl -3.03320100 0.00045300 -0.57079800

 1 2 1.0 11 2.0 12 1.0

 2 3 1.0 5 1.0 6 1.0

 3 4 1.0 7 1.0 8 1.0

 4 9 1.0 10 1.0 12 1.0

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 12 13 1.0

 13 15 1.0 16 1.0 14 1.0

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**complexe reactant CR2**

0 2

 C 1.75746000 0.10250400 -0.18791000

 C 1.74577600 -1.41460400 -0.08625000

 C 0.26528300 -1.76473800 0.13183200

 C -0.35535900 -0.47846100 0.71779800

 H 2.37219100 -1.70205100 0.76325500

 H 2.18256100 -1.85801100 -0.97933600

 H -0.20695000 -1.99422600 -0.82433200

 H 0.12670000 -2.62050100 0.78880000

 H -1.45134500 -0.26300400 0.27917100

 H -0.43452100 -0.51910500 1.80980000

 O 2.63490600 0.81280500 -0.64278100

 N 0.56811200 0.57094900 0.30845800

 C 0.28544300 1.96894400 0.36350800

 H 1.04509700 2.46546600 -0.50872800

 H -0.86539000 2.19305300 0.37339100

 H 0.87061900 2.43419000 1.28853200

 Cl -2.99333000 0.05195500 -0.33184600

 1 2 1.0 11 2.0 12 1.0

 2 3 1.0 5 1.0 6 1.0

 3 4 1.0 7 1.0 8 1.0

 4 10 1.0 12 1.0 9 1.0

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 12 13 1.0

 13 16 1.0 15 1.0 14 1.0

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**complexe reactant CR3**

0 2

 C -1.26130000 0.79336600 -0.15778900

 C -0.19017800 1.39135100 0.74065400

 C 0.63824100 0.16907700 1.18514600

 C -0.31525800 -1.03447200 1.01530900

 H -0.68909100 1.88247700 1.57539800

 H 0.38042100 2.14498100 0.20078900

 H 1.57103800 0.03816100 0.47440600

 H 1.00899700 0.24797300 2.20532500

 H 0.19274900 -1.90757000 0.61742000

 H -0.79279100 -1.32089100 1.96194800

 O -1.96961300 1.38662600 -0.96283400

 N -1.32695600 -0.54023400 0.07438400

 C -2.24340100 -1.38183900 -0.61165100

 H -1.62106400 -1.95960200 -1.53645000

 H -2.41249700 -2.34295600 0.07689800

 H -3.22950100 -0.80499900 -0.91174900

 Cl 2.99227700 -0.17140300 -0.61835400

 1 2 1.0 11 2.0 12 1.0

 2 3 1.0 5 1.0 6 1.0

 3 4 1.0 8 1.0 7 1.0

 4 9 1.0 10 1.0 12 1.0

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 12 13 1.0

 13 16 1.0 14 1.0 15 1.0

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**complexe reactant CR4**

0 2

 C 0.53030100 -0.63153600 0.31589100

 C -0.44098400 0.47307900 0.68159700

 C 0.16816000 1.73432100 0.04891700

 C 1.66699100 1.39957000 -0.10763400

 H -0.48388000 0.53997700 1.77206600

 H -1.52819300 0.21656000 0.30136600

 H -0.27413900 1.90263000 -0.93474300

 H 0.01565700 2.64200600 0.63094200

 H 2.08578500 1.77899400 -1.05219700

 H 2.26104600 1.82335600 0.70228200

 O 0.33512800 -1.83532600 0.35911600

 N 1.70454000 -0.04934500 -0.08484200

 C 2.82480100 -0.84424300 -0.47275300

 H 2.39180615 -1.77177718 -0.74806339

 H 3.54450800 -0.27154600 -1.21012900

 H 3.37661500 -1.25014100 0.50480900

 Cl -3.20109500 -0.18823000 -0.29360200

 1 2 1.0 11 2.0 12 1.0

 2 3 1.0 5 1.0 6 1.0

 3 4 1.0 7 1.0 8 1.0

 4 9 1.0 10 1.0 12 1.0

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 12 13 1.0

 13 15 1.0 16 1.0 14 1.0

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**Transition state TS1**

0 2

 C 0.76586000 0.85540900 0.29080600

 C 2.15189600 0.94020100 -0.32871200

 C 2.42051800 -0.48272800 -0.84361900

 C 1.49358300 -1.38256400 0.00145400

 H 2.85490400 1.24060500 0.45373100

 H 2.17577600 1.70655900 -1.10144700

 H 2.14004000 -0.55640900 -1.89520000

 H 3.46370200 -0.78299500 -0.75696200

 H 1.03850400 -2.18064500 -0.58859600

 H 2.02261200 -1.84635000 0.84134600

 O 0.01871200 1.77796600 0.57447400

 N 0.47204300 -0.46326100 0.49461000

 C -0.76488100 -0.86752300 1.08105200

 H -1.85118400 -0.43860600 0.25590000

 H -0.82191800 -1.95086000 1.16202600

 H -0.94098700 -0.38426400 2.04253000

 Cl -2.93748800 -0.00968800 -0.56925100

 1 2 1.0 11 2.0 12 1.0

 2 3 1.0 5 1.0 6 1.0

 3 4 1.0 7 1.0 8 1.0

 4 9 1.0 10 1.0 12 1.0

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 12 13 1.0

 13 15 1.0 16 1.0

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**Transition state TS2**

0 2

 C 1.76036200 0.10198800 -0.18734000

 C 1.74883300 -1.41508200 -0.08509400

 C 0.26844000 -1.76525000 0.13361100

 C -0.35211100 -0.47879700 0.71928700

 H 2.37555100 -1.70215200 0.76431500

 H 2.18535900 -1.85879700 -0.97815400

 H -0.20409000 -1.99514300 -0.82230900

 H 0.13014200 -2.62077200 0.79095300

 H -1.65933600 -0.22215600 0.19653100

 H -0.43091000 -0.51902900 1.81133100

 O 2.63760200 0.81218400 -0.64277300

 N 0.57114200 0.57052900 0.30924000

 C 0.28837900 1.96852300 0.36384700

 H 1.04770500 2.46477000 -0.50883100

 H -0.86246900 2.19254400 0.37402300

 H 0.87382300 2.43417100 1.28849800

 Cl -2.99047000 0.05100600 -0.32969000

 1 2 1.0 11 2.0 12 1.0

 2 3 1.0 5 1.0 6 1.0

 3 4 1.0 7 1.0 8 1.0

 4 10 1.0 12 1.0

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 12 13 1.0

 13 15 1.0 16 1.0 14 1.0

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**Transition state TS3**

0 2

 C -1.26213100 0.79395400 -0.14219900

 C -0.18658100 1.38091200 0.75822300

 C 0.64167200 0.15281600 1.18668900

 C -0.31434900 -1.04745400 1.00805100

 H -0.68146600 1.86405300 1.59999500

 H 0.38307300 2.13927200 0.22401400

 H 1.81489200 -0.00478200 0.28360200

 H 1.01653300 0.22050100 2.20617300

 H 0.19074400 -1.91711800 0.59908700

 H -0.78862400 -1.34301500 1.95351700

 O -1.97266300 1.39665200 -0.93822700

 N -1.32894800 -0.54189600 0.07630800

 C -2.24937100 -1.37491000 -0.61486700

 H -1.63154900 -1.94393000 -1.54807600

 H -2.41726600 -2.34290400 0.06427800

 H -3.23574000 -0.79348100 -0.90506100

 Cl 2.98811200 -0.17237900 -0.62948500

 1 2 1.0 11 2.0 12 1.0

 2 3 1.0 5 1.0 6 1.0

 3 4 1.0 8 1.0

 4 9 1.0 10 1.0 12 1.0

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 12 13 1.0

 13 14 1.0 15 1.0 16 1.0

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**Transition state TS4**

0 2

 C 0.53435200 -0.63087300 0.31683900

 C -0.43649400 0.47383700 0.68342300

 C 0.17279800 1.73521900 0.05116400

 C 1.67148000 1.40011800 -0.10605900

 H -0.47900200 0.54020500 1.77394000

 H -1.81678800 0.14886200 0.20108400

 H -0.26978500 1.90414400 -0.93226200

 H 0.02075100 2.64265800 0.63369300

 H 2.09006400 1.77989300 -1.05057400

 H 2.26593000 1.82333100 0.70386700

 O 0.33885000 -1.83462900 0.35953000

 N 1.70862200 -0.04881900 -0.08400100

 C 2.82852500 -0.84384300 -0.47268600

 H 2.31608800 -1.94033900 -0.79861200

 H 3.54814600 -0.27098500 -1.21002000

 H 3.38055300 -1.25038600 0.50448700

 Cl -3.19712200 -0.18619800 -0.29117200

 1 2 1.0 11 2.0 12 1.0

 2 3 1.0 5 1.0

 3 4 1.0 7 1.0 8 1.0

 4 9 1.0 10 1.0 12 1.0

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 12 13 1.0

 13 15 1.0 16 1.0 14 1.0

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**complexe product CP1**

0 2

 C 1.29994900 0.82727800 -0.22376800

 C 2.29581200 -0.18861400 -0.75530000

 C 1.69778100 -1.55093600 -0.37865600

 C 0.80030100 -1.24997500 0.83571300

 H 3.25844500 -0.00735500 -0.26698700

 H 2.44315500 -0.04582900 -1.82480200

 H 1.08719100 -1.93141000 -1.19859200

 H 2.45004200 -2.30312700 -0.14586900

 H -0.10749500 -1.85365000 0.85160400

 H 1.32803700 -1.39695400 1.78365800

 O 1.22036100 2.00764700 -0.48225500

 N 0.46054600 0.16651400 0.67780200

 C -0.55350100 0.78468900 1.34788700

 H -2.14339500 0.29606700 0.20988100

 H -0.98179800 0.27290500 2.19687600

 H -0.61309700 1.85785700 1.24499800

 Cl -3.11469700 -0.22646700 -0.51132900

 1 2 1.0 11 2.0 12 1.0

 2 3 1.0 5 1.0 6 1.0

 3 4 1.0 7 1.0 8 1.0

 4 9 1.0 10 1.0 12 1.0

 5

 6

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 12 13 1.0

 13 15 1.0 16 1.0

 14 17 1.0

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**complexe product CP2**

0 2

 C 1.56589900 -0.11971700 -0.44854200

 C 1.14069300 -1.57719800 -0.35008800

 C 0.18232400 -1.63392100 0.85431200

 C -0.16521100 -0.18506800 1.09060200

 H 2.01684700 -2.21676500 -0.25570400

 H 0.64259000 -1.84066700 -1.28613900

 H -0.70010100 -2.24816200 0.67017700

 H 0.68281700 -2.05232500 1.73528500

 H -1.72817000 0.03003300 0.18833100

 H -0.57113500 0.18747600 2.02439200

 O 2.42039000 0.36637500 -1.15400900

 N 0.75975400 0.60284900 0.43134800

 C 0.82667400 2.04953700 0.53696900

 H 1.65593900 2.39087800 -0.07830400

 H -0.10143500 2.50017500 0.18015800

 H 0.99246200 2.34503300 1.57450100

 Cl -2.87491100 0.15009300 -0.50821100

 1 2 1.0 11 2.0 12 1.0

 2 3 1.0 5 1.0 6 1.0

 3 4 1.0 7 1.0 8 1.0

 4 10 1.0 12 1.0

 5

 6

 7

 8

 9 17 1.0

 10

 11

 12 13 1.0

 13 14 1.0 15 1.0 16 1.0

 14

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**complexe product CP3**

0 2

 C -1.58105995 0.83899449 0.08658337

 C -0.50993795 1.43697949 0.98502637

 C 0.31848105 0.21470549 1.42951837

 C -0.63501795 -0.98884351 1.25968137

 H -1.00885095 1.92810549 1.81977037

 H 0.06066105 2.19060949 0.44516137

 H 2.03165185 -0.02975726 0.12024995

 H 0.68923705 0.29360149 2.44969737

 H -0.12701095 -1.86194151 0.86179237

 H -1.11255095 -1.27526251 2.20632037

 O -2.28937295 1.43225449 -0.71846163

 N -1.64671595 -0.49460551 0.31875637

 C -2.56316095 -1.33621051 -0.36727863

 H -1.90255638 -1.77333672 -1.18710927

 H -2.41249700 -2.34295600 0.07689800

 H -3.22950100 -0.80499900 -0.91174900

 Cl 2.99227700 -0.17140300 -0.61835400

 1 2 1.0 11 2.0 12 1.5

 2 3 1.0 5 1.0 6 1.0

 3 4 1.0 8 1.0

 4 9 1.0 10 1.0 12 1.0

 5

 6

 7 17 1.0

 8

 9

 10

 11

 12 13 1.0

 13 14 1.0 15 1.0 16 1.0

 14

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 16

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**complexe product CP4**

0 2

 C 0.25339600 -0.20186700 -0.00056300

 C 0.12886900 1.23674300 -0.00057400

 C 1.46894600 1.87472400 -0.00011500

 C 2.45135500 0.67752800 0.00072700

 H -0.82258700 1.74532100 -0.00101700

 H -4.17918809 1.23666565 -0.00211642

 H 1.61617400 2.51810300 -0.87469900

 H 1.61540000 2.51883700 0.87403300

 H 3.09961000 0.67506300 -0.88091900

 H 3.09785300 0.67498700 0.88368500

 O -0.64321300 -1.06021400 -0.00089600

 N 1.59085100 -0.49587700 -0.00011400

 C 2.11267900 -1.84208900 0.00030000

 H 1.27235100 -2.53303500 0.00069700

 H 2.72672500 -2.02012900 -0.88750300

 H 2.72712700 -2.01937100 0.88797900

 Cl -3.15720482 2.10950771 -0.00134937

 1 2 1.0 11 2.0 12 1.0

 2 3 1.0 5 1.0

 3 4 1.0 7 1.0 8 1.0

 4 9 1.0 10 1.0 12 1.0

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 6 17 1.0

 7

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 12 13 1.0

 13 14 1.0 15 1.0 16 1.0

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| 2-Tables (1-3) Energies B3LYP/6-311G++(2d,pd), CBS-QB3 and G3B3 |

**Table 1**: Energies (Hartree) of reactants and products species involved in the mechanism : In hartree(u.a) as obtained from the DFT calculation. CBS-H enthalpy at 2 98.15 K. CBS-G Gibbs free energy at 298.15 K. CBS-E energy.CBS (0 K) energy at 0 K. a Atomization energy in kcal mol-1 at 0 K. .b Heat of formation at 0 K in kcal mol- 1 . cHeat of formation at 298.15 K in kcal mol-1 d Experimental Heat of formation at 298.15 K in kcal mol-1. (1) CRC Handbook of Chemistry and Physics New York October 2003.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | E-DFT | CBS-H | CBS-G | CBS-E | CBS-0K | D0a | H°f(0K)b | H°f(298K)c | ΔfHd298K |
| NMP | -326,049078 | -325,365587 | -325,408694 | -325,366531 | -325,374519 | 1591,38 | -105,29 | -112,10 | -107,51 |
| R1 | -325,3920739 | -324,719681 | -324,75868 | -324,720625 | -324,727539 | 1499,03 | -64,57 | -71,05 | / |
| R2 | -325,3939165 | -324,720451 | 324,764413 | 324,721395 | -324,72952 | 1500,27 | -65,81 | -71,53 | / |
| R3 | -325,3672691 | -324,693336 | -324,732936 | -324,69428 | -324,701326 | 1482,58 | -48,12 | -54,52 | / |
| R4 | -325,3727367 | -324,699291 | -324,740413 | -324,700235 | -324,7078 | 1486,64 | -52,18 | -58,26 | / |
| CL | -459,477436 | -459,681285 | -459,699322 | -459,67646 | -459,683645 | 0,00 | 28,59 | 28,61 | 28,97 |
| HCL | -460,100058 | -460,344912 | -460,366099 | -460,345856 | -460,348216 | 103,38 | -23,16 | -23,20 | -23,04 |

 **Table 2**: Energies (Hartree) of species involved in the Mechanism Obtained at CBS-QB3//B3LYP/6-311G++(2d,pd) Level . CBS-H enthalpy at 2 98.15 K. CBS-G Gibbs free energy at 298.15 K. CBS-E energy .CBS (0 K) energy at 0 K. a Atomization energy in kcal mol-1 at 0 K. .b Heat of formation at 0 K in kcal mol- 1 . c Heat of formation at 298.15 K in kcal mol-1.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | E-DFT | CBS-H | CBS-G | CBS-E | CBS-0K | D0a | H°f(0K)b | H°f(298K)c | γ |
| NMP+CL | -785,52651 | -785,046872 | -785,10801 | -785,04299 | -785,05816 | 1591,38 | -76,70 | -83,13 |  |
| RC1 | -786.22495 | -785,049597 | -785,09697 | -785,05054 | -785,05961 | 1592,29 | -77,61 | -84,84 |  |
| RC2 | -786.20098 | -785,048959 | -785,07562 | -785,03140 | -785,05975 | 1592,37 | -77,69 | -84,44 |  |
| RC3 | -786.19258 | -785,046565 | -785,06583 | -785,02063 | -785,01488 | 1576,77 | -62,09 | -84,82 |  |
| RC4 | -786.18839 | -785,046707 | -785,06661 | -785,02165 | -785,01027 | 1573,87 | -59,19 | -84,91 |  |
| TS1 | -786.22013 | -785,036605 | -785,10076 | -785,10076 | -785,06557 | 1596,03 | -81,35 | -76,69 | -534.94 |
| TS2 | -786.19486 | -785,036199 | -785,07739 | -785,03414 | -785,04222 | 1581,38 | -66,70 | -70,43 | -732.70 |
| TS3 | -786.18378 | -785,013008 | -785,05664 | -785,01395 | -785,02207 | 1566,01 | -52,33 | -62,16 | -1220.71 |
| TS4 | -786.17631 | -785,015014 | -785,059003 | -785,01595 | -785,02416 | 1570,04 | -55,36 | -63,14 | -1402.26 |
| PC1 | -785,54166 | -785,06813 | -785,08211 | -785,08413 | -785,07825 | 1603,98 | -89,30 | -96,47 |  |
| PC2 | -785,54235 | -785,06801 | -785,10205 | -785,08725 | -785,05207 | 1587,55 | -72,87 | -96,39 |  |
| PC3 | -785,56214 | -785,04135 | -785,11012 | -785,05625 | -785,04094 | 1580,56 | -65,88 | -79,66 |  |
| PC4 | -785,54258 | -785,04552 | -785,11327 | -785,05844 | -785,01287 | 1562,95 | -66,27 | -82,28 |  |
| R1+HCL | -785,49213 | -785,06459 | -785,12477 | -785,06648 | -785,07575 | 1602,42 | -87,74 | -94,25 |  |
| R2+HCL | -785,49397 | -785,065363 | -785,60168 | -135,62446 | -785,07773 | 1603,66 | -88,98 | -94,73 |  |
| R3+HCL | -785,46732 | -785,038248 | -785,09903 | -785,04013 | -785,04954 | 1585,97 | -71,29 | -77,72 |  |
| R4+HCL | -785,47279 | -785,044203 | -785,10651 | -785,04609 | -785,05601 | 1590,03 | -75,35 | -81,46 |  |

**Table 3**: Energies (Hartree) of species involved in the Mechanism Obtained at G3B3//B3LYP/6-311G++(2d,pd) Level . CBS-H enthalpy at 298.15 K. CBS-G Gibbs free energy at 298.15 K. CBS-E energy.CBS (0K) energy at 0 K. a Atomization energy in kcal mol-1 at 0 K. .b Heat of formation at 0 K in kcal mol- 1 . c Heat of formation at 298.15 K in kcal mol-1.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | E-DFT | CBS-H | CBS-G | CBS-E | CBS-0K | D0a | H°f(0K)b | H°f(298K)c | γ (cm-1) |
| NMP+CL | -785,52651 | -785,046435 | -785,069202 | -785,03657 | -785,045215 | 1583,25 | -68,57 | -82,86 |  |
| RC1 | -786.22495 | -785,07103 | -785,04125 | -785,04622 | -785,05961 | 1583,88 | -69,20 | -86,92 |  |
| RC2 | -786.20098 | -785,04622 | -785,04622 | -785,04622 | -785,04622 | 1587,03 | -72,35 | -85,49 |  |
| RC3 | -786.19258 | -785,070252 | -785,02371 | -785,046135 | -785,01488 | 1583,83 | -69,15 | -85,04 |  |
| RC4 | -786.18839 | -785,070285 | -785,02551 | -785,051941 | -785,01027 | 1587,47 | -72,79 | -86,16 |  |
| TS1 | -786,22013 | -785,03661 | -785,10076 | -785,10076 | -785,06557 | 1596,03 | -81,35 | -76,69 | -534.94 |
| TS2 | -786,21486 | -785,03404 | -785,09858 | -785,09499 | -785,06326 | 1594,57 | -80,89 | -74,53 | -732.70 |
| TS3 | -786.18378 | -785,01254 | -785,01532 | -785,01209 | -785,02207 | 1577,46 | -41,13 | -50,41 | -1220.71 |
| TS4 | -786.17631 | -785,01204 | -785,02395 | -785,01236 | -785,02416 | 1572,63 | -42,21 | -52,02 | -1402.26 |
| PC1 | -785,54166 | -785,06176 | -785,07396 | -785,06122 | -785,07019 | 1598,92 | -84,24 | -92,47 |  |
| PC2 | -785,54235 | -785,06146 | -785,07439 | -785,06256 | -785,07054 | 1599,14 | -84,46 | -92,29 |  |
| PC3 | -785,56214 | -785,06042 | -785,07439 | -785,06959 | -785,07014 | 1598,89 | -84,21 | -91,63 |  |
| PC4 | -785,54258 | -785,06018 | -785,07454 | -785,06978 | -785,07006 | 1598,84 | -84,16 | -91,48 |  |
| R1+HCL | -785,49213 | -785,052482 | -785,081619 | -785,059396 | -785,058793 | 1591,77 | -77,09 | -86,65 |  |
| R2+HCL | -785,49397 | -785,052162 | -785,076229 | -135,635732 | -785,058571 | 1591,63 | -76,95 | -86,45 |  |
| R3+HCL | -785,46732 | -785,055322 | -785,079735 | -785,028996 | -785,057356 | 1590,32 | -71,64 | -85,61 |  |
| R4+HCL | -785,47279 | -785,027262 | -785,075412 | -785,026844 | -785,033426 | 1590,85 | -73,17 | -83,83 |  |

|  |
| --- |
| 3-Transmission coefficients |

Table7 :Transmission coefficients, using the formalism of Skodje, and Truhler obtained in the temperature range 273−380 K.

**CBS-QB3**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|   | img δ\*= | β=1/KbT | α=2π/hδ\* | ∆ν# | **(T) |
| TS1 | -534,94 | 1,46459E-59 | -3,95398E-13 | 0,62525698 | 0,999 |
| TS2 | -732,7 | 1,46459E-59 | -2,88678E-13 | 0,58077477 | 1,000 |
| TS3 | -1220,71 | 1,46459E-59 | -1,73271E-13 | 0,69104053 | 1 ,004 |
| TS4 | -1402,26 | 1,46459E-59 | -1,50838E-13 | 0,61836537 | 1,000 |

Table8 :Transmission coefficients, using the formalism of Skodje, and Truhler obtained in the temperature range 273−380 K.

**G3B3**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | img δ\*= | β=1/KbT | α=2π/hδ\* | ∆ν# | **(T) |
| TS1 | -534,94 | 1,4646E-59 | -3,954E-13 | 0,55822041 | 0,996 |
| TS2 | -732,7 | 1,4646E-59 | -2,8868E-13 | 0,55383484 | 1,000 |
| TS3 | -1220,71 | 1,4646E-59 | -1,7327E-13 | 0,69855865 | 1,004 |
| TS4 | -1402,26 | 1,4646E-59 | -1,5084E-13 | 0,55822041 | 1,000 |

Table 9: Transmission coefficients, using the formalism of Wigner obtained in the temperature range 273−380 K.

**CBS-QB3**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| T | QRC1 | QRC2 | QTS1 | QTS2 | QTS1/QRC1 | QTS2/QRC2 | (T) | (T) |
| 273 | 1,51E+51 | 1,57E+52 | 6,31E+39 | 7,53E+40 | 4,19E-12 | 4,25E-12 | 1,001 | 1,001 |
| 280 | 1,86E+51 | 1,02E+52 | 7,76E+39 | 7,27E+40 | 4,18E-12 | 4,09E-12 | 1,001 | 1,001 |
| 290 | 2,48E+51 | 2,34E+52 | 1,04E+40 | 1,24E+40 | 4,18E-12 | 5,31E-13 | 1,001 | 1,003 |
| 298 | 3,12E+51 | 3,08E+51 | 1,31E+40 | 1,56E+40 | 4,19E-12 | 5,08E-12 | 1,001 | 1,003 |
| 300 | 3,31E+51 | 3,15E+51 | 1,39E+40 | 1,66E+40 | 4,19E-12 | 5,26E-12 | 1,001 | 1,003 |
| 310 | 4,38E+51 | 4,57E+51 | 1,84E+40 | 2,20E+40 | 4,20E-12 | 4,82E-12 | 1,001 | 1,001 |
| 313 | 4,76E+51 | 4,72E+51 | 2,00E+40 | 2,40E+40 | 4,21E-12 | 5,07E-12 | 1,001 | 1,003 |
| 320 | 5,77E+51 | 5,73E+51 | 2,44E+40 | 2,91E+40 | 4,22E-12 | 5,08E-12 | 1,001 | 1,003 |
| 330 | 7,57E+51 | 7,58E+51 | 3,21E+40 | 3,85E+40 | 4,24E-12 | 5,07E-12 | 1,001 | 1,003 |
| 333 | 8,21E+51 | 8,15E+51 | 3,49E+40 | 4,18E+40 | 4,25E-12 | 5,12E-12 | 1,001 | 1,003 |
| 340 | 9,90E+51 | 9,88E+51 | 4,23E+40 | 5,06E+40 | 4,27E-12 | 5,12E-12 | 1,001 | 1,003 |
| 350 | 1,29E+52 | 1,20E+52 | 5,54E+40 | 6,64E+40 | 4,30E-12 | 5,55E-12 | 1,001 | 1,003 |
| 353 | 1,39E+52 | 1,67E+52 | 6,01E+40 | 7,20E+40 | 4,31E-12 | 4,32E-12 | 1,001 | 1,001 |
| 360 | 1,67E+52 | 1,93E+52 | 7,25E+40 | 8,68E+40 | 4,33E-12 | 4,50E-12 | 1,001 | 1,001 |
| 380 | 2,79E+52 | 2,22E+52 | 1,23E+40 | 1,47E+40 | 4,41E-13 | 6,64E-13 | 1,001 | 1,004 |

Table 10: Transmission coefficients, using the formalism of Wigner obtained in the temperature range 273−380 K.

**G3B3**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| T | QRC1 | QRC2 | QTS1 | QTS2 | QTS1/QRC1 | QTS2/QRC2 | (T) | (T) |
| 273 | 3,56E+41 | 3,56E+41 | 4,44E+40 | 4,42E+40 | 1,24E-01 | 1,24E-01 | 1,000 | 1,000 |
| 280 | 4,52E+41 | 4,52E+41 | 5,60E+40 | 5,60E+40 | 1,24E-01 | 1,24E-01 | 1,000 | 1,000 |
| 290 | 6,30E+41 | 6,31E+41 | 7,83E+40 | 7,85E+40 | 1,24E-01 | 1,24E-01 | 1,000 | 1,000 |
| **298** | 8,19E+41 | 8,20E+41 | 1,07E+40 | 1,02E+41 | 1,31E-02 | 1,25E-01 | 1,000 | 1,000 |
| 300 | 8,74E+41 | 8,75E+41 | 8,78E+40 | 1,09E+41 | 1,01E-01 | 1,25E-01 | 1,000 | 1,000 |
| 310 | 1,21E+42 | 1,21E+42 | 1,11E+41 | 1,12E+41 | 9,19E-02 | 9,28E-02 | 1,000 | 1,000 |
| 313 | 1,33E+42 | 1,33E+42 | 1,22E+41 | 1,28E+41 | 9,21E-02 | 9,61E-02 | 1,000 | 1,000 |
| 320 | 1,65E+42 | 1,66E+42 | 1,53E+41 | 1,51E+41 | 9,26E-02 | 9,08E-02 | 1,000 | 1,000 |
| 330 | 2,26E+42 | 2,27E+42 | 2,11E+41 | 2,11E+41 | 9,35E-02 | 9,29E-02 | 1,000 | 1,000 |
| 333 | 2,48E+42 | 2,49E+42 | 2,32E+41 | 3,31E+41 | 9,37E-02 | 1,33E-01 | 1,000 | 1,000 |
| 340 | 3,07E+42 | 3,08E+42 | 2,90E+41 | 2,91E+41 | 9,44E-02 | 9,43E-02 | 1,000 | 1,000 |
| 350 | 4,17E+42 | 4,18E+42 | 3,98E+41 | 3,97E+41 | 9,55E-02 | 9,51E-02 | 1,000 | 1,000 |
| 353 | 4,56E+42 | 4,58E+42 | 4,37E+41 | 4,39E+41 | 9,58E-02 | 9,59E-02 | 1,000 | 1,000 |
| 360 | 5,62E+42 | 5,64E+42 | 5,44E+41 | 5,50E+41 | 9,67E-02 | 9,75E-02 | 1,000 | 1,000 |
| 380 | 1,01E+43 | 1,02E+43 | 1,01E+42 | 1,02E+42 | 9,94E-02 | 1,00E-01 | 1,000 | 1,000 |

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**Figue 6: TS1 IRC**

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**Figue 7:TS2 IRC**

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**Figue 8:TS3 IRC**

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**Figue 9:TS4 IRC**