Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Electronic Supplementary Information

# Intersystem crossing rate dependent dual emission and phosphorescence from cyclometalated platinum complexes: A second order cumulant expansionbased approach

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**Contents:**


| S.No. | Title | Page No. |
|---|---|---|
| 1 | One photon absorption data | S3 |
| 2 | Coordinates of the optimised structures of the Pt(II) complexes | S4 |
| 3 | Vibrational frequencies of the various optimised geometries | S16 |
| 4 | Displacement vectors | S26 |
| 5 | Reference | S34 |

## 1. One photon absorption data

Table S1: Adiabatic singlet and triplet excitation wavelengths (λ in nm) accompanied by the major contributing molecular orbitals (MCMO) as obtained by TD-DFT calculations at the B3LYP/cc-pVDZ and LANL2DZ ECP level of theory along with the experimentally observed peaks.[1] Oscillator strengths are given in parentheses.

| Excitation | Complex **1** | | | Complex **2** | | |
|---|---|---|---|---|---|---|
| | Exp λ | Cal | | Exp λ | Cal | |
| | | λ (f) | MCMO | | λ (f) | MCMO |
| $S_0 \rightarrow S_1$ | 429 | 431(0.39) | HOMO →LUMO | 462 | 472 (0.57) | HOMO → LUMO |
| $S_0 \rightarrow S_2$ | 411 | 395 (0.30) | HOMO-1 → LUMO | - | 390 (0.19) | HOMO → LUMO+1 |
| $S_0 \rightarrow S_3$ | - | 376 (0.00) | HOMO-3 →LUMO | - | 380(0.11) | HOMO-1 → LUMO |
| $S_0 \rightarrow S_4$ | - | 367 (0.02) | HOMO-2 →LUMO | - | 372 (0.00) | HOMO-3 → LUMO |
| $S_0 \rightarrow S_5$ | - | 356 (0.29) | HOMO →LUMO+1<br>HOMO-2 →LUMO | - | 357 (0.09) | HOMO → LUMO+2<br>HOMO-2 → LUMO |
| $S_0 \rightarrow S_6$ | 339 | 335 (0.06) | HOMO-1 →LUMO+1 | 354 | 357 (0.24) | HOMO → LUMO+2 |
| $S_0 \rightarrow T_1$ | - | 572 | HOMO → LUMO | - | 722 | HOMO → LUMO |
| $S_0 \rightarrow T_2$ | - | 456 | HOMO-1 → LUMO | - | 471 | HOMO → LUMO+1<br>HOMO →LUMO+2 |
| $S_0 \rightarrow T_3$ | - | 426 | HOMO-1 → LUMO<br>HOMO-2 → LUMO<br>HOMO-4 → LUMO | - | 437 | HOMO → LUMO+1<br>HOMO -1 → LUMO<br>HOMO-2 →LUMO |
| $S_0 \rightarrow T_4$ | - | 415 | HOMO-1 → LUMO+2<br>HOMO-2 → LUMO+2 | - | 427 | HOMO-1 → LUMO<br>HOMO-4 → LUMO |
| $S_0 \rightarrow T_5$ | - | 404 | HOMO → LUMO+1 | - | 413 | HOMO-1 → LUMO+2 |
| $S_0 \rightarrow T_6$ | - | 387 | HOMO-3 → LUMO | - | 385 | HOMO -3 → LUMO |

Table S2: Adiabatic singlet excitation wavelengths (λ in nm) as obtained by RI-CC2 calculations using def-TZVP basis set along with the experimentally observed peaks.[1]

| Excitation | Complex **1** | | Complex **2** | |
|---|---|---|---|---|
| | Exp λ | Cal λ | Exp λ | Cal λ |
| $S_0 \rightarrow S_1$ | 429 | 452 | 462 | 472 |
| $S_0 \rightarrow S_2$ | 411 | 414 | - | 405 |
| $S_0 \rightarrow S_3$ | - | 413 | - | 404 |

## 2. Coordinates of the optimised structure of the Pt (II) complexes

Coordinates of the ground state ($S_0$) optimized geometry of complex **1:**

| | | | |
|---|---|---|---|
| C | -1.46948500 | 7.80167500 | 2.92404200 |
| C | -1.51932600 | 6.84465400 | 1.91473300 |
| C | -0.33673300 | 6.21922500 | 1.51967800 |
| C | 0.89473700 | 6.53765100 | 2.12370600 |
| C | 0.90202100 | 7.50990800 | 3.14180900 |
| C | -0.27246300 | 8.14532200 | 3.54534400 |
| F | -2.60933800 | 8.41184700 | 3.30933100 |
| C | 2.14912900 | 5.86973600 | 1.70103800 |
| C | 2.15570300 | 4.52050800 | 1.32926400 |
| N | 3.26808500 | 3.87761800 | 0.93445100 |
| C | 4.47613100 | 4.52345100 | 0.88108100 |
| C | 4.53469100 | 5.87632300 | 1.24869800 |
| C | 3.38619800 | 6.54295900 | 1.65233500 |
| C | 5.57549900 | 3.68011900 | 0.43247700 |
| C | 5.21524700 | 2.33541900 | 0.13519100 |
| C | 6.20723300 | 1.45737400 | -0.30637400 |
| C | 7.54853600 | 1.87129400 | -0.45136700 |
| C | 7.87980100 | 3.21243100 | -0.14936500 |
| C | 6.90696000 | 4.10443100 | 0.28297700 |
| C | 8.56958300 | 0.91830000 | -0.90066000 |
| C | 8.53237600 | -0.46063500 | -0.88128300 |

| | | | |
|---|---|---|---|
| C | 9.70958800 | -1.07611000 | -1.39558500 |
| C | 10.66538600 | -0.18412200 | -1.81946400 |
| S | 10.10263200 | 1.45806100 | -1.58199900 |
| C | 12.00701600 | -0.47071600 | -2.43507100 |
| C | 12.09221100 | -0.14640800 | -3.93611300 |
| Pt | 3.29270500 | 1.92661400 | 0.39482900 |
| O | 1.18021700 | 1.64620600 | 0.72907900 |
| C | 0.57383500 | 0.54091400 | 0.54785400 |
| C | 1.16024100 | -0.66391100 | 0.10121200 |
| C | 2.50914500 | -0.88153800 | -0.22503600 |
| O | 3.47109500 | -0.03180500 | -0.17942400 |
| C | 2.94348700 | -2.25385300 | -0.68969200 |
| C | -0.90976500 | 0.56533700 | 0.85036900 |
| H | -2.47457300 | 6.60828300 | 1.44388400 |
| H | -0.37023000 | 5.48815500 | 0.70982200 |
| H | 1.83695700 | 7.75820600 | 3.64788800 |
| H | -0.27355600 | 8.89278500 | 4.33993200 |
| H | 1.25651100 | 3.90300700 | 1.35335200 |
| H | 5.48780700 | 6.40300400 | 1.20368500 |
| H | 3.43999700 | 7.60226100 | 1.91098900 |
| H | 5.92239700 | 0.43499500 | -0.55831900 |
| H | 8.91404500 | 3.54988400 | -0.23965200 |
| H | 7.19407500 | 5.13375700 | 0.51132000 |
| H | 7.68745800 | -1.02083200 | -0.48159300 |
| H | 9.85338700 | -2.15687700 | -1.44445200 |
| H | 12.22471900 | -1.53995200 | -2.27439300 |
| H | 12.79297300 | 0.08841200 | -1.89727000 |
| H | 11.90303600 | 0.92263200 | -4.12501400 |
| H | 11.34706600 | -0.72307200 | -4.50714700 |
| H | 13.09266500 | -0.38854800 | -4.33020000 |
| H | 0.49496300 | -1.52057000 | -0.00253700 |
| H | 2.11188200 | -2.96972600 | -0.72778400 |
| H | 3.72264200 | -2.63794600 | -0.01152700 |
| H | 3.39939900 | -2.17194600 | -1.68958500 |

| | | | |
|---|---|---|---|
| H | -1.39666600 | 1.32725800 | 0.22002000 |
| H | -1.06140900 | 0.87061700 | 1.89851900 |
| H | -1.39592200 | -0.40506700 | 0.68299700 |

Coordinates of the first excited singlet state ($S_1$) optimized geometry of complex **1:**

| | | | |
|---|---|---|---|
| C | -1.43853300 | 7.80128300 | 3.02575800 |
| C | -1.53947700 | 6.68103000 | 2.20182000 |
| C | -0.37545900 | 6.05968300 | 1.75897500 |
| C | 0.90629500 | 6.53220600 | 2.12985900 |
| C | 0.95828900 | 7.67499200 | 2.96262800 |
| C | -0.20095600 | 8.30662000 | 3.41123700 |
| F | -2.56703600 | 8.41151800 | 3.45205500 |
| C | 2.13865800 | 5.87715700 | 1.66883900 |
| C | 2.13869600 | 4.52978600 | 1.30211200 |
| N | 3.23594900 | 3.87101600 | 0.88599000 |
| C | 4.47131100 | 4.54139000 | 0.80289700 |
| C | 4.52662100 | 5.89491400 | 1.16380900 |
| C | 3.39767900 | 6.57081200 | 1.59432500 |
| C | 5.54329600 | 3.69843300 | 0.34415400 |
| C | 5.17211300 | 2.31746700 | 0.05813200 |
| C | 6.13557700 | 1.41603000 | -0.39301200 |
| C | 7.47756100 | 1.80312700 | -0.58368600 |
| C | 7.81859800 | 3.16408000 | -0.29635500 |
| C | 6.88218200 | 4.08584600 | 0.15413800 |
| C | 8.47960800 | 0.86463400 | -1.05297600 |
| C | 8.33578800 | -0.47872700 | -1.37827700 |
| C | 9.53673200 | -1.09817800 | -1.80418300 |
| C | 10.63151100 | -0.25819300 | -1.81897700 |
| S | 10.16684200 | 1.34504900 | -1.29126900 |
| C | 12.04155800 | -0.56736000 | -2.23299700 |
| C | 12.45656100 | 0.06491900 | -3.57352300 |
| Pt | 3.28014400 | 1.93280800 | 0.37082400 |
| O | 1.18513700 | 1.64878900 | 0.75862100 |

| | | | |
|---|---|---|---|
| C | 0.57045600 | 0.53897800 | 0.61315900 |
| C | 1.13820600 | -0.67430800 | 0.17289400 |
| C | 2.47826500 | -0.90413900 | -0.19003300 |
| O | 3.44116400 | -0.05801800 | -0.18818700 |
| C | 2.89043000 | -2.28685900 | -0.64225200 |
| C | -0.90206000 | 0.57866500 | 0.95654200 |
| H | -2.52542000 | 6.31971200 | 1.90514400 |
| H | -0.46507300 | 5.20566400 | 1.08587900 |
| H | 1.92355400 | 8.06014900 | 3.29376100 |
| H | -0.15645100 | 9.18139800 | 4.06206800 |
| H | 1.23860600 | 3.91716700 | 1.35742800 |
| H | 5.48036400 | 6.42097900 | 1.09315000 |
| H | 3.45848800 | 7.63168900 | 1.83278400 |
| H | 5.82148100 | 0.39186400 | -0.59618300 |
| H | 8.85025300 | 3.49510000 | -0.43459400 |
| H | 7.19949700 | 5.11044200 | 0.35677300 |
| H | 7.38419700 | -1.00393100 | -1.30823800 |
| H | 9.60355800 | -2.14810300 | -2.09437400 |
| H | 12.13744400 | -1.66420400 | -2.29542000 |
| H | 12.74310200 | -0.23923100 | -1.44540300 |
| H | 12.39461400 | 1.16426700 | -3.53233400 |
| H | 11.80171100 | -0.27701200 | -4.39074700 |
| H | 13.49444700 | -0.20745400 | -3.82480800 |
| H | 0.46696200 | -1.52957500 | 0.10425000 |
| H | 2.05548600 | -2.99957100 | -0.63863600 |
| H | 3.69081500 | -2.66051000 | 0.01675000 |
| H | 3.31222600 | -2.22547700 | -1.65853500 |
| H | -1.40084500 | 1.33043600 | 0.32344300 |
| H | -1.02068700 | 0.90980400 | 2.00097000 |
| H | -1.39803200 | -0.39205200 | 0.82482900 |

Coordinates of the first excited triplet state ($T_1$) optimized geometry of complex **1:**

| | | | |
|---|---|---|---|
| C | -1.41017400 | 7.81412600 | 2.98160700 |

| | | | |
|---|---|---|---|
| C | -1.50775200 | 6.73009300 | 2.11287000 |
| C | -0.34142100 | 6.09827200 | 1.68671500 |
| C | 0.93219900 | 6.53106200 | 2.11856200 |
| C | 0.98292400 | 7.63415900 | 2.99866200 |
| C | -0.17642400 | 8.27605500 | 3.43101100 |
| F | -2.53704200 | 8.43181400 | 3.39526500 |
| C | 2.16453000 | 5.86124000 | 1.66851800 |
| C | 2.15929400 | 4.50195700 | 1.30669600 |
| N | 3.24535800 | 3.84401000 | 0.89432900 |
| C | 4.48059200 | 4.49315100 | 0.79878300 |
| C | 4.54300900 | 5.86715100 | 1.15595100 |
| C | 3.41821400 | 6.53564800 | 1.58172900 |
| C | 5.53508500 | 3.66879600 | 0.34591600 |
| C | 5.17131400 | 2.28066800 | 0.05752200 |
| C | 6.13454700 | 1.41471400 | -0.38621000 |
| C | 7.50960400 | 1.82834400 | -0.58123200 |
| C | 7.83856700 | 3.21292700 | -0.28586800 |
| C | 6.89761300 | 4.09432500 | 0.15731300 |
| C | 8.48430900 | 0.92797000 | -1.03793200 |
| C | 8.33516200 | -0.45138200 | -1.37046900 |
| C | 9.51693700 | -1.06184500 | -1.79649000 |
| C | 10.62885000 | -0.22260800 | -1.82064700 |
| S | 10.19031100 | 1.39807100 | -1.29136800 |
| C | 12.02923700 | -0.54838200 | -2.24342100 |
| C | 12.45022600 | 0.09764400 | -3.57682600 |
| Pt | 3.25763200 | 1.89623100 | 0.38137600 |
| O | 1.15222400 | 1.62746500 | 0.78086100 |
| C | 0.53922900 | 0.52130300 | 0.63582900 |
| C | 1.10815300 | -0.69365000 | 0.19256700 |
| C | 2.44562000 | -0.92282200 | -0.17160400 |
| O | 3.41174000 | -0.07797200 | -0.17158300 |
| C | 2.85756700 | -2.30634900 | -0.62527500 |
| C | -0.93522200 | 0.55498600 | 0.98074600 |
| H | -2.49041200 | 6.40179200 | 1.77100700 |

| | | | |
|---|---|---|---|
| H | -0.42330200 | 5.26935500 | 0.98200300 |
| H | 1.94506500 | 7.98202300 | 3.37796700 |
| H | -0.13671800 | 9.12183700 | 4.11904100 |
| H | 1.25627900 | 3.89232900 | 1.36419200 |
| H | 5.49507600 | 6.39265300 | 1.07807300 |
| H | 3.48336400 | 7.59719400 | 1.82442300 |
| H | 5.84867900 | 0.38378900 | -0.59653100 |
| H | 8.86706900 | 3.55350800 | -0.42356700 |
| H | 7.18408500 | 5.12653500 | 0.36818800 |
| H | 7.38071400 | -0.96772000 | -1.29202200 |
| H | 9.58201800 | -2.11185700 | -2.08725300 |
| H | 12.11127400 | -1.64540200 | -2.32061700 |
| H | 12.73712400 | -0.23733800 | -1.45372400 |
| H | 12.40016700 | 1.19674300 | -3.52087100 |
| H | 11.79187000 | -0.22675500 | -4.39826700 |
| H | 13.48490500 | -0.18334200 | -3.83099100 |
| H | 0.43672800 | -1.54910400 | 0.12422500 |
| H | 2.02241400 | -3.01916100 | -0.62077600 |
| H | 3.65844800 | -2.68143000 | 0.03239800 |
| H | 3.27752600 | -2.24567800 | -1.64242100 |
| H | -1.43901400 | 1.30392100 | 0.34805000 |
| H | -1.05578600 | 0.88372500 | 2.02579600 |
| H | -1.42758100 | -0.41779000 | 0.84877800 |

Coordinates of the second excited triplet state ($T_2$) optimized geometry of complex **1:**

| | | | |
|---|---|---|---|
| C | -1.48133300 | 7.79666200 | 3.02398100 |
| C | -1.56582000 | 6.72852900 | 2.13415200 |
| C | -0.39220300 | 6.11834300 | 1.69580200 |
| C | 0.87780000 | 6.55059900 | 2.13976600 |
| C | 0.91435500 | 7.63839000 | 3.04016600 |
| C | -0.25250100 | 8.26166800 | 3.48191900 |
| F | -2.61705100 | 8.39660500 | 3.44696400 |
| C | 2.11899900 | 5.90089600 | 1.68295500 |

| | | | |
|---|---|---|---|
| C | 2.13749700 | 4.55348900 | 1.31476400 |
| N | 3.24334000 | 3.91555700 | 0.90083500 |
| C | 4.46985700 | 4.57919800 | 0.81358600 |
| C | 4.50770600 | 5.94397500 | 1.17914300 |
| C | 3.37089400 | 6.59506400 | 1.60531100 |
| C | 5.54069100 | 3.75334600 | 0.35561200 |
| C | 5.17629400 | 2.38725300 | 0.07308700 |
| C | 6.15364000 | 1.47034400 | -0.38734900 |
| C | 7.50878500 | 1.85359300 | -0.58631800 |
| C | 7.83196200 | 3.20672500 | -0.29859000 |
| C | 6.88883100 | 4.12480700 | 0.15519200 |
| C | 8.47524300 | 0.88835300 | -1.05712800 |
| C | 8.28687000 | -0.46747900 | -1.37516200 |
| C | 9.46046100 | -1.12173000 | -1.80827000 |
| C | 10.58476200 | -0.31764400 | -1.84230600 |
| S | 10.17116000 | 1.32137300 | -1.31525700 |
| C | 11.98173400 | -0.66643200 | -2.26138900 |
| C | 12.42967000 | -0.01037300 | -3.57982100 |
| Pt | 3.30475700 | 1.95651700 | 0.37498500 |
| O | 1.23253800 | 1.62779500 | 0.75656900 |
| C | 0.62379600 | 0.51183000 | 0.61167500 |
| C | 1.20626000 | -0.69130200 | 0.16797500 |
| C | 2.55190200 | -0.89652100 | -0.19611800 |
| O | 3.49308300 | -0.02779100 | -0.18840900 |
| C | 2.99232600 | -2.26800200 | -0.65302800 |
| C | -0.84659600 | 0.53859500 | 0.95931800 |
| H | -2.54461100 | 6.39858000 | 1.78237700 |
| H | -0.46452700 | 5.30649500 | 0.97002000 |
| H | 1.87266300 | 7.98857500 | 3.42721900 |
| H | -0.22100500 | 9.09603600 | 4.18440900 |
| H | 1.24388800 | 3.93042900 | 1.36662600 |
| H | 5.45349800 | 6.48343000 | 1.10993900 |
| H | 3.42039300 | 7.65577400 | 1.85459800 |
| H | 5.83071900 | 0.44834700 | -0.58656300 |

| | | | |
|---|---|---|---|
| H | 8.86049700 | 3.54792200 | -0.43697700 |
| H | 7.21192800 | 5.14895100 | 0.35516400 |
| H | 7.32235000 | -0.96609300 | -1.29214900 |
| H | 9.49162600 | -2.17530200 | -2.09195500 |
| H | 12.03765400 | -1.76401000 | -2.35621300 |
| H | 12.69265700 | -0.38851200 | -1.46171200 |
| H | 12.40450700 | 1.08889600 | -3.50748800 |
| H | 11.77014000 | -0.30552300 | -4.41151800 |
| H | 13.45998500 | -0.30981900 | -3.83195800 |
| H | 0.54879100 | -1.55695200 | 0.09714900 |
| H | 2.17125800 | -2.99651300 | -0.65339900 |
| H | 3.79847200 | -2.62873000 | 0.00595400 |
| H | 3.41405400 | -2.19445500 | -1.66838500 |
| H | -1.35349000 | 1.28843300 | 0.33060300 |
| H | -0.96484900 | 0.86471500 | 2.00526900 |
| H | -1.33430700 | -0.43590800 | 0.82538200 |

Coordinates of the ground state ($S_0$) optimized geometry of complex **2:**

| | | | |
|---|---|---|---|
| C | 5.31802800 | 3.74605000 | 0.24714900 |
| C | 5.25942900 | 2.35457400 | 0.32540700 |
| C | 6.48917700 | 1.80412600 | 0.77145400 |
| C | 7.46977500 | 2.75137800 | 1.03023300 |
| S | 6.87814700 | 4.38704200 | 0.72735600 |
| C | -2.14482700 | 6.79442400 | -2.46048500 |
| C | -2.08308000 | 5.69370200 | -1.61109500 |
| C | -0.83612000 | 5.25352900 | -1.16694900 |
| C | 0.35145100 | 5.89763600 | -1.56515000 |
| C | 0.24509000 | 7.00623900 | -2.42688600 |
| C | -0.99539400 | 7.46017100 | -2.87558300 |
| F | -3.34836000 | 7.22731800 | -2.89137300 |
| C | 1.67428700 | 5.42523300 | -1.09240900 |
| C | 1.92880900 | 4.05972000 | -0.91177100 |
| N | 3.10802000 | 3.58555900 | -0.48191200 |

| | | | |
|---|---|---|---|
| C | 4.14865400 | 4.44317000 | -0.19713100 |
| C | 3.95902800 | 5.82607700 | -0.36422400 |
| C | 2.73629700 | 6.30891100 | -0.80505600 |
| Pt | 3.51262400 | 1.60322200 | -0.21156000 |
| O | 1.56312200 | 0.96945200 | -0.82788900 |
| C | 1.19921100 | -0.25172700 | -0.87595200 |
| C | 1.99268800 | -1.36833200 | -0.53490700 |
| C | 3.32294400 | -1.35861900 | -0.08198800 |
| O | 4.07501600 | -0.33521100 | 0.10814700 |
| C | 4.00539800 | -2.67028500 | 0.23522900 |
| C | -0.22158800 | -0.47672900 | -1.34700400 |
| C | 10.98353300 | 1.53859600 | 2.36527200 |
| C | 11.06457700 | 2.88769400 | 2.11360200 |
| C | 9.85635500 | 3.45729600 | 1.62267000 |
| C | 8.82677500 | 2.54533600 | 1.49162700 |
| S | 9.37468200 | 0.94811000 | 1.99465700 |
| C | 12.05879700 | 0.61138700 | 2.85951100 |
| C | 12.58720200 | -0.36306800 | 1.79314500 |
| H | 6.65600500 | 0.73358300 | 0.89186500 |
| H | -3.00583000 | 5.20303700 | -1.29814600 |
| H | -0.78906600 | 4.40834900 | -0.47776700 |
| H | 1.14856600 | 7.51005300 | -2.77585100 |
| H | -1.08138600 | 8.31336500 | -3.54999400 |
| H | 1.18165000 | 3.29450500 | -1.12842200 |
| H | 4.77741200 | 6.50890000 | -0.13243400 |
| H | 2.58887600 | 7.38583200 | -0.90780400 |
| H | 1.52379900 | -2.34693900 | -0.63286000 |
| H | 4.34029200 | -2.66153300 | 1.28502900 |
| H | 4.90814300 | -2.77090200 | -0.38868700 |
| H | 3.35183900 | -3.53690200 | 0.07007200 |
| H | -0.91543300 | 0.05650300 | -0.67680300 |
| H | -0.49683400 | -1.53932900 | -1.37930000 |
| H | -0.34478300 | -0.03938100 | -2.35112000 |
| H | 11.97800300 | 3.46131200 | 2.27847100 |

| | | | |
|---|---|---|---|
| H | 9.74752900 | 4.51140900 | 1.36509100 |
| H | 11.68730500 | 0.03609100 | 3.72585600 |
| H | 12.88734200 | 1.23454100 | 3.23553700 |
| H | 13.00512400 | 0.18268900 | 0.93218600 |
| H | 11.78412700 | -1.01684500 | 1.41648000 |
| H | 13.37856900 | -1.00532200 | 2.21246400 |

Coordinates of the first excited singlet state ($S_1$) optimized geometry of complex **2:**

| | | | |
|---|---|---|---|
| C | 5.32296100 | 3.73930100 | 0.25751900 |
| C | 5.24384300 | 2.30880300 | 0.35286300 |
| C | 6.45097400 | 1.74817400 | 0.80530900 |
| C | 7.45683300 | 2.67689800 | 1.06221700 |
| S | 6.88044900 | 4.35596800 | 0.72599500 |
| C | -2.09559800 | 6.78734200 | -2.54907600 |
| C | -2.03122100 | 5.58494900 | -1.84687300 |
| C | -0.79810500 | 5.14251200 | -1.37577500 |
| C | 0.38791600 | 5.88035500 | -1.59802900 |
| C | 0.27298900 | 7.09592800 | -2.31096100 |
| C | -0.95623800 | 7.54992200 | -2.78699000 |
| F | -3.29100200 | 7.22325000 | -3.00260500 |
| C | 1.69375900 | 5.41460000 | -1.10390100 |
| C | 1.93282700 | 4.05188600 | -0.90100100 |
| N | 3.10545500 | 3.55740200 | -0.46348300 |
| C | 4.16916700 | 4.44241400 | -0.18896100 |
| C | 3.98587800 | 5.81874000 | -0.37869700 |
| C | 2.77394200 | 6.31738000 | -0.83113300 |
| Pt | 3.50072000 | 1.60277800 | -0.17291500 |
| O | 1.54286000 | 0.98357500 | -0.78191200 |
| C | 1.16420800 | -0.23487500 | -0.81753500 |
| C | 1.94018500 | -1.35949700 | -0.46641500 |
| C | 3.27151400 | -1.36806700 | -0.01206200 |
| O | 4.03913000 | -0.35691600 | 0.16920000 |
| C | 3.92931000 | -2.68932900 | 0.31678000 |

| | | | |
|---|---|---|---|
| C | -0.25919700 | -0.44316600 | -1.28622100 |
| C | 10.98745700 | 1.51332500 | 2.33952900 |
| C | 10.99755400 | 2.88950400 | 2.22608800 |
| C | 9.77761700 | 3.44270000 | 1.77177200 |
| C | 8.79074900 | 2.48703100 | 1.52254000 |
| S | 9.42211400 | 0.87117500 | 1.87168800 |
| C | 12.10294500 | 0.60462000 | 2.76662100 |
| C | 12.69905200 | -0.23959300 | 1.62535300 |
| H | 6.59266500 | 0.67607900 | 0.94368000 |
| H | -2.94635400 | 5.01928400 | -1.66498300 |
| H | -0.76170800 | 4.21818800 | -0.79720000 |
| H | 1.16628900 | 7.68379900 | -2.52649700 |
| H | -1.04071800 | 8.48293000 | -3.34647300 |
| H | 1.17684300 | 3.29542200 | -1.11393200 |
| H | 4.81307700 | 6.49546400 | -0.15456700 |
| H | 2.63507700 | 7.39245400 | -0.93745800 |
| H | 1.45559900 | -2.33111900 | -0.55591600 |
| H | 4.26277600 | -2.67743000 | 1.36704300 |
| H | 4.83110500 | -2.81067300 | -0.30487200 |
| H | 3.26085700 | -3.54558100 | 0.15778900 |
| H | -0.94405500 | 0.10550500 | -0.61928300 |
| H | -0.54986500 | -1.50174600 | -1.31104700 |
| H | -0.37588800 | -0.00993900 | -2.29284900 |
| H | 11.87627700 | 3.48764900 | 2.47244000 |
| H | 9.61177000 | 4.51080700 | 1.62866200 |
| H | 11.74933400 | -0.06916200 | 3.56767800 |
| H | 12.89134500 | 1.23213400 | 3.21452500 |
| H | 13.10175100 | 0.40396300 | 0.82715200 |
| H | 11.93777500 | -0.89632900 | 1.17464500 |
| H | 13.51599500 | -0.87579400 | 2.00253200 |

Coordinates of the first excited triplet state ($T_1$) optimized geometry of complex **2:**

| | | | |
|---|---|---|---|
| C | 5.32422500 | 3.73853400 | 0.25434000 |

| | | | |
|---|---|---|---|
| C | 5.25816200 | 2.28160000 | 0.35561200 |
| C | 6.44220400 | 1.74849400 | 0.80003700 |
| C | 7.47520800 | 2.70646500 | 1.06633500 |
| S | 6.88132800 | 4.38799800 | 0.72378100 |
| C | -2.08926500 | 6.78962800 | -2.51822000 |
| C | -2.02870900 | 5.61957000 | -1.76582200 |
| C | -0.79034800 | 5.17464800 | -1.30695400 |
| C | 0.39823100 | 5.88164300 | -1.59173800 |
| C | 0.28960200 | 7.06237700 | -2.35727800 |
| C | -0.94329300 | 7.51952600 | -2.82045700 |
| F | -3.28641400 | 7.22681200 | -2.96264300 |
| C | 1.70802000 | 5.40846400 | -1.10721400 |
| C | 1.95171700 | 4.03751400 | -0.90669300 |
| N | 3.11657000 | 3.55164200 | -0.47217700 |
| C | 4.18086500 | 4.41732200 | -0.19007700 |
| C | 3.99424600 | 5.81235700 | -0.37703500 |
| C | 2.78698700 | 6.29694900 | -0.82658300 |
| Pt | 3.50217200 | 1.57862500 | -0.18097900 |
| O | 1.54179900 | 0.97355800 | -0.79853000 |
| C | 1.15795500 | -0.24204900 | -0.83748100 |
| C | 1.92993100 | -1.36974900 | -0.48537000 |
| C | 3.25928500 | -1.38149200 | -0.02771200 |
| O | 4.02970600 | -0.37228100 | 0.15710600 |
| C | 3.91443200 | -2.70419900 | 0.30176100 |
| C | -0.26527700 | -0.44606900 | -1.31071700 |
| C | 10.98088700 | 1.53200700 | 2.34246100 |
| C | 10.99191700 | 2.91440100 | 2.22936100 |
| C | 9.78576600 | 3.47340000 | 1.77763500 |
| C | 8.77681500 | 2.51106700 | 1.51913000 |
| S | 9.41156200 | 0.88308600 | 1.87085000 |
| C | 12.09496200 | 0.62367900 | 2.77139000 |
| C | 12.68061500 | -0.23515900 | 1.63578500 |
| H | 6.60450100 | 0.68000600 | 0.94496000 |
| H | -2.94837900 | 5.07898600 | -1.53731400 |

| | | | |
|---|---|---|---|
| H | -0.75261800 | 4.27447500 | -0.69135700 |
| H | 1.18819400 | 7.62193900 | -2.62240400 |
| H | -1.02590000 | 8.42680500 | -3.42068800 |
| H | 1.19582600 | 3.27978300 | -1.11893500 |
| H | 4.81748500 | 6.49077100 | -0.14777400 |
| H | 2.64793100 | 7.37302600 | -0.93994600 |
| H | 1.44332800 | -2.34021700 | -0.57730500 |
| H | 4.24506900 | -2.69417500 | 1.35289400 |
| H | 4.81762900 | -2.82674700 | -0.31753800 |
| H | 3.24480300 | -3.55911000 | 0.14008000 |
| H | -0.95154000 | 0.10200000 | -0.64464900 |
| H | -0.55809500 | -1.50407100 | -1.33813300 |
| H | -0.37882100 | -0.01176400 | -2.31727400 |
| H | 11.87378200 | 3.50714200 | 2.47860500 |
| H | 9.62254100 | 4.54151900 | 1.63589500 |
| H | 11.74225300 | -0.04077800 | 3.58093800 |
| H | 12.88917000 | 1.25117300 | 3.20929700 |
| H | 13.08402000 | 0.39794600 | 0.82953400 |
| H | 11.91295400 | -0.89066200 | 1.19432500 |
| H | 13.49500600 | -0.87341700 | 2.01488600 |

## 3. Vibrational frequencies of the various optimised geometries

Vibrational frequencies of complex **1** in $cm^{-1}$:

| $S_1$ | $T_1$ | $T_2$ |
|---|---|---|
| 30.242 | 30.041 | i21.535 |
| 45.844 | 44.509 | 30.079 |
| 52.426 | 51.058 | 40.917 |
| 57.247 | 55.763 | 46.059 |
| 59.63 | 59.446 | 51.628 |
| 66.296 | 63.692 | 56.614 |
| 82.965 | 75.118 | 64.58 |

| | | |
|---|---|---|
| 92.912 | 89.829 | 70.442 |
| 95.392 | 92.417 | 88.282 |
| 101.64 | 96.105 | 92.375 |
| 117.038 | 111.702 | 102.192 |
| 135.365 | 129.302 | 112.387 |
| 146.156 | 144.846 | 124.422 |
| 151.626 | 148.829 | 130.288 |
| 163.729 | 157.11 | 151.499 |
| 166.309 | 161.932 | 158.452 |
| 181.518 | 178 | 174.551 |
| 186.448 | 181.689 | 178.932 |
| 192.938 | 183.651 | 182.446 |
| 200.335 | 198.161 | 192.763 |
| 222.169 | 220.641 | 213.927 |
| 241.393 | 228.184 | 220.856 |
| 255.804 | 247.333 | 236.552 |
| 262.355 | 259.452 | 241.122 |
| 276.128 | 278.284 | 266.825 |
| 296.03 | 291.194 | 279.51 |
| 297.056 | 294.686 | 293.481 |
| 300.99 | 296.74 | 295.112 |
| 309.75 | 301.196 | 298.7 |
| 326.876 | 314.46 | 309.345 |
| 333.963 | 321.312 | 319.426 |
| 367.588 | 356.057 | 356.613 |
| 375.182 | 370.227 | 370.079 |
| 385.28 | 376.638 | 379.372 |
| 410.938 | 395.163 | 397.757 |
| 426.372 | 421.202 | 414.22 |
| 431.934 | 432.68 | 425.446 |
| 438.922 | 436.678 | 435.475 |
| 441.109 | 438.99 | 439.47 |
| 452.246 | 441.289 | 442.142 |

| | | |
|---|---|---|
| 457.902 | 447.839 | 444.99 |
| 473.996 | 464.094 | 464.564 |
| 483.628 | 473.853 | 474.456 |
| 528.232 | 502.545 | 502.4 |
| 543.093 | 520.998 | 515.872 |
| 550.513 | 539.458 | 537.615 |
| 573.273 | 554.417 | 541.768 |
| 583.763 | 568.839 | 555.249 |
| 601.787 | 578.05 | 569.468 |
| 608.044 | 583.367 | 583.724 |
| 614.416 | 595.5 | 590.728 |
| 626.607 | 609.661 | 608.773 |
| 639.129 | 614.655 | 616.832 |
| 647.239 | 622.822 | 621.305 |
| 656.858 | 645.69 | 644.717 |
| 670.284 | 654.744 | 658.265 |
| 679.232 | 672.038 | 666.769 |
| 689.592 | 681.986 | 681.509 |
| 699.2 | 688.719 | 688.872 |
| 719.366 | 702.996 | 700.965 |
| 737.585 | 708.96 | 706.834 |
| 743.493 | 729.385 | 728.746 |
| 754.278 | 738.3 | 736.547 |
| 783.975 | 760.03 | 752.081 |
| 795.892 | 773.546 | 776.152 |
| 826.61 | 790.517 | 802.541 |
| 830.174 | 813.276 | 812.479 |
| 837.39 | 825.705 | 818.941 |
| 841.001 | 827.853 | 824.94 |
| 848.837 | 832.227 | 831.042 |
| 858.41 | 845.869 | 835.69 |
| 869.085 | 857.569 | 848.224 |
| 884.727 | 877.63 | 856.54 |

| | | |
|---|---|---|
| 919.089 | 908.714 | 875.902 |
| 939.084 | 915.411 | 914.876 |
| 941.595 | 921.896 | 921.057 |
| 944.607 | 937.747 | 941.957 |
| 948.793 | 939.962 | 942.752 |
| 976.152 | 948.634 | 950.217 |
| 976.801 | 951.629 | 972.002 |
| 984.357 | 983.096 | 981.193 |
| 992.244 | 987.001 | 983.067 |
| 996.374 | 992.024 | 988.068 |
| 1002.355 | 994.834 | 993.766 |
| 1006.758 | 1001.199 | 997.666 |
| 1014.258 | 1003.739 | 1000.581 |
| 1022.413 | 1023.192 | 1023.98 |
| 1034.971 | 1026.336 | 1029.354 |
| 1047.378 | 1033.446 | 1033.871 |
| 1056.456 | 1043.064 | 1041.606 |
| 1058.091 | 1055.77 | 1056.449 |
| 1062.294 | 1062.226 | 1060.855 |
| 1063.353 | 1062.789 | 1063.033 |
| 1078.208 | 1071.474 | 1077.861 |
| 1094.281 | 1077.827 | 1081.509 |
| 1103.899 | 1089.818 | 1093.942 |
| 1131.234 | 1094.294 | 1100.917 |
| 1133.939 | 1128.064 | 1126.832 |
| 1170.039 | 1139.139 | 1138.319 |
| 1177.868 | 1176.674 | 1169.274 |
| 1191.336 | 1183.979 | 1180.566 |
| 1196.866 | 1188.286 | 1182.479 |
| 1203.26 | 1220.606 | 1193.508 |
| 1231.563 | 1232.169 | 1218 |
| 1239.345 | 1248.843 | 1230.251 |
| 1247.428 | 1251.398 | 1257.153 |

| | | |
|---|---|---|
| 1260.362 | 1262.989 | 1260.508 |
| 1269.854 | 1265.678 | 1265.523 |
| 1270.296 | 1267.406 | 1272.676 |
| 1279.649 | 1283.493 | 1284.58 |
| 1310.458 | 1300.953 | 1297.322 |
| 1318.111 | 1316.859 | 1305.427 |
| 1332.092 | 1322.298 | 1322.671 |
| 1339.464 | 1332.801 | 1330.677 |
| 1352.059 | 1337.705 | 1339.601 |
| 1359.768 | 1357.676 | 1358.271 |
| 1379.445 | 1364.07 | 1364.655 |
| 1387.205 | 1385.162 | 1374.785 |
| 1413.218 | 1405.698 | 1392.554 |
| 1416.768 | 1412.73 | 1401.869 |
| 1418.373 | 1416.445 | 1408.332 |
| 1419.45 | 1418.985 | 1417.502 |
| 1430.236 | 1419.821 | 1418.763 |
| 1436.023 | 1431.549 | 1422.948 |
| 1445.413 | 1446.357 | 1433.079 |
| 1476.206 | 1465.16 | 1444.987 |
| 1484.807 | 1470.136 | 1479.379 |
| 1485.411 | 1479.91 | 1484.401 |
| 1488.707 | 1485.123 | 1485.142 |
| 1490.559 | 1485.778 | 1485.812 |
| 1497.155 | 1488.647 | 1488.11 |
| 1502.438 | 1494.495 | 1493.936 |
| 1506.682 | 1502.551 | 1499.979 |
| 1516.675 | 1506.164 | 1501.469 |
| 1522.37 | 1506.624 | 1506.811 |
| 1534.87 | 1517.025 | 1509.808 |
| 1540.999 | 1523.626 | 1517.646 |
| 1546.837 | 1538.304 | 1522.963 |
| 1559.376 | 1540.665 | 1537.936 |

| | | |
|---|---|---|
| 1578.869 | 1568.252 | 1541.461 |
| 1585.644 | 1585.286 | 1552.429 |
| 1598.549 | 1589.168 | 1575.501 |
| 1621.84 | 1601.891 | 1585.867 |
| 1631.265 | 1621.204 | 1615.333 |
| 2924.227 | 2917.205 | 2916.786 |
| 2934.449 | 2936.379 | 2934.219 |
| 2947.808 | 2947.02 | 2948.208 |
| 2950.443 | 2949.732 | 2951.777 |
| 2964.269 | 2966.906 | 2960.358 |
| 2992.782 | 2994.911 | 2993.399 |
| 2995.805 | 2995.967 | 2996.971 |
| 3000.461 | 3000.229 | 2999.718 |
| 3001.404 | 3003.23 | 3002.359 |
| 3035.092 | 3032.54 | 3035.076 |
| 3038.801 | 3036.558 | 3035.944 |
| 3078.416 | 3084.471 | 3075.863 |
| 3094.267 | 3097.531 | 3092.149 |
| 3098.517 | 3098.659 | 3094.433 |
| 3098.97 | 3099.881 | 3095.387 |
| 3100.717 | 3100.388 | 3100.831 |
| 3101.321 | 3105.219 | 3102.195 |
| 3108.674 | 3108.591 | 3112.23 |
| 3110.974 | 3113.001 | 3112.524 |
| 3113.304 | 3114.775 | 3113.694 |
| 3116.032 | 3114.938 | 3115.145 |
| 3125.401 | 3118.268 | 3115.241 |
| 3129.591 | 3119.672 | 3120.077 |
| 3130.625 | 3143.232 | 3131.973 |

Vibrational frequencies of complex **2** in $cm^{-1}$:

| $S_1$ | $T_1$ |
|---|---|

| | |
|---|---|
| 28.727 | 29.01 |
| 43.411 | 41.68 |
| 51.646 | 50.073 |
| 55.091 | 53.779 |
| 59.683 | 55.927 |
| 66.806 | 65.449 |
| 85.904 | 80.447 |
| 92.482 | 84.632 |
| 94.91 | 87.151 |
| 99.792 | 94.083 |
| 115.213 | 110.225 |
| 136.996 | 129.552 |
| 143.151 | 137.896 |
| 150.186 | 147.616 |
| 163.091 | 157.304 |
| 177.194 | 173.19 |
| 180.904 | 174.837 |
| 182.949 | 181.908 |
| 189.627 | 183.5 |
| 207.49 | 205.691 |
| 222.126 | 216.557 |
| 236.877 | 224.853 |
| 260.409 | 250.545 |
| 261.815 | 261.634 |
| 274.107 | 273.996 |
| 279.77 | 281.878 |
| 293.822 | 293.541 |
| 299.67 | 299.631 |
| 309.385 | 301.836 |
| 317.899 | 311.738 |
| 325.485 | 319.52 |
| 363.538 | 355.47 |
| 368.922 | 362.192 |

| | |
|---|---|
| 374.098 | 370.841 |
| 397.99 | 393.571 |
| 406.705 | 399.907 |
| 434.347 | 429.252 |
| 436.013 | 436.427 |
| 439.419 | 439.127 |
| 442.991 | 442.205 |
| 463.141 | 453.709 |
| 488.598 | 465.762 |
| 502.663 | 479.896 |
| 527.941 | 506.617 |
| 544.593 | 530.825 |
| 564.184 | 546.152 |
| 583.15 | 568.368 |
| 589.617 | 574.917 |
| 599.901 | 583.117 |
| 607.823 | 598.689 |
| 616.786 | 612.439 |
| 624.352 | 620.796 |
| 630.355 | 622.291 |
| 647.824 | 637.015 |
| 660.294 | 644.997 |
| 662.776 | 648.841 |
| 681.542 | 684.475 |
| 689.151 | 687.257 |
| 690.307 | 689.652 |
| 713.872 | 692.489 |
| 738.589 | 731.085 |
| 763.052 | 747.417 |
| 769.774 | 748.286 |
| 786.643 | 761.508 |
| 827.066 | 779.068 |
| 827.638 | 826.582 |

| | |
|---|---|
| 835.638 | 827.764 |
| 836.075 | 833.761 |
| 858.811 | 846.018 |
| 863.529 | 857.008 |
| 881.767 | 867.698 |
| 884.669 | 876.59 |
| 900.769 | 884.623 |
| 913.925 | 911.201 |
| 940.743 | 940.154 |
| 947.848 | 948.411 |
| 950.068 | 949.243 |
| 969.039 | 963.143 |
| 983.247 | 982.429 |
| 992.257 | 992.678 |
| 1000.811 | 999.886 |
| 1005.429 | 1006.282 |
| 1019.505 | 1023.116 |
| 1021.926 | 1028.83 |
| 1040.247 | 1036.605 |
| 1041.7 | 1037.969 |
| 1057.336 | 1049.819 |
| 1062.613 | 1057.131 |
| 1063.62 | 1062.89 |
| 1078.459 | 1063.44 |
| 1093.724 | 1078.273 |
| 1103.938 | 1095.258 |
| 1129.396 | 1103.3 |
| 1133.701 | 1128.954 |
| 1169.122 | 1132.755 |
| 1172.705 | 1155.064 |
| 1186.105 | 1168.028 |
| 1191.213 | 1179.39 |
| 1206.733 | 1188.159 |

| | |
|---|---|
| 1215.628 | 1232.366 |
| 1232.312 | 1244.68 |
| 1248.094 | 1261.817 |
| 1263.184 | 1263.454 |
| 1267.38 | 1264.463 |
| 1268.623 | 1268.297 |
| 1287.781 | 1281.164 |
| 1309.881 | 1297.109 |
| 1325.591 | 1304.29 |
| 1334.895 | 1329.666 |
| 1338.628 | 1333.837 |
| 1367.742 | 1352.176 |
| 1373.166 | 1367.813 |
| 1390.517 | 1390.012 |
| 1407.36 | 1414.122 |
| 1415.081 | 1416.201 |
| 1417.886 | 1417.725 |
| 1420.279 | 1420.195 |
| 1431.817 | 1428.535 |
| 1445.809 | 1433.124 |
| 1464.471 | 1452.918 |
| 1483.787 | 1470.042 |
| 1483.919 | 1483.884 |
| 1485.054 | 1485.27 |
| 1488.175 | 1488.268 |
| 1492.177 | 1488.397 |
| 1498.687 | 1494.886 |
| 1502.352 | 1497.912 |
| 1506.871 | 1502.547 |
| 1517.263 | 1506.305 |
| 1530.722 | 1516.897 |
| 1539.59 | 1529.027 |
| 1545.675 | 1538.797 |

| | |
|---|---|
| 1553.106 | 1541.902 |
| 1579.406 | 1571.599 |
| 1584.533 | 1581.433 |
| 1618.501 | 1588.098 |
| 1630.975 | 1624.038 |
| 2926.225 | 2922.066 |
| 2939.266 | 2939.505 |
| 2945.788 | 2945.676 |
| 2946.16 | 2946.313 |
| 2966.284 | 2964.61 |
| 2993.404 | 2993.772 |
| 2994.653 | 2994.598 |
| 2999.616 | 3000.096 |
| 3004.236 | 3004.155 |
| 3032.327 | 3031.973 |
| 3038.151 | 3037.386 |
| 3094.422 | 3096.12 |
| 3097.171 | 3096.784 |
| 3097.942 | 3100.973 |
| 3102.152 | 3101.337 |
| 3105.341 | 3104.429 |
| 3112.365 | 3113.011 |
| 3115.17 | 3113.928 |
| 3118.476 | 3117.323 |
| 3121.255 | 3118.633 |
| 3127.336 | 3119.624 |
| 3128.061 | 3125.408 |

**4. <u>Displacement vectors:</u>**

Displacement vector for complex **1** in ($a_0$ amu$^{1/2}$)**:**

| $S_1 \rightarrow T_1$ | $S_1 \rightarrow T_2$ |
|---|---|
| -0.65587 | -3.25E-03 |
| -1.00837 | 1.329374 |

| | |
|---|---|
| -0.18929 | 0.94615 |
| 0.465875 | -1.5519 |
| 0.123625 | -0.31583 |
| 8.15E-02 | 0.194338 |
| 8.97E-02 | 0.464669 |
| 0.976859 | 1.173596 |
| 0.536275 | 0.245765 |
| -0.14402 | -7.20E-02 |
| 0.389121 | -0.58939 |
| -2.11E-02 | -0.25327 |
| 0.207474 | -0.17271 |
| -0.7867 | 0.172342 |
| 4.66E-02 | 0.267956 |
| -0.65718 | -0.31086 |
| -3.95E-02 | 4.57E-02 |
| 0.265279 | -0.13366 |
| 4.57E-02 | -0.1474 |
| 0.369832 | 9.09E-02 |
| -0.12576 | -5.65E-02 |
| -9.23E-02 | -2.45E-04 |
| 0.135303 | -0.11409 |
| -0.13269 | 0.112115 |
| 0.166332 | 6.79E-02 |
| -3.38E-02 | -4.60E-03 |
| 3.18E-02 | 5.44E-03 |
| 2.61E-03 | 1.71E-03 |
| -0.2432 | 1.73E-02 |
| -0.27733 | -1.82E-02 |
| -0.23677 | 8.97E-02 |
| -8.63E-02 | -3.97E-02 |
| 9.41E-02 | -1.99E-03 |
| 9.37E-02 | -6.82E-03 |
| -1.61E-02 | -1.52E-02 |
| 7.23E-04 | -2.60E-02 |
| -2.46E-04 | 6.85E-02 |
| 2.69E-02 | 3.31E-02 |
| -4.07E-02 | 1.43E-03 |
| 4.31E-02 | 1.33E-02 |
| -8.63E-02 | -8.69E-03 |
| 4.86E-02 | 7.69E-03 |
| 1.06E-02 | 1.20E-02 |
| 1.14E-02 | 5.27E-03 |
| 3.32E-02 | -2.35E-02 |
| 2.71E-02 | 1.19E-02 |
| -6.16E-03 | 4.37E-02 |
| -2.08E-04 | 6.25E-04 |

| | |
|---|---|
| -3.41E-02 | 2.18E-02 |
| -2.57E-02 | 7.60E-03 |
| 4.24E-02 | -3.59E-02 |
| 6.38E-02 | 3.79E-02 |
| -5.41E-04 | -5.85E-03 |
| 3.04E-02 | -3.09E-02 |
| -0.11212 | -0.15102 |
| -8.12E-02 | 6.02E-02 |
| -7.24E-03 | -4.41E-02 |
| 2.73E-04 | 1.18E-03 |
| 5.04E-02 | 2.30E-02 |
| 0.114712 | -5.22E-02 |
| -1.38E-02 | -1.68E-02 |
| 8.86E-03 | 7.85E-03 |
| -6.56E-02 | -4.77E-02 |
| -6.54E-03 | -1.97E-03 |
| 5.87E-02 | -8.50E-02 |
| 6.14E-04 | -9.24E-04 |
| -2.78E-02 | -1.72E-02 |
| 3.22E-02 | 8.35E-02 |
| -2.39E-03 | -6.92E-03 |
| 1.81E-03 | -1.16E-03 |
| 1.14E-02 | 2.72E-02 |
| -1.03E-02 | -6.02E-03 |
| -1.11E-02 | -6.74E-03 |
| 1.91E-03 | -2.18E-03 |
| -3.67E-03 | 5.47E-04 |
| 9.91E-03 | -1.64E-03 |
| -3.47E-02 | 7.50E-03 |
| 4.42E-03 | -1.52E-02 |
| -8.39E-02 | -3.87E-02 |
| -1.39E-02 | -5.73E-03 |
| 1.48E-03 | -3.03E-04 |
| 2.83E-05 | 3.02E-03 |
| -3.03E-02 | -4.66E-02 |
| -8.48E-03 | -1.89E-02 |
| -1.11E-02 | -8.87E-04 |
| -4.65E-03 | 2.60E-02 |
| -7.06E-03 | -5.17E-03 |
| 4.63E-02 | 1.02E-02 |
| -1.16E-02 | 6.47E-03 |
| 1.36E-03 | -6.95E-03 |
| -1.74E-03 | 1.14E-02 |
| -7.28E-03 | 2.88E-03 |
| 1.21E-03 | -7.42E-04 |
| -4.52E-04 | -4.65E-04 |

| | |
|---|---|
| 4.77E-02 | 1.90E-02 |
| 4.03E-02 | 9.84E-03 |
| -1.39E-02 | -1.16E-02 |
| -7.62E-03 | -2.03E-02 |
| -6.96E-02 | -1.96E-02 |
| 8.23E-03 | -2.21E-02 |
| -3.28E-02 | -3.53E-02 |
| 4.26E-02 | 4.57E-02 |
| -5.62E-02 | 6.29E-04 |
| 8.75E-03 | -4.10E-03 |
| -1.85E-02 | -2.97E-02 |
| 2.58E-02 | 5.68E-03 |
| 1.23E-02 | -1.23E-02 |
| -1.08E-03 | 1.31E-02 |
| -1.95E-02 | 7.76E-03 |
| 0.148991 | -1.29E-02 |
| -9.61E-03 | 1.18E-02 |
| 5.17E-02 | 2.63E-02 |
| -2.08E-02 | -2.76E-02 |
| -2.22E-02 | -2.21E-02 |
| 6.30E-02 | 5.82E-02 |
| 3.69E-02 | -3.56E-04 |
| -3.19E-02 | -4.64E-02 |
| 1.91E-02 | -1.95E-02 |
| -1.86E-02 | 6.57E-02 |
| -3.05E-02 | 6.22E-02 |
| 2.25E-02 | -3.92E-02 |
| 1.49E-02 | -2.10E-02 |
| -2.91E-02 | -1.60E-02 |
| -2.28E-02 | 3.24E-03 |
| -3.67E-02 | -1.84E-02 |
| -0.15542 | -7.28E-02 |
| 9.03E-06 | -1.03E-04 |
| -4.87E-04 | -4.18E-04 |
| 3.24E-03 | 6.77E-03 |
| -2.24E-02 | -4.25E-03 |
| 3.48E-03 | 3.71E-05 |
| 5.85E-03 | -7.47E-03 |
| 2.04E-03 | 6.71E-04 |
| 1.82E-02 | 1.32E-02 |
| 3.11E-02 | 8.15E-03 |
| -2.58E-02 | -3.70E-02 |
| -4.40E-03 | 3.57E-03 |
| 7.09E-02 | 2.56E-02 |
| 3.91E-02 | -2.85E-02 |
| 4.21E-02 | -1.64E-03 |

| | |
|---|---|
| 1.95E-02 | 1.00E-02 |
| 0.181982 | 1.75E-03 |
| 1.22E-02 | 3.07E-02 |
| -4.83E-02 | -4.98E-02 |
| 2.29E-04 | -1.84E-03 |
| -7.92E-04 | -2.65E-03 |
| 1.41E-04 | -6.32E-04 |
| 3.27E-04 | -3.44E-04 |
| 4.40E-04 | 1.45E-03 |
| 1.65E-04 | 8.38E-04 |
| -5.04E-05 | 8.36E-05 |
| 3.17E-05 | 1.29E-05 |
| -1.96E-04 | -7.57E-04 |
| 9.45E-05 | -4.33E-05 |
| 1.96E-04 | -2.22E-04 |
| 7.43E-04 | 1.13E-03 |
| 1.30E-04 | -1.50E-03 |
| -8.57E-04 | 4.56E-04 |
| -2.68E-03 | -1.19E-03 |
| 1.91E-04 | -1.65E-03 |
| -1.99E-03 | -1.39E-03 |
| -1.41E-03 | -9.30E-04 |
| 5.31E-04 | -3.57E-04 |
| -3.91E-03 | -5.12E-03 |
| 3.85E-03 | 4.86E-03 |
| 9.90E-04 | 2.47E-03 |
| -6.09E-04 | -4.74E-04 |
| 3.95E-03 | 2.06E-03 |

Displacement vector for complex **2** in ($a_0$ amu$^{1/2}$)**:**

| $S_1 \rightarrow T_1$ |
|---|
| 0.410432 |
| 0.40772 |
| 1.89E-02 |
| 0.158287 |
| -0.118 |
| 0.125535 |
| -0.29066 |
| 0.202405 |
| -1.103 |
| -0.10754 |
| 0.18761 |
| -0.18389 |

| |
|---|
| 0.217589 |
| 0.19713 |
| -9.91E-02 |
| -0.17722 |
| -2.96E-02 |
| -1.96E-03 |
| 6.97E-02 |
| -9.28E-02 |
| -2.56E-02 |
| 4.62E-02 |
| 1.27E-02 |
| -3.95E-03 |
| 6.54E-02 |
| 0.199241 |
| -1.43E-03 |
| -4.47E-03 |
| -6.12E-02 |
| 0.232501 |
| -7.40E-02 |
| -0.15823 |
| -3.44E-02 |
| 5.91E-02 |
| 8.15E-02 |
| -5.85E-02 |
| 4.67E-03 |
| -3.68E-02 |
| 1.80E-02 |
| -5.80E-03 |
| 3.92E-03 |
| -1.76E-02 |
| 2.12E-02 |
| -5.31E-02 |
| 2.41E-02 |
| 6.68E-02 |
| -3.54E-04 |
| -2.20E-02 |
| -3.29E-02 |
| 2.18E-02 |
| 1.82E-02 |
| -2.17E-03 |
| -3.56E-02 |
| 1.46E-02 |
| -5.80E-03 |
| 0.132614 |
| -1.93E-02 |
| -1.67E-02 |

| |
|---|
| 4.66E-04 |
| 8.41E-02 |
| 1.69E-02 |
| 6.95E-02 |
| 6.56E-03 |
| -4.64E-02 |
| 2.51E-04 |
| 1.85E-02 |
| -2.23E-02 |
| -3.64E-02 |
| -1.48E-02 |
| -1.05E-02 |
| -6.35E-03 |
| -6.02E-04 |
| 2.53E-02 |
| 6.33E-04 |
| 1.07E-03 |
| 3.61E-03 |
| 2.01E-03 |
| -2.32E-02 |
| 6.69E-04 |
| -1.02E-02 |
| 2.21E-03 |
| -1.45E-02 |
| -3.25E-03 |
| -2.69E-03 |
| -3.77E-03 |
| -8.29E-03 |
| -4.29E-04 |
| 2.95E-03 |
| -5.74E-04 |
| 5.24E-04 |
| 3.95E-02 |
| -2.53E-02 |
| 2.65E-02 |
| -3.11E-02 |
| 7.48E-02 |
| -9.48E-03 |
| 0.10011 |
| -7.90E-03 |
| -1.44E-02 |
| -1.91E-03 |
| 8.17E-05 |
| -1.35E-02 |
| -1.76E-03 |
| -7.19E-02 |

| |
|---|
| -1.51E-02 |
| 7.46E-02 |
| -2.62E-02 |
| -7.19E-02 |
| -2.31E-02 |
| -4.26E-03 |
| 1.86E-02 |
| 1.74E-02 |
| 1.39E-02 |
| -5.55E-02 |
| -1.82E-02 |
| -4.06E-03 |
| -2.95E-03 |
| 3.75E-03 |
| 2.42E-02 |
| -3.81E-02 |
| 2.99E-02 |
| 1.61E-03 |
| 1.74E-03 |
| -2.98E-02 |
| -0.13441 |
| -3.24E-02 |
| -8.42E-04 |
| 1.64E-03 |
| 3.61E-02 |
| -2.55E-02 |
| 1.11E-03 |
| 9.87E-02 |
| 4.84E-02 |
| -2.70E-03 |
| -1.04E-02 |
| 6.32E-02 |
| -4.82E-02 |
| 8.61E-05 |
| -2.04E-04 |
| 1.87E-04 |
| -7.77E-05 |
| 1.09E-05 |
| 3.16E-05 |
| -2.28E-05 |
| 1.19E-04 |
| -1.51E-05 |
| 2.52E-05 |
| -1.18E-04 |
| -3.05E-03 |
| -4.91E-05 |

| |
|---|
| -6.53E-04 |
| -1.13E-03 |
| -1.46E-04 |
| 3.16E-03 |
| -3.27E-03 |
| 1.90E-03 |
| -1.37E-03 |
| -8.42E-04 |
| 1.86E-03 |

## 5. Reference:

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