# Polypyridyl iron(II) complexes showing remarkable photocytotoxicity in visible light

ADITYA GARAI[a], UTTARA BASU[a], ILA PANT[b], PATURU KONDAIAH*[,b] AND AKHIL R. CHAKRAVARTY*[,a]

[a] Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore 560012, India

E-mail: arc@ipc.iisc.ernet.in

[b] Department of Molecular Reproduction, Development and Genetics, Indian Institute of Science, Bangalore 560012, India

E-mail: paturu@mrdg.iisc.ernet.in

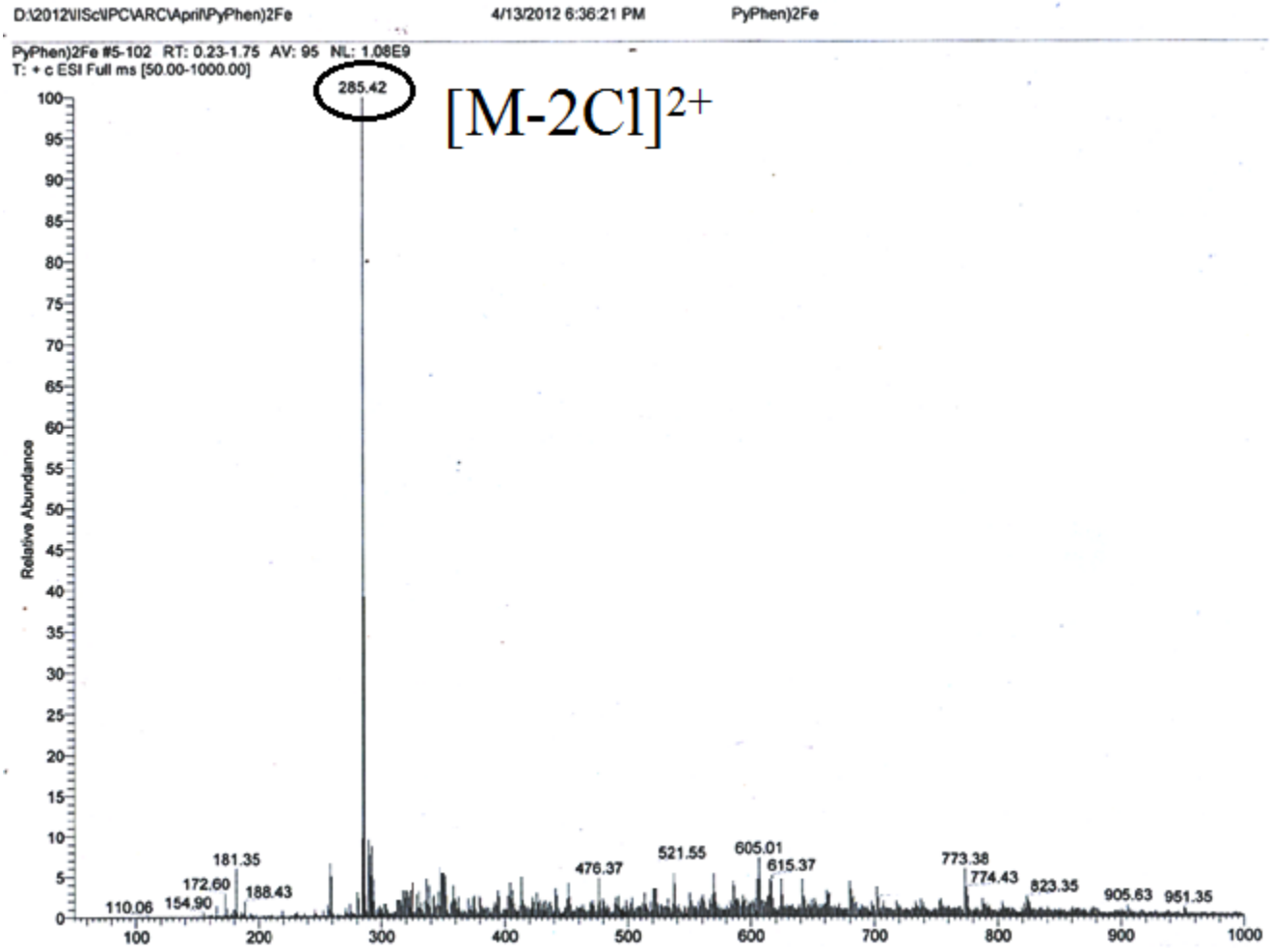


**Figure S1**. ESI-MS spectrum of complex **1** in MeOH showing a prominent peak corresponding to $[M - 2Cl]^{2+}$ at 285.42 (m/z).

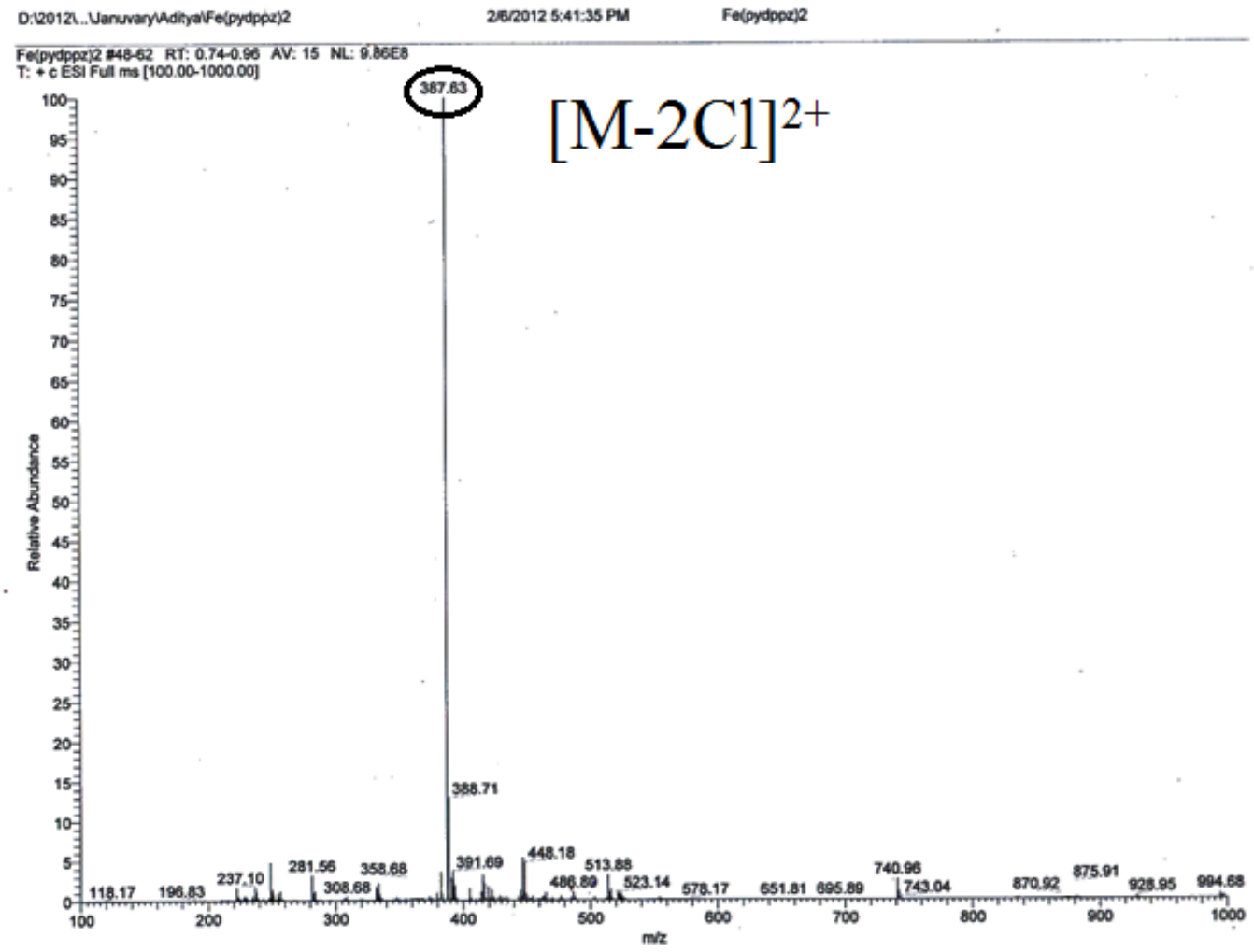


**Figure S2**. ESI-MS spectrum of complex **2** in MeOH showing a prominent peak corresponding to $[M - 2Cl]^{2+}$ at 387.63 (m/z).

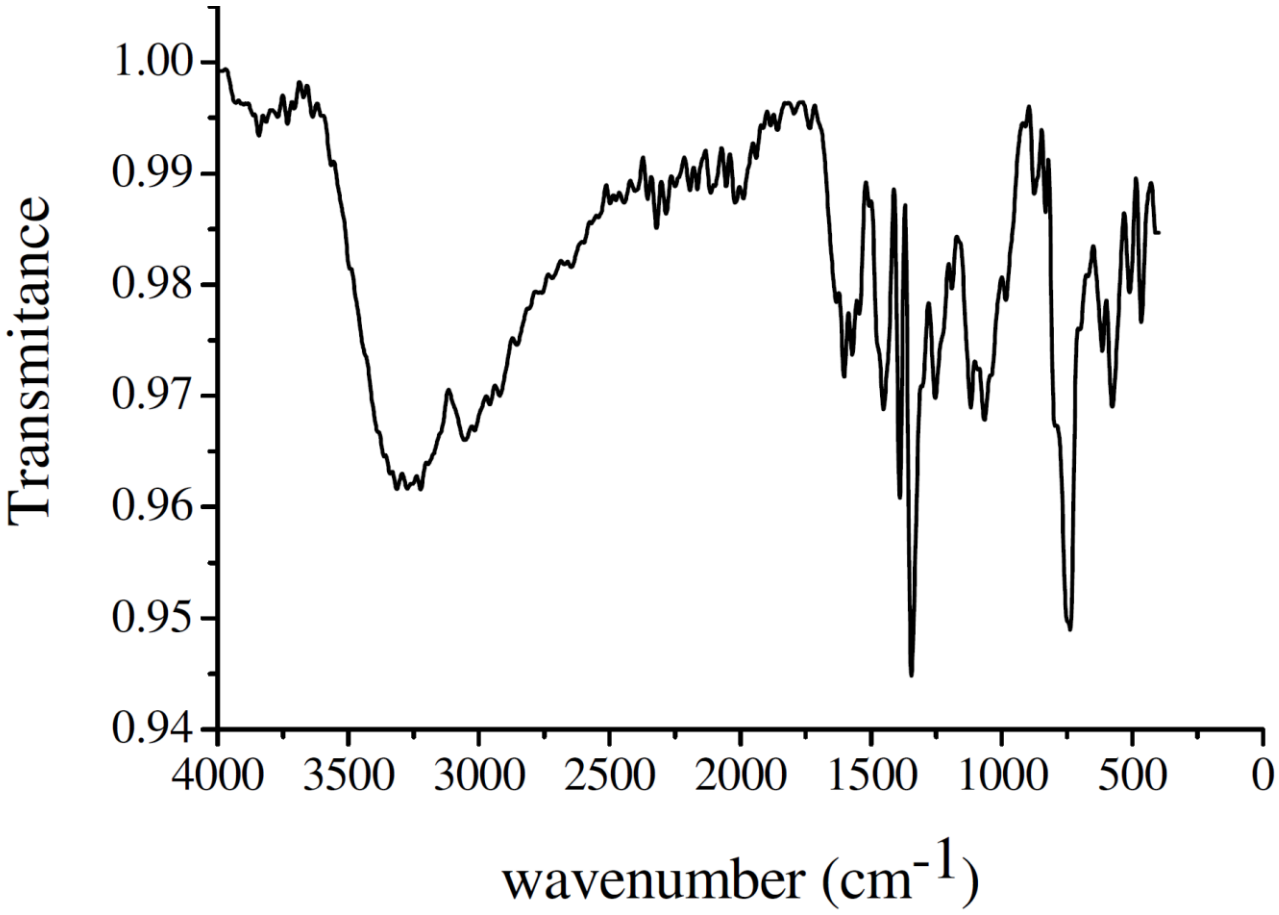


**Figure S3**. IR spectrum of complex **1** in the solid phase.

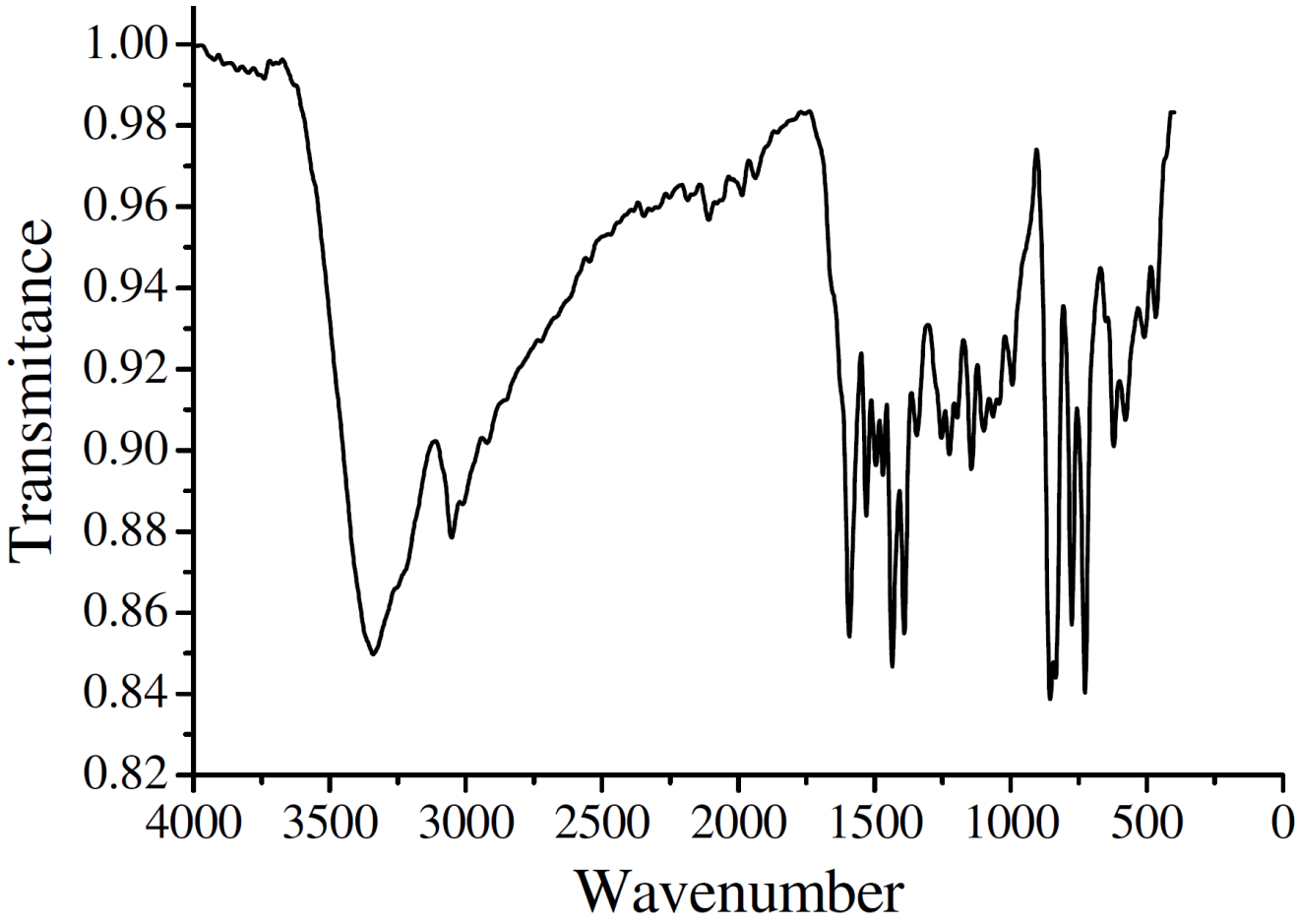


**Figure S4**. IR spectrum of complex **2** in the solid phase.

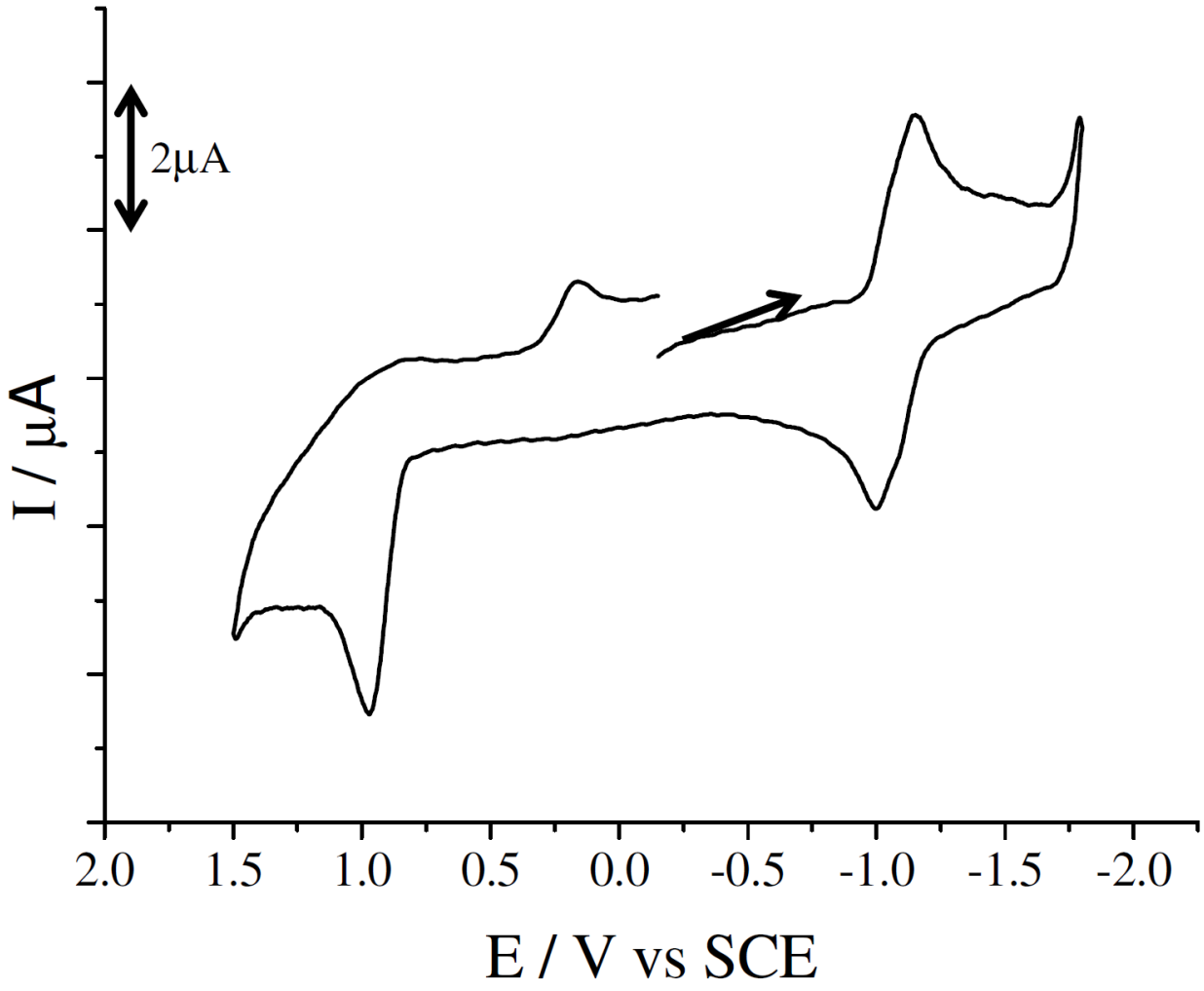


**Figure S5.** Cyclic voltammogram of complex **1** showing irreversible Fe(III)/Fe(II) couple and quasi-reversible ligand centered peak in DMF–0.1M TBAP at a scan rate of 50 mV $s^{-1}$.

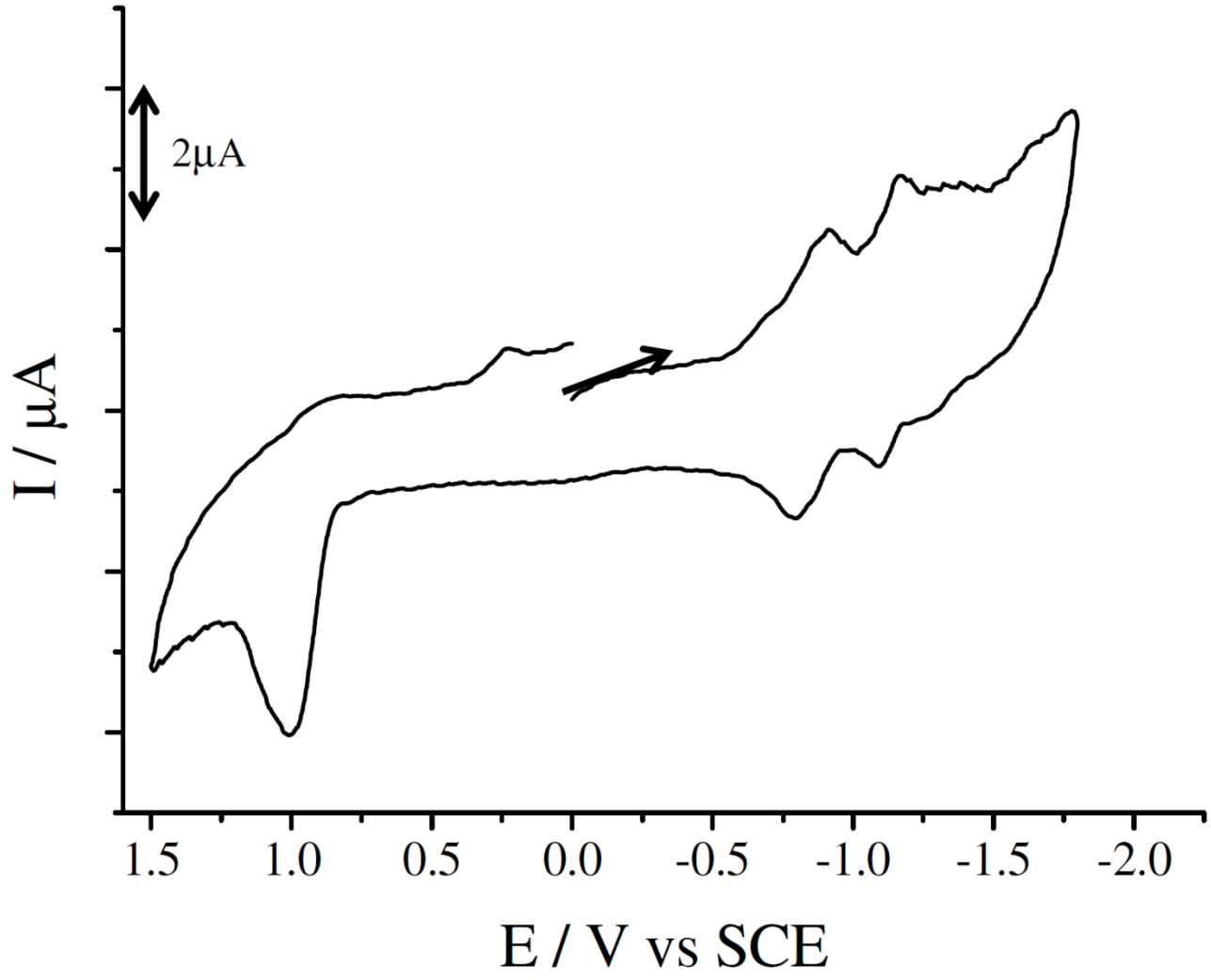


**Figure S6.** Cyclic voltammogram of complex **2** showing irreversible Fe(III)/Fe(II) couple and quasi-reversible ligand centered peak in DMF–0.1M TBAP at a scan rate of 50 mV $s^{-1}$.

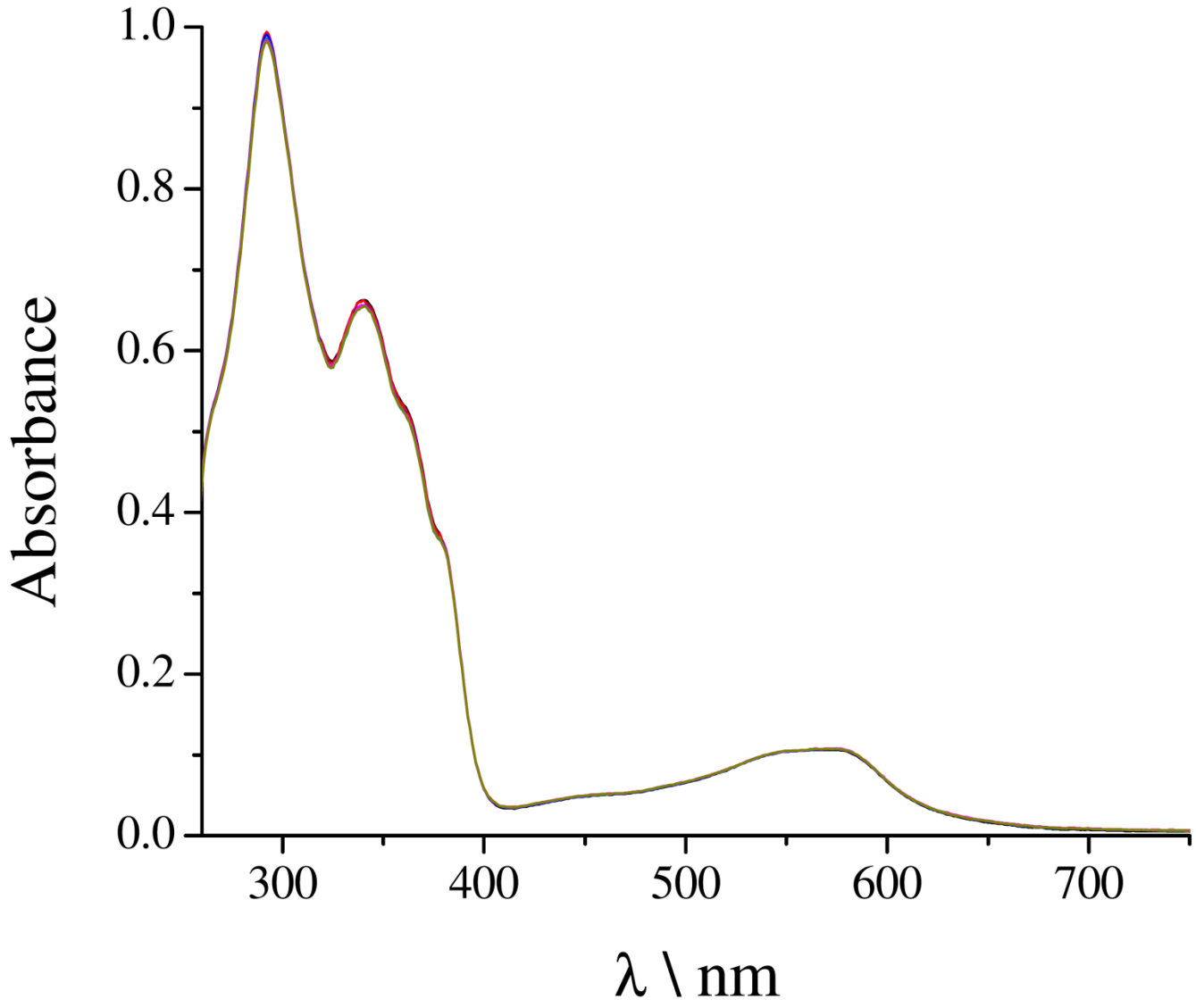


**Figure S7.** Spectral traces of complex **1** recorded in 50% aqueous DMSO over a time period of 24 h showing no pronounced change in the intensity or position of the absorption bands.

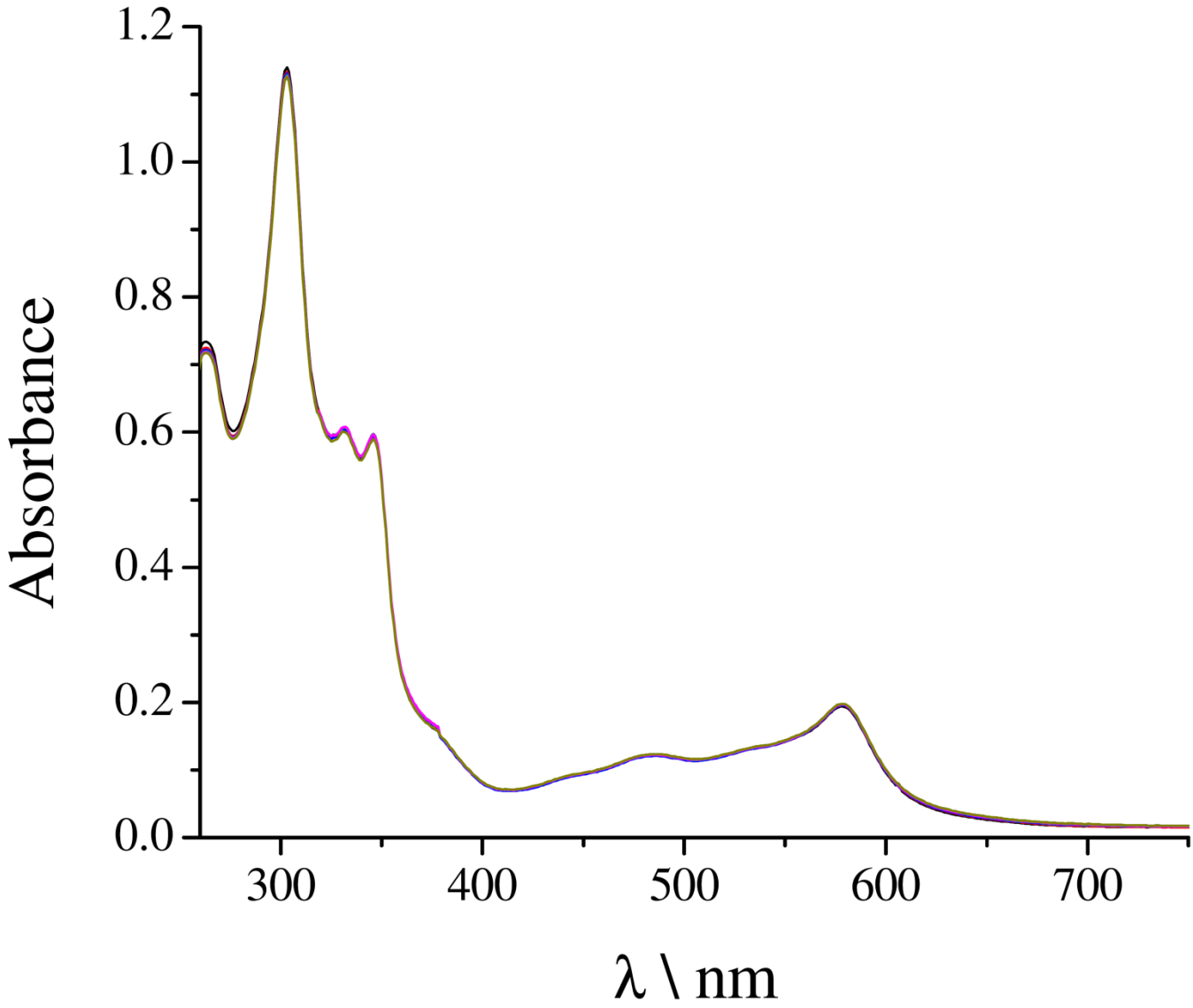


**Figure S8.** Spectral traces of complex **2** recorded in 50% aqueous DMSO over a time period of 24 h showing no pronounced change in the intensity or position of the absorption bands.

Table S1. Table showing the various transitions corresponding to the excited states of geometrically optimized complex **2** with their respective contributions, oscillator strength and the type of transition

| Excited states dppz | Contribution (%) | Oscillator strength | Wavelength (nm) | Type of Transition |
|---|---|---|---|---|
| Excited State 2 | | 0.0016 | 559.17 | |
| HOMO →LUMO | 60.63 | | | MLCT |
| HOMO-2→ LUMO+1 | 10.58 | | | MLCT |
| HOMO→LUMO+ 3 | 11.19 | | | MLCT |
| Excited state 3 | | 0.0025 | 558.17 | |
| HOMO→LUMO | 57 | | | MLCT |
| HOMO→LUMO+ 2 | 12.35 | | | MLCT |
| HOMO-2→LUMO | 8.73 | | | MLCT |
| Excited State 8 | | 0.0935 | 478.80 | |
| HOMO-3→ LUMO+1 | 38.68 | | | MLCT |
| HOMO-4→ LUMO | 29.16 | | | MLCT |
| HOMO-2→LUMO | 17.53 | | | MLCT |
| Excited State 9 | | 0.0128 | 473.47 | |
| HOMO→LUMO+ 3 | 36.58 | | | MLCT |
| HOMO-3→LUMO | 21.88 | | | MLCT |
| HOMO-4→ LUMO+1 | 13.21 | | | MLCT |

| | | | | |
|---|---|---|---|---|
| HOMO-2→LUMO+1 | 12.87 | | | MLCT |
| Excited State 10 | | 0.0040 | 445.96 | |
| HOMO-3→LUMO+3 | 67.67 | | | MLCT |
| HOMO→LUMO+2 | 10.71 | | | MLCT |
| HOMO-3→LUMO+4 | 9.7 | | | MLCT |

Table S2: Computational Data of Complex **1**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.003274 | 0.184210 | 0.003040 |
| 2 | 6 | 0 | 2.693349 | -0.621252 | 0.141514 |
| 3 | 6 | 0 | 2.153015 | 0.947877 | 1.655638 |
| 4 | 6 | 0 | 4.018177 | -0.701617 | 0.594702 |
| 5 | 6 | 0 | 2.122775 | -1.353301 | -0.900475 |
| 6 | 6 | 0 | 3.446918 | 0.964416 | 2.199882 |
| 7 | 6 | 0 | 4.424199 | 0.114849 | 1.662467 |
| 8 | 6 | 0 | 4.927625 | -1.711456 | -0.130802 |
| 9 | 6 | 0 | 2.895371 | -2.287275 | -1.599480 |
| 10 | 1 | 0 | 3.679862 | 1.619356 | 3.013043 |
| 11 | 1 | 0 | 5.413840 | 0.104110 | 2.073523 |
| 12 | 6 | 0 | 4.370675 | -2.458945 | -1.180704 |
| 13 | 6 | 0 | 2.234880 | -2.975281 | -2.626111 |
| 14 | 6 | 0 | 0.218744 | -1.712864 | -2.101752 |
| 15 | 1 | 0 | 2.749690 | -3.708684 | -3.209544 |
| 16 | 6 | 0 | 0.885103 | -2.681255 | -2.866603 |
| 17 | 1 | 0 | -0.807179 | -1.468172 | -2.274850 |
| 18 | 1 | 0 | 0.362948 | -3.198904 | -3.643698 |
| 19 | 6 | 0 | -2.113083 | -1.389697 | 0.863911 |
| 20 | 6 | 0 | -0.202770 | -1.746804 | 2.074051 |
| 21 | 6 | 0 | -2.875602 | -2.337653 | 1.556354 |
| 22 | 6 | 0 | -2.684621 | -0.628447 | -0.156189 |
| 23 | 6 | 0 | -0.860268 | -2.735021 | 2.824186 |
| 24 | 1 | 0 | 0.817157 | -1.484165 | 2.252855 |
| 25 | 6 | 0 | -2.207451 | -3.036440 | 2.572566 |
| 26 | 6 | 0 | -4.350360 | -2.508444 | 1.137147 |
| 27 | 6 | 0 | -4.008944 | -0.712483 | -0.605918 |
| 28 | 1 | 0 | -0.333741 | -3.265149 | 3.591876 |
| 29 | 1 | 0 | -2.716997 | -3.787245 | 3.140337 |
| 30 | 6 | 0 | -4.909029 | -1.741733 | 0.103520 |
| 31 | 6 | 0 | -4.426611 | 0.123320 | -1.653370 |
| 32 | 6 | 0 | -2.166988 | 0.982571 | -1.637635 |
| 33 | 1 | 0 | -5.420294 | 0.120393 | -2.054311 |
| 34 | 6 | 0 | -3.462939 | 0.996888 | -2.179010 |
| 35 | 1 | 0 | -3.707862 | 1.666030 | -2.978155 |
| 36 | 7 | 0 | -1.756177 | 0.196666 | -0.640060 |
| 37 | 7 | 0 | -0.826536 | -1.093408 | 1.087609 |
| 38 | 7 | 0 | 0.834656 | -1.058299 | -1.111967 |
| 39 | 7 | 0 | 1.749840 | 0.172077 | 0.646221 |
| 40 | 6 | 0 | -1.292218 | 2.168605 | 1.563967 |
| 41 | 6 | 0 | 0.925266 | 1.779974 | 2.051215 |
| 42 | 6 | 0 | 0.961176 | 2.720007 | 3.086779 |
| 43 | 6 | 0 | -0.225662 | 3.404253 | 3.366923 |
| 44 | 6 | 0 | -1.360596 | 3.116558 | 2.598248 |
| 45 | 1 | 0 | -2.161199 | 1.962664 | 0.972660 |
| 46 | 1 | 0 | 1.856684 | 2.900183 | 3.642838 |

| | | | | | |
|---|---|---|---|---|---|
| 47 | 1 | 0 | -0.250116 | 4.122751 | 4.159366 |
| 48 | 1 | 0 | -2.270444 | 3.635783 | 2.821840 |
| 49 | 6 | 0 | -0.978478 | 2.762726 | -3.043554 |
| 50 | 6 | 0 | -0.931993 | 1.807747 | -2.024050 |
| 51 | 6 | 0 | 1.272367 | 2.211493 | -1.523403 |
| 52 | 6 | 0 | 1.332380 | 3.176292 | -2.540240 |
| 53 | 6 | 0 | 0.199857 | 3.465339 | -3.311690 |
| 54 | 1 | 0 | -1.880636 | 2.945720 | -3.587570 |
| 55 | 1 | 0 | 2.143136 | 2.013675 | -0.933073 |
| 56 | 1 | 0 | 2.237276 | 3.707538 | -2.752789 |
| 57 | 1 | 0 | 0.216936 | 4.198582 | -4.089389 |
| 58 | 7 | 0 | 0.148046 | 1.524250 | -1.284602 |
| 59 | 7 | 0 | -0.154428 | 1.508749 | 1.306512 |
| 60 | 1 | 0 | 5.947654 | -1.817365 | 0.177648 |
| 61 | 1 | 0 | 5.006752 | -3.157748 | -1.680709 |
| 62 | 1 | 0 | -5.929019 | -1.846635 | -0.202509 |
| 63 | 1 | 0 | -4.982705 | -3.220100 | 1.623085 |

Table S3: Computational Data of Complex **2**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.000001 | 1.107545 | 0.000001 |
| 2 | 6 | 0 | 2.639642 | 0.256169 | 0.438667 |
| 3 | 6 | 0 | 1.928382 | 1.927428 | 1.941019 |
| 4 | 6 | 0 | 3.909564 | 0.167889 | 1.022322 |
| 5 | 6 | 0 | 2.229286 | -0.542603 | -0.680630 |
| 6 | 6 | 0 | 3.184444 | 1.890942 | 2.576784 |
| 7 | 6 | 0 | 4.169264 | 1.016699 | 2.119636 |
| 8 | 6 | 0 | 4.848419 | -0.789224 | 0.447919 |
| 9 | 6 | 0 | 3.111303 | -1.467852 | -1.254362 |
| 10 | 1 | 0 | 3.390842 | 2.535485 | 3.417781 |
| 11 | 1 | 0 | 5.138609 | 0.973209 | 2.593089 |
| 12 | 6 | 0 | 4.452641 | -1.595669 | -0.677937 |
| 13 | 6 | 0 | 2.644498 | -2.215870 | -2.351487 |
| 14 | 6 | 0 | 0.523638 | -1.058174 | -2.176477 |
| 15 | 1 | 0 | 3.300737 | -2.936467 | -2.815534 |
| 16 | 6 | 0 | 1.347949 | -2.003168 | -2.806015 |
| 17 | 1 | 0 | -0.484586 | -0.881386 | -2.516420 |
| 18 | 1 | 0 | 0.962156 | -2.561430 | -3.645647 |
| 19 | 6 | 0 | -2.229281 | -0.542615 | 0.680621 |
| 20 | 6 | 0 | -0.523624 | -1.058204 | 2.176451 |
| 21 | 6 | 0 | -3.111295 | -1.467871 | 1.254346 |
| 22 | 6 | 0 | -2.639642 | 0.256169 | -0.438667 |
| 23 | 6 | 0 | -1.347932 | -2.003207 | 2.805982 |
| 24 | 1 | 0 | 0.484602 | -0.881421 | 2.516391 |
| 25 | 6 | 0 | -2.644483 | -2.215902 | 2.351459 |
| 26 | 6 | 0 | -4.452635 | -1.595682 | 0.677926 |
| 27 | 6 | 0 | -3.909568 | 0.167896 | -1.022315 |
| 28 | 1 | 0 | -0.962134 | -2.561480 | 3.645604 |
| 29 | 1 | 0 | -3.300720 | -2.936504 | 2.815501 |
| 30 | 6 | 0 | -4.848420 | -0.789224 | -0.447918 |
| 31 | 6 | 0 | -4.169274 | 1.016719 | -2.119618 |
| 32 | 6 | 0 | -1.928391 | 1.927446 | -1.941004 |
| 33 | 1 | 0 | -5.138621 | 0.973235 | -2.593066 |
| 34 | 6 | 0 | -3.184456 | 1.890967 | -2.576762 |
| 35 | 1 | 0 | -3.390860 | 2.535521 | -3.417750 |
| 36 | 7 | 0 | -1.692303 | 1.109911 | -0.888985 |
| 37 | 7 | 0 | -0.945600 | -0.329418 | 1.124714 |
| 38 | 7 | 0 | 0.945607 | -0.329402 | -1.124728 |
| 39 | 7 | 0 | 1.692301 | 1.109907 | 0.888989 |
| 40 | 6 | 0 | 8.723331 | -3.643880 | -0.690386 |
| 41 | 6 | 0 | 7.466305 | -3.527848 | -1.238608 |
| 42 | 6 | 0 | 6.545103 | -2.601908 | -0.687065 |
| 43 | 6 | 0 | 6.939817 | -1.793722 | 0.441884 |
| 44 | 6 | 0 | 8.242859 | -1.938154 | 0.983304 |
| 45 | 6 | 0 | 9.113129 | -2.846017 | 0.425172 |

| | | | | | |
|---|---|---|---|---|---|
| 46 | 1 | 0 | 9.430370 | -4.347387 | -1.105996 |
| 47 | 1 | 0 | 7.150183 | -4.121694 | -2.083141 |
| 48 | 1 | 0 | 8.516117 | -1.323336 | 1.827814 |
| 49 | 1 | 0 | 10.107385 | -2.961531 | 0.832136 |
| 50 | 6 | 0 | -9.113129 | -2.846018 | -0.425173 |
| 51 | 6 | 0 | -8.242863 | -1.938147 | -0.983298 |
| 52 | 6 | 0 | -6.939818 | -1.793722 | -0.441884 |
| 53 | 6 | 0 | -6.545097 | -2.601922 | 0.687052 |
| 54 | 6 | 0 | -7.466296 | -3.527869 | 1.238590 |
| 55 | 6 | 0 | -8.723324 | -3.643895 | 0.690372 |
| 56 | 1 | 0 | -10.107386 | -2.961528 | -0.832134 |
| 57 | 1 | 0 | -8.516126 | -1.323318 | -1.827799 |
| 58 | 1 | 0 | -7.150168 | -4.121726 | 2.083113 |
| 59 | 1 | 0 | -9.430360 | -4.347409 | 1.105977 |
| 60 | 6 | 0 | -1.461673 | 3.220043 | 1.624506 |
| 61 | 6 | 0 | 0.755644 | 2.754736 | 2.251711 |
| 62 | 6 | 0 | 0.686583 | 3.700839 | 3.274647 |
| 63 | 6 | 0 | -0.493516 | 4.419617 | 3.468950 |
| 64 | 6 | 0 | -1.582914 | 4.174304 | 2.632175 |
| 65 | 1 | 0 | -2.281430 | 3.004176 | 0.958291 |
| 66 | 1 | 0 | 1.540601 | 3.875567 | 3.911679 |
| 67 | 1 | 0 | -0.559841 | 5.154628 | 4.257418 |
| 68 | 1 | 0 | -2.511540 | 4.710666 | 2.754180 |
| 69 | 6 | 0 | -0.686596 | 3.700869 | -3.274621 |
| 70 | 6 | 0 | -0.755654 | 2.754757 | -2.251692 |
| 71 | 6 | 0 | 1.461667 | 3.220055 | -1.624494 |
| 72 | 6 | 0 | 1.582905 | 4.174323 | -2.632157 |
| 73 | 6 | 0 | 0.493503 | 4.419646 | -3.468923 |
| 74 | 1 | 0 | -1.540616 | 3.875603 | -3.911647 |
| 75 | 1 | 0 | 2.281426 | 3.004181 | -0.958283 |
| 76 | 1 | 0 | 2.511533 | 4.710683 | -2.754162 |
| 77 | 1 | 0 | 0.559826 | 5.154663 | -4.257386 |
| 78 | 7 | 0 | 0.324362 | 2.517194 | -1.423452 |
| 79 | 7 | 0 | -0.324369 | 2.517181 | 1.423465 |
| 80 | 7 | 0 | -5.296404 | -2.478633 | 1.221936 |
| 81 | 7 | 0 | -6.068750 | -0.897065 | -0.985538 |
| 82 | 7 | 0 | 5.296413 | -2.478613 | -1.221953 |
| 83 | 7 | 0 | 6.068747 | -0.897072 | 0.985545 |