# Structure, Vibrations and Raman Modes in Electron Doped Metal Phthalocyanines - Supplement

Jaroslav Tóbik[1*] and Erio Tosatti[1,2]
[1] International School for Advanced Studies (SISSA),
and INFM Democritos National Simulation Center,
Via Beirut 2-4, I-34014 Trieste, Italy
[2] The Abdus Salam International Centre for Theoretical Physics (ICTP)
P.O.Box 586, I-34014 Trieste, Italy

Before giving tables with calculated quantities we would like to make some remarks about symmetry properties of $\mathrm{D_{2h}}$ group, the symmetry group of JT distorted molecule. Quantities tabulated in table III are related to this. In the parallel with equation (4) from our paper, proper vibrations can be classified according irreducible representations as follows:

$$\begin{aligned}\Gamma_{\mathrm{vib}} = \; & 28\mathrm{A_g} + 27\mathrm{B_{1g}} + 13\mathrm{B_{2g}} + 13\mathrm{B_{3g}} + \\ & + 13\mathrm{A_u} + 15\mathrm{B_{1u}} + 28\mathrm{B_{2u}} + 28\mathrm{B_{3u}}\end{aligned} \tag{1}$$

Among these, infrared active modes are of $\mathrm{B_{1u}}$, $\mathrm{B_{2u}}$ and $\mathrm{B_{3u}}$ symmetry.

Raman active modes have $\mathrm{A_g}$, $\mathrm{B_{1g}}$, $\mathrm{B_{2g}}$ and $\mathrm{B_{3g}}$ symmetry. In parallel with equation (5) from our paper, Raman tensors in $\mathrm{D_{2h}}$ symmetry are constrained to have form

$$\mathrm{A_g}: \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix}, \quad \mathrm{B_{1g}}: \begin{pmatrix} 0 & d & 0 \\ d & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathrm{B_{2g}}: \begin{pmatrix} 0 & 0 & e \\ 0 & 0 & 0 \\ e & 0 & 0 \end{pmatrix}, \quad \mathrm{B_{3g}}: \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & f \\ 0 & f & 0 \end{pmatrix} \tag{2}$$

Infrared active modes are $\mathrm{B_{1u}}$, $\mathrm{B_{2u}}$ and $\mathrm{B_{3u}}$.

In the following tables we give frequency of vibration modes, symmetry assignment and Raman tensor components or amplitude of vibration induced dipole moments. The ordering of tensor components is alphabetical. Atomic units are used in tables, namely $1a_0$ for distance, 1Ry for energy, 1e for charge, and 1amu for mass.

| frequency | symmetry | Raman or Infra red intensity | Jahn-Teller parameters |
|---|---|---|---|
| 24 | $\mathrm{E_g}$ | Ra e=0.54, f=3.73 | - |
| 35 | $\mathrm{B_{2g}}$ | Ra d=18.48 | k=0.006, q=0.0691, L=0.4 |
| 73 | $\mathrm{B_{2u}}$ | - | - |
| 116 | $\mathrm{E_u}$ | IR 0.121465 | - |
| 117 | $\mathrm{A_{2u}}$ | IR 0.400072 | - |
| 125 | $\mathrm{B_{1u}}$ | - | - |
| 141 | $\mathrm{E_g}$ | Ra e=0.27, f=2.96 | - |
| 146 | $\mathrm{A_{1u}}$ | - | - |
| 162 | $\mathrm{B_{2u}}$ | - | - |
| 168 | $\mathrm{A_{2u}}$ | IR 0.694770 | - |
| 184 | $\mathrm{B_{1g}}$ | Ra c=49.50 | k=0.281, q=0.0267, L=7.5 |
| 197 | $\mathrm{A_{2g}}$ | - | - |
| 219 | $\mathrm{B_{2g}}$ | Ra d=32.85 | k=0.581, q=0.0589, L=34.2 |
| 232 | $\mathrm{E_g}$ | Ra e=-0.38, f=2.39 | - |
| 232 | $\mathrm{B_{1u}}$ | - | - |
| 233 | $\mathrm{B_{2u}}$ | - | - |
| 262 | $\mathrm{A_{1g}}$ | Ra a=57.78, b=5.18 | k=0.539, q=0.0841 (0.0774), L=45.3 (41.7) |
| 264 | $\mathrm{A_{2u}}$ | IR 0.177599 | - |
| 276 | $\mathrm{E_u}$ | IR 0.302859 | - |
| 288 | $\mathrm{E_g}$ | Ra e=0.79, f=-0.20 | - |
| 349 | $\mathrm{A_{2u}}$ | IR 0.087985 | - |
| 415 | $\mathrm{E_g}$ | Ra e=0.12, f=-0.07 | - |
| 421 | $\mathrm{B_{2u}}$ | - | - |
| 427 | $\mathrm{E_u}$ | IR 0.158089 | - |
| 435 | $\mathrm{A_{1u}}$ | - | - |
| 441 | $\mathrm{A_{2u}}$ | IR 0.527469 | - |
| 477 | $\mathrm{B_{2g}}$ | Ra d=24.06 | k=1.271, q=0.0681, L=86.5 |

| frequency | symmetry | Raman or Infra red intensity | Jahn-Teller parameters |
|---|---|---|---|
| 500 | $E_g$ | Ra e=0.16, f=0.53 | - |
| 506 | $E_u$ | IR 0.230344 | - |
| 526 | $B_{1u}$ | - | - |
| 561 | $B_{1g}$ | Ra c=29.10 | k=2.628, q=0.0121, L=31.9 |
| 576 | $A_{2g}$ | - | - |
| 579 | $E_u$ | IR 0.404429 | - |
| 589 | $A_{1g}$ | Ra a=1.28, b=-0.96 | k=3.227, q=0.0287(0.0285), L=92.6(92.0) |
| 614 | $A_{2g}$ | - | - |
| 637 | $A_{1u}$ | - | - |
| 654 | $E_u$ | IR 0.033897 | - |
| 655 | $E_g$ | Ra e=0.12, f=-0.03 | - |
| 676 | $A_{1g}$ | Ra a=20.41, b=-3.83 | k=4.321, q=0.0605(0.0602), L=261.4(260.1) |
| 692 | $B_{2g}$ | Ra d=16.86 | k=3.533, q=0.0027, L=9.5 |
| 703 | $E_g$ | Ra e=0.34, f=-0.05 | - |
| 704 | $B_{1u}$ | - | - |
| 707 | $B_{2u}$ | - | - |
| 759 | $B_{1g}$ | Ra c=59.00 | k=6.061, q=0.0393, L=238.1 |
| 760 | $E_u$ | IR 0.470902 | - |
| 769 | $A_{2u}$ | IR 1.179033 | - |
| 778 | $B_{2u}$ | - | - |
| 779 | $E_g$ | Ra e=0.03, f=2.80 | - |
| 794 | $B_{1g}$ | Ra c=10.93 | k=4.440, q=0.0247, L=109.7 |
| 798 | $A_{1u}$ | - | - |
| 802 | $B_{1u}$ | - | - |
| 803 | $E_g$ | Ra e=2.49, f=1.42 | - |
| 809 | $A_{2u}$ | IR 0.912525 | - |
| 817 | $E_u$ | IR 0.319912 | - |
| 839 | $A_{1g}$ | Ra a=52.92, b=8.03 | k=5.339, q=0.0104 (0.0082), L=55.5(43.9) |
| 850 | $A_{2g}$ | - | - |
| 877 | $E_g$ | Ra e=0.09, f=1.04 | - |
| 877 | $B_{1u}$ | - | - |
| 878 | $A_{1u}$ | - | - |
| 894 | $E_u$ | IR 0.369663 | - |
| 934 | $B_{2g}$ | Ra d=0.38 | k=9.163, q=0.0183, L=167.7 |
| 951 | $B_{2u}$ | - | - |
| 951 | $E_g$ | Ra e=0.00, f=0.36 | - |
| 952 | $A_{2u}$ | IR 0.206490 | - |
| 983 | $A_{1u}$ | - | - |
| 983 | $E_g$ | Ra e=0.24, f=0.08 | - |
| 984 | $B_{1u}$ | - | - |
| 1000 | $E_u$ | IR 0.525074 | - |
| 1002 | $B_{1g}$ | Ra c=13.50 | k=1.839, q=0.0063, L=11.6 |
| 1014 | $A_{1g}$ | Ra a=23.91, b=3.03 | k=1.865, q=0.0139(0.0161), L=25.9(30.1) |
| 1038 | $B_{2g}$ | Ra d=6.88 | k=8.233, q=0.0052, L=42.7 |
| 1066 | $E_u$ | IR 0.059541 | - |
| 1079 | $A_{2g}$ | - | - |
| 1092 | $B_{2g}$ | Ra d=13.23 | k=1.655, q=0.0414, L=68.4 |
| 1102 | $E_u$ | IR 0.353613 | - |
| 1117 | $A_{1g}$ | Ra a=17.80, b=2.31 | |
| 1121 | $B_{1g}$ | Ra c=12.63 | k=1.535, q=0.0532, L=81.6 |
| 1124 | $E_u$ | IR 0.003464 | - |
| 1157 | $A_{2g}$ | - | - |
| 1158 | $A_{1g}$ | Ra a=36.42, b=2.04 | k=3.123, q=0.0286(0.0305), L=89.2(95.4) |
| 1176 | $E_u$ | IR 0.255071 | - |
| 1193 | $A_{2g}$ | - | - |
| 1195 | $E_u$ | IR 0.202789 | - |
| 1195 | $B_{1g}$ | Ra c=67.84 | k=5.271, q=0.0263, L=138.4 |
| 1210 | $B_{2g}$ | Ra d=4.87 | k=3.880, q=0.0587, L=227.6 |
| 1277 | $E_u$ | IR 0.226052 | - |
| 1279 | $A_{2g}$ | - | - |
| 1289 | $B_{2g}$ | Ra d=14.26 | k=3.789, q=0.0533, L=202.1 |
| 1328 | $B_{1g}$ | Ra c=238.92 | k=18.812, q=0.0108, L=203.4 |
| 1344 | $E_u$ | IR 1.429662 | - |

| frequency | symmetry | Raman or Infra red intensity | Jahn-Teller parameters |
|---|---|---|---|
| 1379 | $A_{1g}$ | Ra a=200.59, b=2.08 | k=23.275, q=0.0048(0.0060), L=112.6(140.5) |
| 1403 | $E_u$ | IR 0.729572 | - |
| 1406 | $B_{1g}$ | Ra c=29.48 | k=10.570, q=0.0170, L=180.0 |
| 1407 | $A_{1g}$ | Ra a=29.84, b=2.56 | k=5.630, q=0.0019(0.0017), L=10.6(9.7) |
| 1411 | $E_u$ | IR 0.654896 | - |
| 1437 | $A_{1g}$ | Ra a=21.46, b=2.21 | k=16.936, q=0.0013(0.0014), L=16.9(16.9) |
| 1443 | $B_{1g}$ | Ra c=33.20 | k=7.829, q=0.0373, L=292.7 |
| 1447 | $B_{2g}$ | Ra d=37.92 | k=14.366, q=0.0223, L=320.7 |
| 1467 | $A_{2g}$ | - | - |
| 1467 | $E_u$ | IR 0.492994 | - |
| 1477 | $B_{2g}$ | Ra d=27.75 | k=9.204, q=0.0013, L=12.0 |
| 1492 | $E_u$ | IR 0.761032 | - |
| 1518 | $A_{2g}$ | - | - |
| 1521 | $A_{1g}$ | Ra a=74.16, b=-1.94 | k=23.937, q=0.0139(0.0123), L=332.2(295.3) |
| 1533 | $E_u$ | IR 0.132082 | - |
| 1587 | $B_{1g}$ | Ra c=405.18 | k=29.069, q=0.0443, L=1287.6 |
| 1604 | $E_u$ | IR 0.024565 | - |
| 1606 | $B_{1g}$ | Ra c=40.20 | k=21.857, q=0.0176, L=358.3 |
| 1606 | $A_{1g}$ | Ra a=19.89, b=-1.94 | k=20.514, q=0.0038(0.0040), L=77.7 (81.4) |
| 1628 | $A_{2g}$ | - | - |
| 1630 | $E_u$ | IR 0.338197 | - |
| 1632 | $B_{2g}$ | Ra d=6.60 | k=22.065, q=0.0067, L=148.2 |
| 3076 | $B_{2g}$ | Ra d=28.26 | k=10.577, q=0.0000, L=0.0 |
| 3076 | $A_{2g}$ | - | - |
| 3076 | $E_u$ | IR 0.101160 | - |
| 3086 | $A_{1g}$ | Ra a=27.38, b=-0.46 | k=10.684, q=0.000, L=0.0 |
| 3086 | $B_{1g}$ | Ra c=46.79 | k=10.683, q=0.000, L=0.0 |
| 3087 | $E_u$ | IR 0.141285 | - |
| 3096 | $A_{2g}$ | - | - |
| 3096 | $E_u$ | IR 0.051209 | - |
| 3097 | $B_{2g}$ | Ra d=39.61 | k=10.812, q=0.000, L=0.0 |
| 3101 | $B_{1g}$ | Ra c=52.22 | k=10.889, q=0.000, L=0.0 |
| 3102 | $A_{1g}$ | Ra a=88.43, b=8.62 | k=10.892, q=0.000, L=0.0 |
| 3103 | $E_u$ | IR 0.401503 | - |

TABLE I: Vibration spectra of MgPc neutral molecule. In the first column is energy of the vibration in $cm^{-1}$, next column is assignment of irreducible representation of the mode (we note that $E_g$ and $E_u$ modes are two–fold degenerated), then Raman tensor components for Raman active modes and induced dipole momenta per displacement amplitude for infra–red active modes. Atomic units are used (Ry for energy, e for charge, $a_0$ for distance and amu for mass). Notation of tensor components follows equation (5) in the paper. Last column contains parameters for linear Jahn-Teller effect - force constant $k$ in $eV/a_0^2$, displacement $q$ after addition of one electron in $a_0$, linear coupling constant $L$ in $eV/a_0$. For $A_{1g}$ modes is possible to obtain coupling constants from the position of the minima as well as from the saddle point (in brackets).

| freq. | sym. | Ra or IR |
|---|---|---|
| 2.56i | $A_{2u}$ | IR 1.13 |
| 0.19i | $E_g$ | Ra -0.05, -0.18 |
| 0.11i | $B_{1u}$ | - |
| 0.11i | $A_{1u}$ | - |
| 0.08i | $B_{2u}$ | - |
| 0.06i | $E_g$ | Ra 1.59, -2.46 |
| 93 | $E_u$ | IR 0.26 |
| 103 | $B_{2g}$ | Ra -16.89 |
| 137 | $A_{2u}$ | IR 1.28 |
| 178 | $B_{2u}$ | - |
| 178 | $B_{1g}$ | Ra 60.14 |
| 201 | $A_{2g}$ | - |
| 205 | $B_{1u}$ | - |
| 218 | $E_g$ | Ra 0.18, 0.06 |
| 221 | $B_{2g}$ | Ra 44.78 |
| 224 | $A_{1g}$ | Ra 61.08, 4.81 |
| 242 | $B_{2u}$ | - |
| 244 | $A_{2u}$ | IR 0.52 |
| 269 | $E_u$ | IR 0.38 |
| 271 | $E_g$ | Ra 1.02, 0.06 |
| 347 | $A_{2u}$ | IR 0.38 |
| 363 | $A_{2u}$ | IR 0.66 |
| 414 | $E_g$ | Ra -0.01, -0.01 |
| 416 | $A_{1u}$ | - |
| 422 | $E_u$ | IR 0.09 |
| 423 | $B_{2u}$ | - |
| 475 | $B_{2g}$ | Ra -24.81 |
| 494 | $E_g$ | Ra -0.04, 0.06 |
| 505 | $E_u$ | IR 0.85 |
| 527 | $B_{1u}$ | - |
| 565 | $A_{2u}$ | IR 1.23 |
| 568 | $B_{1g}$ | Ra -34.79 |
| 575 | $A_{2g}$ | - |
| 578 | $E_u$ | IR 0.46 |
| 586 | $A_{1g}$ | Ra -11.35, 1.17 |
| 612 | $A_{2g}$ | - |
| 630 | $A_{1u}$ | - |
| 635 | $E_g$ | Ra -1.14, -1.36 |
| 645 | $E_u$ | IR 0.23 |
| 665 | $E_g$ | Ra -0.69, 2.44 |
| 678 | $A_{1g}$ | Ra -8.15, -4.12 |
| 685 | $B_{2g}$ | Ra -15.83 |
| 686 | $B_{1u}$ | - |
| 697 | $B_{2u}$ | - |
| 733 | $B_{1g}$ | Ra -77.01 |
| 757 | $E_u$ | IR 1.58 |
| 764 | $B_{2u}$ | - |
| 772 | $E_g$ | Ra 4.70, 0.27 |
| 774 | $A_{2u}$ | IR 0.84 |
| 793 | $A_{1u}$ | - |
| 795 | $B_{1u}$ | - |
| 795 | $E_g$ | Ra -1.50, 1.50 |
| 800 | $B_{1g}$ | Ra 14.92 |
| 812 | $E_u$ | IR 0.44 |
| 841 | $A_{1g}$ | Ra -41.84, -6.31 |
| 848 | $A_{2g}$ | - |
| 861 | $B_{1u}$ | - |
| 862 | $A_{1u}$ | - |
| 864 | $E_g$ | Ra 0.65, -0.07 |
| 893 | $E_u$ | IR 0.48 |
| 926 | $B_{2g}$ | Ra 8.25 |
| 935 | $A_{2u}$ | IR 0.05 |
| 938 | $E_g$ | Ra -0.06, -2.10 |
| 938 | $B_{2u}$ | - |
| 964 | $A_{1u}$ | - |
| 965 | $E_g$ | Ra -0.04, 0.18 |
| 965 | $B_{1u}$ | - |
| 984 | $A_{1g}$ | Ra -29.91, -3.34 |
| 991 | $B_{1g}$ | Ra 17.24 |
| 995 | $E_u$ | IR 0.73 |
| 1030 | $B_{2g}$ | Ra 3.89 |
| 1068 | $E_u$ | IR 0.98 |
| 1084 | $A_{2g}$ | - |
| 1090 | $B_{2g}$ | Ra 18.31 |
| 1098 | $E_u$ | IR 0.81 |
| 1099 | $B_{1g}$ | Ra -20.20 |
| 1116 | $A_{1g}$ | Ra -15.33, -2.04 |
| 1120 | $E_u$ | IR 0.17 |
| 1152 | $A_{1g}$ | Ra -32.35, -2.26 |
| 1158 | $A_{2g}$ | - |
| 1177 | $B_{1g}$ | Ra 46.43 |
| 1183 | $E_u$ | IR 1.50 |
| 1187 | $B_{2g}$ | Ra 4.03 |
| 1205 | $E_u$ | IR 0.08 |
| 1208 | $A_{2g}$ | - |
| 1263 | $B_{2g}$ | Ra 9.15 |
| 1272 | $E_u$ | IR 0.19 |
| 1275 | $A_{2g}$ | - |
| 1289 | $B_{1g}$ | Ra -160.27 |
| 1329 | $E_u$ | IR 0.31 |
| 1350 | $B_{1g}$ | Ra 44.86 |
| 1369 | $A_{1g}$ | Ra -163.90, -1.86 |
| 1399 | $E_u$ | IR 0.22 |
| 1404 | $A_{1g}$ | Ra 32.46, 2.77 |
| 1405 | $B_{1g}$ | Ra -0.52 |
| 1412 | $E_u$ | IR 1.65 |
| 1433 | $B_{2g}$ | Ra -32.17 |
| 1433 | $A_{1g}$ | Ra 60.48, 3.89 |
| 1466 | $E_u$ | IR 1.32 |
| 1469 | $A_{2g}$ | - |
| 1480 | $B_{2g}$ | Ra 28.56 |
| 1482 | $B_{1g}$ | Ra 57.07 |
| 1487 | $E_u$ | IR 2.36 |
| 1515 | $A_{1g}$ | Ra 57.82, -3.10 |
| 1518 | $E_u$ | IR 0.67 |
| 1520 | $A_{2g}$ | - |
| 1590 | $B_{1g}$ | Ra 72.49 |
| 1590 | $E_u$ | IR 0.93 |
| 1593 | $A_{1g}$ | Ra -53.02, 1.89 |
| 1612 | $A_{2g}$ | - |
| 1615 | $E_u$ | IR 0.38 |
| 1616 | $B_{2g}$ | Ra -23.29 |
| 3061 | $A_{2g}$ | - |
| 3061 | $E_u$ | IR 0.17 |
| 3061 | $B_{2g}$ | Ra 35.39 |
| 3075 | $E_u$ | IR 0.29 |
| 3075 | $B_{1g}$ | Ra -59.18 |
| 3076 | $A_{1g}$ | Ra -45.11, -0.61 |
| 3092 | $B_{2g}$ | Ra 38.26 |
| 3093 | $E_u$ | IR 0.51 |
| 3094 | $A_{1g}$ | Ra 84.52, 7.69 |
| 3095 | $B_{1g}$ | Ra 48.02 |
| 3098 | $E_u$ | IR 0.36 |
| 3100 | $A_{2g}$ | - |

TABLE II: Vibration spectra of symmetrized $D_{4h}$ $MgPc^-$ anion.

| freq. | sym. | Ra or IR | 679 | $B_{1g}$ | Ra -54.28 | | | |
|---|---|---|---|---|---|---|---|---|
| 1.85i | $B_{1u}$ | IR 1.13 | 684 | $B_{1u}$ | IR 0.18 | 1199 | $B_{1g}$ | Ra 5.39 |
| 0.66i | $A_u$ | - | 723 | $B_{3g}$ | Ra 0.77 | 1200 | $B_{3u}$ | IR 0.82 |
| 0.64i | $B_{3g}$ | Ra -2.61 | 747 | $B_{1u}$ | IR 0.25 | 1252 | $B_{1g}$ | Ra 17.03 |
| 0.27i | $B_{1u}$ | IR 0.46 | 749 | $A_u$ | - | 1270 | $B_{3u}$ | IR 0.23 |
| 0.19i | $B_{2g}$ | Ra 0.84 | 750 | $B_{2g}$ | Ra 3.37 | 1277 | $B_{2u}$ | IR 0.77 |
| 0.13i | $A_u$ | - | 751 | $B_{3u}$ | IR 1.48 | 1280 | $B_{1g}$ | Ra -2.33 |
| 112 | $B_{1g}$ | Ra 29.50 | 754 | $B_{2u}$ | IR 1.46 | 1307 | $A_g$ | Ra 107.81, -285.42, 7.08 |
| 113 | $B_{3u}$ | IR 0.29 | 755 | $A_g$ | Ra -2.30, -63.88, 7.30 | 1315 | $B_{2u}$ | IR 0.25 |
| 115 | $B_{1u}$ | IR 1.05 | 760 | $B_{3g}$ | Ra 1.52 | 1338 | $B_{3u}$ | IR 0.36 |
| 119 | $B_{2u}$ | IR 0.34 | 773 | $B_{1u}$ | IR 0.45 | 1366 | $A_g$ | Ra 137.39, 124.04, -5.92 |
| 133 | $B_{2g}$ | Ra -5.33 | 783 | $B_{3g}$ | Ra -3.03 | 1394 | $B_{3u}$ | IR 0.14 |
| 165 | $A_u$ | - | 784 | $B_{1g}$ | Ra -487.12 | 1394 | $A_g$ | Ra -25.24, -7.92, -4.09 |
| 174 | $B_{1g}$ | Ra -49.67 | 789 | $A_g$ | Ra 24.12, 8.67, -4.02 | 1395 | $B_{2u}$ | IR 1.98 |
| 176 | $A_g$ | Ra -59.94, 58.78, 0.33 | 796 | $A_u$ | - | 1404 | $B_{2u}$ | IR 0.79 |
| 180 | $B_{1u}$ | IR 0.64 | 799 | $B_{2g}$ | Ra 0.99 | 1406 | $B_{1g}$ | Ra -47.32 |
| 191 | $B_{3g}$ | Ra 0.36 | 804 | $B_{3u}$ | IR 0.80 | 1408 | $A_g$ | Ra -45.71, -42.31, 0.42 |
| 195 | $B_{3g}$ | Ra -3.06 | 814 | $B_{2u}$ | IR 0.04 | 1424 | $B_{3u}$ | IR 1.90 |
| 201 | $B_{1g}$ | Ra 7.09 | 829 | $A_g$ | Ra 34.44, 46.85, 8.85 | 1432 | $A_g$ | Ra 28.86, -1.99, 10.80 |
| 205 | $B_{1u}$ | IR 0.58 | 837 | $A_u$ | - | 1442 | $A_g$ | Ra 61.72, 64.28, -7.51 |
| 212 | $B_{3g}$ | Ra 3.79 | 839 | $B_{3g}$ | Ra -0.08 | 1461 | $B_{2u}$ | IR 1.47 |
| 214 | $B_{2g}$ | Ra 5.74 | 841 | $B_{1g}$ | Ra -0.97 | 1462 | $B_{3u}$ | IR 2.60 |
| 225 | $A_g$ | Ra -63.40, -55.35, -0.51 | 864 | $A_u$ | - | 1466 | $B_{1g}$ | Ra -7.29 |
| 249 | $B_{1u}$ | IR 0.63 | 865 | $B_{2g}$ | Ra -0.45 | 1472 | $B_{3u}$ | IR 1.16 |
| 261 | $B_{2g}$ | Ra 1.63 | 889 | $B_{2u}$ | IR 0.87 | 1480 | $B_{1g}$ | Ra -30.81 |
| 284 | $B_{2u}$ | IR 0.48 | 894 | $B_{3u}$ | IR 0.09 | 1485 | $B_{2u}$ | IR 0.87 |
| 293 | $B_{3u}$ | IR 0.23 | 906 | $B_{1u}$ | IR 0.18 | 1506 | $A_g$ | Ra 40.75, -99.25, 8.09 |
| 323 | $B_{1u}$ | IR 0.27 | 919 | $A_u$ | - | 1526 | $B_{3u}$ | IR 1.72 |
| 324 | $A_u$ | - | 923 | $B_{3g}$ | Ra -0.35 | 1533 | $B_{1g}$ | Ra 102.84 |
| 328 | $B_{1u}$ | IR 0.60 | 932 | $B_{1u}$ | IR 0.05 | 1547 | $B_{2u}$ | IR 1.65 |
| 356 | $B_{3g}$ | Ra -2.44 | 934 | $B_{3g}$ | Ra -0.95 | 1577 | $B_{3u}$ | IR 0.96 |
| 364 | $B_{2g}$ | Ra -0.89 | 934 | $B_{2g}$ | Ra -1.48 | 1577 | $A_g$ | Ra 81.15, -95.85, 8.42 |
| 402 | $B_{1g}$ | Ra 171.94 | 963 | $A_u$ | - | 1592 | $A_g$ | Ra 196.21, 527.85, -48.35 |
| 415 | $B_{1u}$ | IR 0.13 | 964 | $B_{2g}$ | Ra 0.82 | 1599 | $B_{2u}$ | IR 0.67 |
| 421 | $B_{3u}$ | IR 0.26 | 979 | $B_{1g}$ | Ra -266.85 | 1602 | $A_g$ | Ra -68.87, -123.31, 21.10 |
| 423 | $B_{3g}$ | Ra 0.32 | 993 | $B_{3u}$ | IR 0.77 | 1612 | $B_{1g}$ | Ra 45.58 |
| 428 | $B_{2u}$ | IR 0.03 | 995 | $A_g$ | Ra -36.18, -3.72, -0.44 | 1614 | $B_{2u}$ | IR 0.76 |
| 468 | $A_u$ | - | 1000 | $B_{2u}$ | IR 0.51 | 1618 | $B_{1g}$ | Ra -114.80 |
| 500 | $B_{3u}$ | IR 1.09 | 1001 | $A_g$ | Ra 9.82, 26.07, 2.49 | 1624 | $B_{3u}$ | IR 0.14 |
| 500 | $B_{2g}$ | Ra 0.31 | 1038 | $B_{1g}$ | Ra -37.21 | 3071 | $B_{1g}$ | Ra -12.41 |
| 504 | $B_{2u}$ | IR 0.56 | 1052 | $B_{2u}$ | IR 0.98 | 3071 | $B_{2u}$ | IR 0.06 |
| 550 | $A_g$ | Ra -38.21, 30.43, 3.29 | 1062 | $B_{3u}$ | IR 0.52 | 3074 | $B_{3u}$ | IR 0.18 |
| 555 | $B_{1u}$ | IR 1.13 | 1073 | $B_{1g}$ | Ra -0.42 | 3074 | $B_{1g}$ | Ra -8.79 |
| 565 | $B_{3g}$ | Ra -1.11 | 1096 | $B_{2u}$ | IR 0.63 | 3075 | $B_{3u}$ | IR 0.26 |
| 572 | $B_{3u}$ | IR 0.36 | 1097 | $B_{3u}$ | IR 1.39 | 3077 | $A_g$ | Ra -64.26, 38.52, 0.92 |
| 575 | $B_{1g}$ | Ra 18.32 | 1110 | $B_{1g}$ | Ra 36.26 | 3079 | $B_{1g}$ | Ra 8.77 |
| 576 | $A_u$ | - | 1116 | $A_g$ | Ra 20.21, 2.49, 2.47 | 3080 | $B_{2u}$ | IR 0.09 |
| 578 | $B_{2u}$ | IR 0.54 | 1120 | $B_{3u}$ | IR 0.01 | 3081 | $B_{2u}$ | IR 0.45 |
| 593 | $A_g$ | Ra -1.60, -26.25, -12.45 | 1123 | $A_g$ | Ra 20.12, 26.09, -1.83 | 3082 | $A_g$ | Ra 15.83, -57.72, 1.06 |
| 611 | $B_{1g}$ | Ra 0.30 | 1123 | $B_{2u}$ | IR 0.40 | 3082 | $B_{3u}$ | IR 0.31 |
| 612 | $B_{2g}$ | Ra -3.34 | 1153 | $B_{1g}$ | Ra 4.70 | 3087 | $B_{1g}$ | Ra 42.82 |
| 634 | $B_{3u}$ | IR 0.33 | 1153 | $A_g$ | Ra -20.41, -31.20, 0.17 | 3090 | $B_{3u}$ | IR 0.57 |
| 647 | $B_{2u}$ | IR 0.13 | 1181 | $B_{2u}$ | IR 1.57 | 3092 | $B_{2u}$ | IR 0.55 |
| 659 | $B_{2g}$ | Ra -2.78 | 1188 | $B_{3u}$ | IR 0.84 | 3093 | $A_g$ | Ra 42.71, -40.08, 0.38 |
| 667 | $A_g$ | Ra 16.86, 8.92, 8.92 | 1191 | $A_g$ | Ra 30.13, -74.43, 4.83 | 3096 | $A_g$ | Ra 96.27, 90.82, 8.07 |
| 677 | $A_u$ | - | 1197 | $B_{2u}$ | IR 0.74 | | | |

TABLE III: Vibration frequencies, symmetry and Raman tensor components or induced dipole moment for $MgPc^{-}$ Jahn–Teller distorted $D_{2h}$ anion.