
 TD-DFT/TDA EXCITED STATES

the weight of the individual excitations are printed if larger than 1.0e-02

STATE 1: E= 0.104081 au 2.832 eV 22843.0 cm⁻¹ <S²> = 9.547072
 205a -> 212a : 0.013482 (c= 0.11611288)
 209a -> 212a : 0.099537 (c= -0.31549488)
 210a -> 211a : 0.582352 (c= -0.76311963)
 210a -> 213a : 0.138182 (c= 0.37172823)
 205b -> 207b : 0.014230 (c= -0.11928856)

STATE 2: E= 0.105900 au 2.882 eV 23242.4 cm⁻¹ <S²> = 9.600350
 205a -> 213a : 0.014695 (c= 0.12122263)
 209a -> 211a : 0.292572 (c= 0.54089903)
 209a -> 213a : 0.167606 (c= 0.40939693)
 210a -> 212a : 0.322574 (c= 0.56795606)
 210a -> 214a : 0.014193 (c= 0.11913446)
 202b -> 206b : 0.023028 (c= -0.15175000)
 204b -> 207b : 0.010120 (c= 0.10059691)
 205b -> 208b : 0.015685 (c= 0.12524079)

STATE 3: E= 0.108836 au 2.962 eV 23886.8 cm⁻¹ <S²> = 9.555729
 207a -> 213a : 0.023731 (c= 0.15404751)
 209a -> 211a : 0.011810 (c= -0.10867461)
 209a -> 212a : 0.047900 (c= 0.21886143)
 209a -> 213a : 0.026663 (c= -0.16328666)
 209a -> 214a : 0.016227 (c= 0.12738616)
 209a -> 215a : 0.068363 (c= -0.26146375)
 210a -> 211a : 0.068615 (c= 0.26194393)
 210a -> 212a : 0.041855 (c= 0.20458541)
 210a -> 213a : 0.501826 (c= 0.70839690)
 203b -> 206b : 0.012406 (c= 0.11138379)
 204b -> 206b : 0.015828 (c= -0.12580827)

STATE 4: E= 0.109850 au 2.989 eV 24109.3 cm⁻¹ <S²> = 9.623078
 208a -> 212a : 0.015648 (c= -0.12509143)
 209a -> 211a : 0.138137 (c= 0.37166775)
 209a -> 212a : 0.201274 (c= -0.44863622)
 209a -> 213a : 0.016864 (c= 0.12986291)
 209a -> 214a : 0.031266 (c= 0.17682065)
 209a -> 216a : 0.017618 (c= 0.13273400)
 210a -> 211a : 0.084002 (c= 0.28983079)
 210a -> 212a : 0.128870 (c= -0.35898476)
 210a -> 213a : 0.046454 (c= 0.21553213)
 210a -> 214a : 0.020263 (c= -0.14234694)
 210a -> 215a : 0.032738 (c= -0.18093564)
 210a -> 216a : 0.032500 (c= -0.18027655)
 203b -> 207b : 0.010628 (c= -0.10309058)
 205b -> 206b : 0.011443 (c= 0.10697129)

STATE 5: E= 0.110403 au 3.004 eV 24230.8 cm⁻¹ <S²> = 9.673010
 208a -> 211a : 0.012300 (c= 0.11090452)

208a -> 213a : 0.013988 (c= -0.11827121)
 209a -> 211a : 0.145831 (c= 0.38187861)
 209a -> 212a : 0.267165 (c= 0.51688025)
 209a -> 214a : 0.015331 (c= -0.12381654)
 210a -> 211a : 0.029516 (c= -0.17180077)
 210a -> 212a : 0.106760 (c= -0.32674186)
 210a -> 214a : 0.059731 (c= -0.24439983)
 210a -> 215a : 0.030521 (c= -0.17470300)
 210a -> 216a : 0.051980 (c= 0.22799018)
 201b -> 207b : 0.012374 (c= -0.11123830)
 204b -> 210b : 0.011442 (c= -0.10696799)
 205b -> 207b : 0.011383 (c= -0.10669304)
 205b -> 210b : 0.013024 (c= -0.11412247)

STATE 6: E= 0.110943 au 3.019 eV 24349.2 cm⁻¹ <S²> = 9.778646

205a -> 211a : 0.012978 (c= -0.11392092)
 207a -> 212a : 0.012720 (c= -0.11278459)
 209a -> 211a : 0.068546 (c= 0.26181220)
 209a -> 212a : 0.039174 (c= -0.19792515)
 209a -> 213a : 0.438332 (c= -0.66206669)
 209a -> 216a : 0.021285 (c= 0.14589530)
 210a -> 212a : 0.080216 (c= 0.28322413)
 210a -> 213a : 0.019909 (c= -0.14109810)
 210a -> 214a : 0.030757 (c= -0.17537710)
 201b -> 206b : 0.029631 (c= 0.17213650)
 202b -> 208b : 0.030538 (c= 0.17475077)
 204b -> 207b : 0.018778 (c= 0.13703300)
 204b -> 209b : 0.018786 (c= 0.13706102)
 205b -> 206b : 0.013430 (c= -0.11588979)

STATE 7: E= 0.118768 au 3.232 eV 26066.5 cm⁻¹ <S²> = 9.377061

205a -> 216a : 0.012458 (c= -0.11161321)
 209a -> 211a : 0.190575 (c= -0.43654932)
 209a -> 213a : 0.063853 (c= 0.25269082)
 209a -> 216a : 0.025492 (c= 0.15966140)
 210a -> 212a : 0.163835 (c= 0.40476498)
 210a -> 214a : 0.303037 (c= -0.55048815)
 210a -> 215a : 0.092831 (c= -0.30468111)

STATE 8: E= 0.120141 au 3.269 eV 26367.9 cm⁻¹ <S²> = 9.495268

205a -> 215a : 0.015891 (c= 0.12606132)
 209a -> 212a : 0.078095 (c= -0.27945512)
 209a -> 214a : 0.212815 (c= -0.46131837)
 209a -> 215a : 0.127107 (c= 0.35652131)
 210a -> 211a : 0.128548 (c= 0.35853546)
 210a -> 213a : 0.111020 (c= 0.33319683)
 210a -> 215a : 0.019412 (c= 0.13932699)
 210a -> 216a : 0.100292 (c= 0.31668972)
 202b -> 209b : 0.014346 (c= 0.11977504)
 203b -> 208b : 0.010513 (c= -0.10253055)
 205b -> 211b : 0.011215 (c= 0.10589989)

STATE 9: E= 0.120886 au 3.289 eV 26531.4 cm⁻¹ <S²> = 9.429304

205a -> 214a : 0.015065 (c= -0.12273828)

209a -> 212a : 0.109119 (c= 0.33033186)
 209a -> 213a : 0.015931 (c= -0.12621795)
 209a -> 215a : 0.216157 (c= 0.46492685)
 210a -> 211a : 0.011825 (c= -0.10874092)
 210a -> 212a : 0.012600 (c= 0.11225015)
 210a -> 213a : 0.105616 (c= 0.32498574)
 210a -> 216a : 0.335811 (c= -0.57949221)
 202b -> 211b : 0.010088 (c= -0.10044077)
 205b -> 207b : 0.012316 (c= 0.11097695)
 205b -> 209b : 0.010418 (c= -0.10207072)

STATE 10: E= 0.125409 au 3.413 eV 27524.2 cm⁻¹ <S²> = 9.273796

207a -> 215a : 0.011800 (c= -0.10862894)
 209a -> 211a : 0.027542 (c= -0.16595662)
 209a -> 213a : 0.077054 (c= -0.27758609)
 209a -> 215a : 0.017063 (c= 0.13062522)
 209a -> 219a : 0.015877 (c= 0.12600560)
 210a -> 214a : 0.249427 (c= 0.49942703)
 210a -> 215a : 0.457940 (c= -0.67671248)

STATE 11: E= 0.127364 au 3.466 eV 27953.3 cm⁻¹ <S²> = 9.385511

208a -> 214a : 0.012980 (c= -0.11392925)
 209a -> 211a : 0.013168 (c= 0.11475115)
 209a -> 212a : 0.041664 (c= -0.20411823)
 209a -> 214a : 0.316488 (c= -0.56257297)
 209a -> 215a : 0.176450 (c= -0.42005993)
 209a -> 216a : 0.041834 (c= -0.20453279)
 210a -> 211a : 0.018683 (c= -0.13668444)
 210a -> 214a : 0.014325 (c= -0.11968518)
 210a -> 215a : 0.030403 (c= -0.17436388)
 210a -> 216a : 0.098631 (c= -0.31405646)
 210a -> 217a : 0.015878 (c= 0.12600935)
 210a -> 219a : 0.013385 (c= 0.11569457)
 204b -> 206b : 0.012155 (c= -0.11024787)

STATE 12: E= 0.128013 au 3.483 eV 28095.6 cm⁻¹ <S²> = 9.485720

207a -> 212a : 0.011478 (c= -0.10713620)
 208a -> 216a : 0.019791 (c= 0.14068164)
 209a -> 211a : 0.042278 (c= -0.20561645)
 209a -> 213a : 0.035374 (c= 0.18808060)
 209a -> 214a : 0.069865 (c= -0.26432013)
 209a -> 215a : 0.021054 (c= -0.14509828)
 209a -> 216a : 0.408736 (c= 0.63932498)
 209a -> 217a : 0.012458 (c= 0.11161747)
 210a -> 212a : 0.043170 (c= -0.20777317)
 210a -> 214a : 0.017853 (c= 0.13361370)
 210a -> 215a : 0.016736 (c= 0.12936890)
 210a -> 218a : 0.047031 (c= 0.21686604)
 204b -> 207b : 0.025588 (c= 0.15996186)

STATE 13: E= 0.137850 au 3.751 eV 30254.5 cm⁻¹ <S²> = 9.751905

198a -> 212a : 0.010153 (c= -0.10076411)
 208a -> 211a : 0.071246 (c= -0.26691965)
 208a -> 213a : 0.015277 (c= 0.12360092)

208a -> 216a : 0.010275 (c= 0.10136634)
 209a -> 214a : 0.011778 (c= 0.10852700)
 209a -> 219a : 0.016411 (c= 0.12810369)
 210a -> 212a : 0.016407 (c= -0.12808816)
 210a -> 214a : 0.195297 (c= -0.44192441)
 210a -> 215a : 0.059754 (c= -0.24444641)
 210a -> 216a : 0.032383 (c= 0.17995381)
 210a -> 218a : 0.115476 (c= 0.33981815)
 194b -> 207b : 0.023450 (c= -0.15313276)
 201b -> 206b : 0.015117 (c= -0.12295018)
 201b -> 207b : 0.013582 (c= 0.11654007)
 203b -> 207b : 0.032771 (c= 0.18102719)
 205b -> 207b : 0.015196 (c= 0.12327030)
 205b -> 208b : 0.037708 (c= 0.19418644)
 205b -> 210b : 0.013873 (c= 0.11778414)

STATE 14: E= 0.138465 au 3.768 eV 30389.5 cm**-1 <S**2> = 9.781963

197a -> 211a : 0.013367 (c= -0.11561548)
 198a -> 211a : 0.010259 (c= -0.10128635)
 207a -> 211a : 0.023944 (c= 0.15473892)
 208a -> 212a : 0.062948 (c= -0.25089425)
 209a -> 212a : 0.056187 (c= 0.23703842)
 209a -> 214a : 0.153087 (c= -0.39126329)
 209a -> 215a : 0.051404 (c= -0.22672523)
 209a -> 218a : 0.019722 (c= -0.14043568)
 210a -> 216a : 0.045993 (c= 0.21445902)
 210a -> 217a : 0.079104 (c= -0.28125426)
 210a -> 218a : 0.027277 (c= -0.16515650)
 210a -> 219a : 0.029072 (c= -0.17050466)
 194b -> 206b : 0.014644 (c= 0.12101431)
 194b -> 208b : 0.015046 (c= -0.12266108)
 201b -> 207b : 0.050377 (c= 0.22444807)
 202b -> 207b : 0.013474 (c= -0.11607791)
 204b -> 206b : 0.019545 (c= 0.13980515)
 204b -> 208b : 0.013868 (c= -0.11776082)
 205b -> 207b : 0.018509 (c= 0.13604951)

STATE 15: E= 0.138715 au 3.775 eV 30444.3 cm**-1 <S**2> = 9.659082

197a -> 211a : 0.010981 (c= 0.10478978)
 208a -> 212a : 0.031563 (c= 0.17765872)
 208a -> 214a : 0.014351 (c= 0.11979399)
 208a -> 215a : 0.012276 (c= 0.11079583)
 209a -> 214a : 0.039586 (c= -0.19896326)
 209a -> 216a : 0.011025 (c= 0.10499967)
 209a -> 217a : 0.012918 (c= 0.11365686)
 209a -> 218a : 0.028252 (c= -0.16808292)
 210a -> 211a : 0.024504 (c= 0.15653811)
 210a -> 213a : 0.017672 (c= -0.13293563)
 210a -> 214a : 0.021909 (c= -0.14801584)
 210a -> 215a : 0.012374 (c= -0.11123701)
 210a -> 216a : 0.205820 (c= -0.45367360)
 210a -> 217a : 0.092227 (c= -0.30368834)
 210a -> 219a : 0.062093 (c= -0.24918562)
 194b -> 208b : 0.010610 (c= 0.10300277)

203b -> 206b : 0.027050 (c= 0.16446837)
 203b -> 208b : 0.010114 (c= -0.10056624)
 205b -> 206b : 0.016566 (c= -0.12871066)
 205b -> 207b : 0.050471 (c= -0.22465694)

STATE 16: E= 0.139609 au 3.799 eV 30640.7 cm⁻¹ <S²> = 9.486102

207a -> 212a : 0.013024 (c= 0.11412131)
 208a -> 211a : 0.022050 (c= -0.14849240)
 209a -> 213a : 0.011476 (c= -0.10712491)
 209a -> 215a : 0.017148 (c= 0.13095178)
 209a -> 216a : 0.235798 (c= 0.48559067)
 209a -> 217a : 0.118846 (c= -0.34474116)
 210a -> 215a : 0.034911 (c= 0.18684371)
 210a -> 217a : 0.026327 (c= 0.16225519)
 210a -> 218a : 0.258089 (c= -0.50802479)

STATE 17: E= 0.139789 au 3.804 eV 30680.1 cm⁻¹ <S²> = 9.672542

205a -> 213a : 0.016860 (c= 0.12984527)
 207a -> 214a : 0.018867 (c= 0.13735877)
 207a -> 215a : 0.020739 (c= -0.14401151)
 208a -> 213a : 0.021311 (c= -0.14598413)
 209a -> 211a : 0.029559 (c= -0.17192774)
 209a -> 213a : 0.038646 (c= -0.19658527)
 209a -> 216a : 0.064183 (c= -0.25334440)
 209a -> 217a : 0.060304 (c= -0.24556789)
 209a -> 219a : 0.147668 (c= 0.38427612)
 210a -> 214a : 0.025782 (c= -0.16056811)
 210a -> 215a : 0.133982 (c= 0.36603530)
 210a -> 218a : 0.011136 (c= 0.10552637)
 201b -> 208b : 0.024694 (c= -0.15714344)
 202b -> 206b : 0.034387 (c= -0.18543622)
 204b -> 207b : 0.016807 (c= 0.12964151)
 205b -> 206b : 0.023688 (c= 0.15390946)

STATE 18: E= 0.139907 au 3.807 eV 30706.1 cm⁻¹ <S²> = 9.840150

196a -> 213a : 0.023035 (c= -0.15177353)
 197a -> 213a : 0.023405 (c= 0.15298801)
 207a -> 211a : 0.026109 (c= 0.16158246)
 207a -> 213a : 0.084784 (c= 0.29117619)
 209a -> 214a : 0.069394 (c= -0.26342732)
 209a -> 215a : 0.226737 (c= 0.47616960)
 209a -> 216a : 0.015974 (c= -0.12638971)
 209a -> 217a : 0.010906 (c= 0.10443348)
 209a -> 220a : 0.016219 (c= 0.12735479)
 210a -> 213a : 0.012249 (c= -0.11067646)
 210a -> 218a : 0.012449 (c= 0.11157549)
 192b -> 208b : 0.010379 (c= 0.10187835)
 194b -> 206b : 0.030985 (c= 0.17602678)
 194b -> 208b : 0.020399 (c= 0.14282344)
 203b -> 206b : 0.020572 (c= 0.14342976)
 203b -> 208b : 0.024850 (c= 0.15763942)
 204b -> 206b : 0.046871 (c= -0.21649689)
 204b -> 208b : 0.032327 (c= -0.17979710)

STATE 19: E= 0.144828 au 3.941 eV 31786.0 cm⁻¹ <S²> = 9.584921

| | | |
|----------------|----------|------------------|
| 189a -> 211a : | 0.010224 | (c= 0.10111152) |
| 205a -> 212a : | 0.034658 | (c= 0.18616553) |
| 207a -> 211a : | 0.041840 | (c= 0.20454949) |
| 208a -> 214a : | 0.014072 | (c= 0.11862441) |
| 209a -> 212a : | 0.018790 | (c= 0.13707700) |
| 209a -> 214a : | 0.012295 | (c= -0.11088078) |
| 209a -> 215a : | 0.014415 | (c= -0.12006276) |
| 209a -> 218a : | 0.021619 | (c= 0.14703474) |
| 210a -> 211a : | 0.015159 | (c= 0.12312119) |
| 210a -> 217a : | 0.442743 | (c= 0.66538967) |
| 210a -> 218a : | 0.027205 | (c= 0.16494067) |
| 210a -> 221a : | 0.011087 | (c= 0.10529384) |
| 202b -> 206b : | 0.012294 | (c= -0.11087936) |
| 202b -> 207b : | 0.026222 | (c= -0.16193063) |
| 204b -> 206b : | 0.023541 | (c= 0.15343044) |
| 204b -> 208b : | 0.023055 | (c= -0.15183922) |
| 205b -> 207b : | 0.025886 | (c= -0.16089266) |

STATE 20: E= 0.145906 au 3.970 eV 32022.6 cm⁻¹ <S²> = 9.579615

| | | |
|----------------|----------|------------------|
| 205a -> 213a : | 0.031036 | (c= 0.17617022) |
| 208a -> 211a : | 0.022428 | (c= -0.14976049) |
| 209a -> 211a : | 0.014214 | (c= -0.11922186) |
| 209a -> 216a : | 0.024807 | (c= -0.15750227) |
| 209a -> 217a : | 0.168261 | (c= 0.41019585) |
| 209a -> 219a : | 0.140468 | (c= -0.37479017) |
| 210a -> 217a : | 0.041044 | (c= 0.20259217) |
| 210a -> 218a : | 0.150292 | (c= -0.38767482) |
| 210a -> 219a : | 0.032384 | (c= -0.17995466) |
| 210a -> 220a : | 0.020416 | (c= 0.14288425) |
| 201b -> 208b : | 0.014190 | (c= -0.11912010) |
| 202b -> 206b : | 0.032754 | (c= -0.18098134) |
| 203b -> 207b : | 0.012557 | (c= 0.11205763) |
| 204b -> 207b : | 0.021205 | (c= 0.14562036) |
| 205b -> 208b : | 0.027871 | (c= 0.16694658) |

STATE 21: E= 0.146684 au 3.991 eV 32193.3 cm⁻¹ <S²> = 9.293119

| | | |
|----------------|----------|------------------|
| 209a -> 217a : | 0.026190 | (c= -0.16183295) |
| 209a -> 219a : | 0.013707 | (c= 0.11707867) |
| 209a -> 220a : | 0.051565 | (c= 0.22707957) |
| 210a -> 217a : | 0.059275 | (c= 0.24346394) |
| 210a -> 218a : | 0.024267 | (c= 0.15577768) |
| 210a -> 219a : | 0.665681 | (c= -0.81589292) |

STATE 22: E= 0.148582 au 4.043 eV 32609.9 cm⁻¹ <S²> = 9.323307

| | | |
|----------------|----------|------------------|
| 209a -> 216a : | 0.015180 | (c= -0.12320876) |
| 209a -> 217a : | 0.133216 | (c= 0.36498782) |
| 209a -> 218a : | 0.180883 | (c= -0.42530380) |
| 209a -> 219a : | 0.303823 | (c= 0.55120150) |
| 209a -> 221a : | 0.019058 | (c= -0.13804955) |
| 210a -> 217a : | 0.094073 | (c= 0.30671337) |
| 210a -> 218a : | 0.038172 | (c= -0.19537741) |
| 210a -> 220a : | 0.010615 | (c= -0.10302855) |
| 210a -> 221a : | 0.020994 | (c= 0.14489393) |

STATE 23: E= 0.149141 au 4.058 eV 32732.7 cm**-1 <S**2> = 9.300261
 209a -> 216a : 0.012109 (c= -0.11003884)
 209a -> 217a : 0.013833 (c= 0.11761419)
 209a -> 218a : 0.526817 (c= 0.72582143)
 209a -> 219a : 0.152250 (c= 0.39019220)
 209a -> 222a : 0.014268 (c= -0.11944872)
 210a -> 217a : 0.011006 (c= -0.10491030)
 210a -> 218a : 0.056662 (c= -0.23803881)
 210a -> 222a : 0.054563 (c= -0.23358648)

STATE 24: E= 0.149533 au 4.069 eV 32818.7 cm**-1 <S**2> = 9.625900
 205a -> 211a : 0.059826 (c= -0.24459362)
 207a -> 212a : 0.056718 (c= -0.23815477)
 208a -> 213a : 0.023589 (c= 0.15358595)
 208a -> 216a : 0.024069 (c= 0.15514138)
 209a -> 213a : 0.031707 (c= 0.17806547)
 209a -> 216a : 0.048638 (c= -0.22054099)
 209a -> 217a : 0.228009 (c= -0.47750260)
 209a -> 221a : 0.021574 (c= 0.14687959)
 210a -> 212a : 0.028820 (c= -0.16976576)
 210a -> 215a : 0.047668 (c= -0.21833088)
 210a -> 218a : 0.065560 (c= -0.25604784)
 210a -> 220a : 0.031205 (c= -0.17665078)
 202b -> 208b : 0.024430 (c= 0.15630243)
 204b -> 207b : 0.024620 (c= 0.15690739)
 205b -> 206b : 0.018417 (c= -0.13570784)

 ABSORPTION SPECTRUM VIA TRANSITION ELECTRIC DIPOLE MOMENTS

| State | Energy (cm-1) | Wavelength (nm) | fosc | T2 (au**2) | TX (au) | TY (au) | TZ (au) |
|-------|------------------|--------------------|-------------|---------------|------------|------------|------------|
| 1 | 22843.0 | 437.8 | 0.090156067 | 1.29932 | -0.97610 | -0.15999 | 0.56653 |
| 2 | 23242.4 | 430.2 | 0.066664030 | 0.94425 | -0.52118 | 0.09589 | -0.81451 |
| 3 | 23886.8 | 418.6 | 0.007933201 | 0.10934 | -0.08621 | -0.31590 | 0.04597 |
| 4 | 24109.3 | 414.8 | 0.009789405 | 0.13367 | -0.24637 | 0.12393 | 0.24003 |
| 5 | 24230.8 | 412.7 | 0.007334245 | 0.09965 | 0.25243 | -0.18775 | -0.02601 |
| 6 | 24349.2 | 410.7 | 0.006481930 | 0.08764 | 0.12863 | -0.08768 | 0.25180 |
| 7 | 26066.5 | 383.6 | 0.009359540 | 0.11821 | 0.17119 | -0.05179 | 0.29363 |
| 8 | 26367.9 | 379.2 | 0.008699878 | 0.10862 | 0.27080 | 0.02612 | -0.18602 |
| 9 | 26531.4 | 376.9 | 0.018109963 | 0.22472 | 0.04251 | 0.46652 | 0.07260 |
| 10 | 27524.2 | 363.3 | 0.000083229 | 0.00100 | 0.02739 | 0.01098 | 0.01118 |
| 11 | 27953.3 | 357.7 | 0.000263888 | 0.00311 | -0.02357 | -0.04127 | -0.02914 |
| 12 | 28095.6 | 355.9 | 0.000695486 | 0.00815 | 0.02306 | -0.05073 | 0.07102 |
| 13 | 30254.5 | 330.5 | 0.031208298 | 0.33959 | 0.14475 | -0.23423 | 0.51359 |
| 14 | 30389.5 | 329.1 | 0.034665422 | 0.37553 | 0.37168 | -0.35647 | -0.33214 |
| 15 | 30444.3 | 328.5 | 0.043254026 | 0.46773 | 0.58155 | 0.35922 | -0.02215 |
| 16 | 30640.7 | 326.4 | 0.003342492 | 0.03591 | 0.07531 | 0.00016 | 0.17390 |
| 17 | 30680.1 | 325.9 | 0.022898206 | 0.24571 | 0.29227 | 0.00396 | 0.40034 |
| 18 | 30706.1 | 325.7 | 0.014880147 | 0.15954 | 0.13143 | 0.32949 | -0.18357 |
| 19 | 31786.0 | 314.6 | 0.064801363 | 0.67116 | 0.75192 | 0.06341 | -0.31899 |
| 20 | 32022.6 | 312.3 | 0.039793503 | 0.40910 | 0.10826 | -0.10681 | 0.62127 |

| | | | | | | | |
|----|---------|-------|-------------|---------|----------|----------|----------|
| 21 | 32193.3 | 310.6 | 0.011986543 | 0.12258 | -0.33855 | -0.01580 | 0.08782 |
| 22 | 32609.9 | 306.7 | 0.007705949 | 0.07780 | -0.23640 | 0.04030 | -0.14242 |
| 23 | 32732.7 | 305.5 | 0.001805096 | 0.01815 | -0.06453 | 0.01285 | -0.11758 |
| 24 | 32818.7 | 304.7 | 0.001363823 | 0.01368 | 0.02724 | -0.01657 | 0.11254 |

 ABSORPTION SPECTRUM VIA TRANSITION VELOCITY DIPOLE MOMENTS

| State | Energy (cm-1) | Wavelength (nm) | fosc | P2 (au**2) | PX (au) | PY (au) | PZ (au) |
|-------|------------------|--------------------|-------------|---------------|------------|------------|------------|
| 1 | 22843.0 | 437.8 | 0.008476076 | 0.00132 | 0.02935 | 0.01325 | -0.01691 |
| 2 | 23242.4 | 430.2 | 0.002299685 | 0.00037 | 0.01154 | -0.00238 | 0.01505 |
| 3 | 23886.8 | 418.6 | 0.001000421 | 0.00016 | -0.01107 | 0.00475 | 0.00428 |
| 4 | 24109.3 | 414.8 | 0.001130921 | 0.00019 | 0.00067 | -0.00161 | 0.01354 |
| 5 | 24230.8 | 412.7 | 0.000976227 | 0.00016 | 0.01007 | -0.00125 | 0.00766 |
| 6 | 24349.2 | 410.7 | 0.000708737 | 0.00012 | 0.00573 | -0.00354 | 0.00852 |
| 7 | 26066.5 | 383.6 | 0.001127818 | 0.00020 | -0.00800 | 0.00211 | -0.01151 |
| 8 | 26367.9 | 379.2 | 0.001408856 | 0.00025 | -0.01345 | -0.00323 | 0.00791 |
| 9 | 26531.4 | 376.9 | 0.000332636 | 0.00006 | -0.00592 | 0.00313 | 0.00394 |
| 10 | 27524.2 | 363.3 | 0.000632514 | 0.00012 | 0.00390 | -0.00149 | 0.01008 |
| 11 | 27953.3 | 357.7 | 0.001533621 | 0.00029 | -0.01529 | -0.00185 | 0.00746 |
| 12 | 28095.6 | 355.9 | 0.000271312 | 0.00005 | -0.00500 | -0.00068 | 0.00516 |
| 13 | 30254.5 | 330.5 | 0.000679090 | 0.00014 | 0.00482 | 0.00562 | -0.00925 |
| 14 | 30389.5 | 329.1 | 0.000600785 | 0.00012 | -0.00864 | 0.00258 | 0.00659 |
| 15 | 30444.3 | 328.5 | 0.006324021 | 0.00132 | -0.03102 | -0.01545 | 0.01071 |
| 16 | 30640.7 | 326.4 | 0.000106911 | 0.00002 | 0.00460 | -0.00099 | -0.00053 |
| 17 | 30680.1 | 325.9 | 0.004093022 | 0.00086 | -0.01422 | 0.00213 | -0.02552 |
| 18 | 30706.1 | 325.7 | 0.000484282 | 0.00010 | 0.00603 | -0.00781 | 0.00207 |
| 19 | 31786.0 | 314.6 | 0.021473065 | 0.00466 | -0.06247 | -0.00482 | 0.02719 |
| 20 | 32022.6 | 312.3 | 0.011846973 | 0.00259 | -0.00769 | 0.01265 | -0.04872 |
| 21 | 32193.3 | 310.6 | 0.004677839 | 0.00103 | 0.02988 | 0.00979 | -0.00638 |
| 22 | 32609.9 | 306.7 | 0.002485504 | 0.00055 | 0.01927 | 0.00626 | 0.01197 |
| 23 | 32732.7 | 305.5 | 0.000568203 | 0.00013 | 0.00376 | -0.00826 | 0.00668 |
| 24 | 32818.7 | 304.7 | 0.001129059 | 0.00025 | -0.00547 | 0.00412 | -0.01437 |