

Supporting information

**Glutathione Radical Cation in the Gas Phase; Generation, Structure and  
Fragmentation**

Junfang Zhao, K.W. Michael Siu and Alan C. Hopkinson\*

Department of Chemistry and Centre for Research in Mass Spectrometry, York  
University, 4700 Keele Street, Toronto, Ontario, Canada M3J 1P3

To whom correspondence should be addressed. Tel: (416)7362100 ext. 77839; FAX:

(416)736-5936; E-mail: [ach@yorku.ca](mailto:ach@yorku.ca)

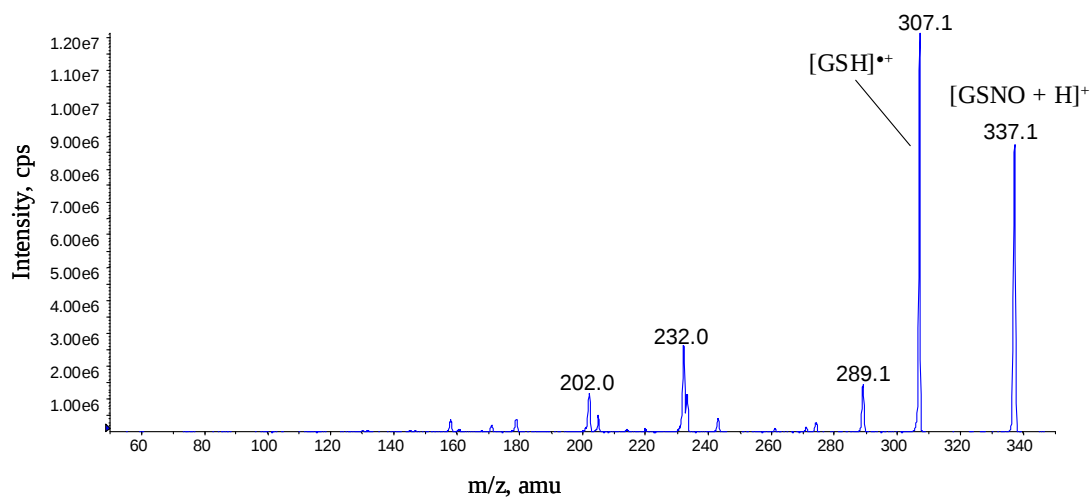


Figure S1: CID of protonated GSNO

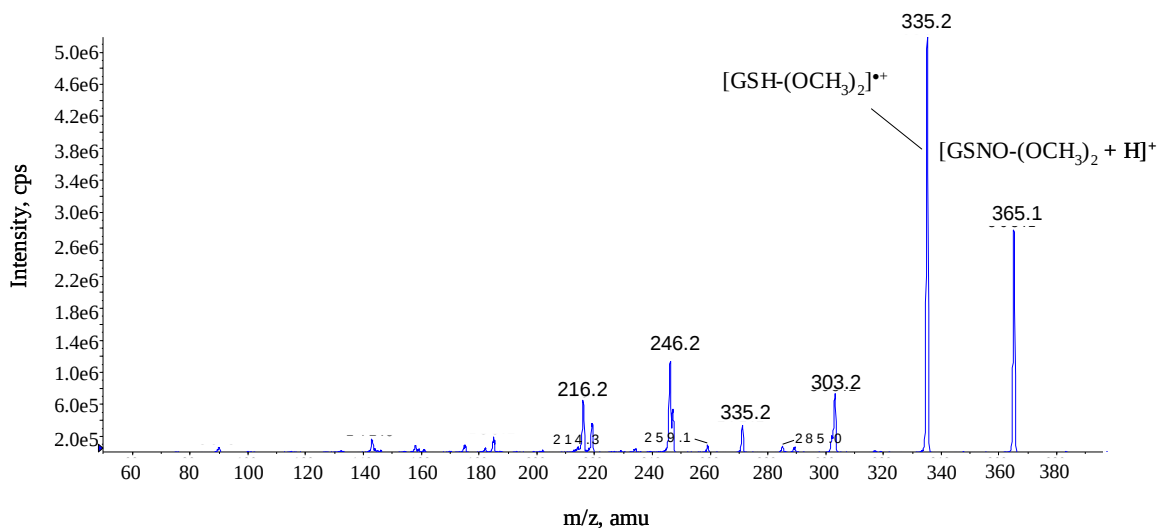


Figure S2: CID of protonated GSNO-(OCH<sub>3</sub>)<sub>2</sub>

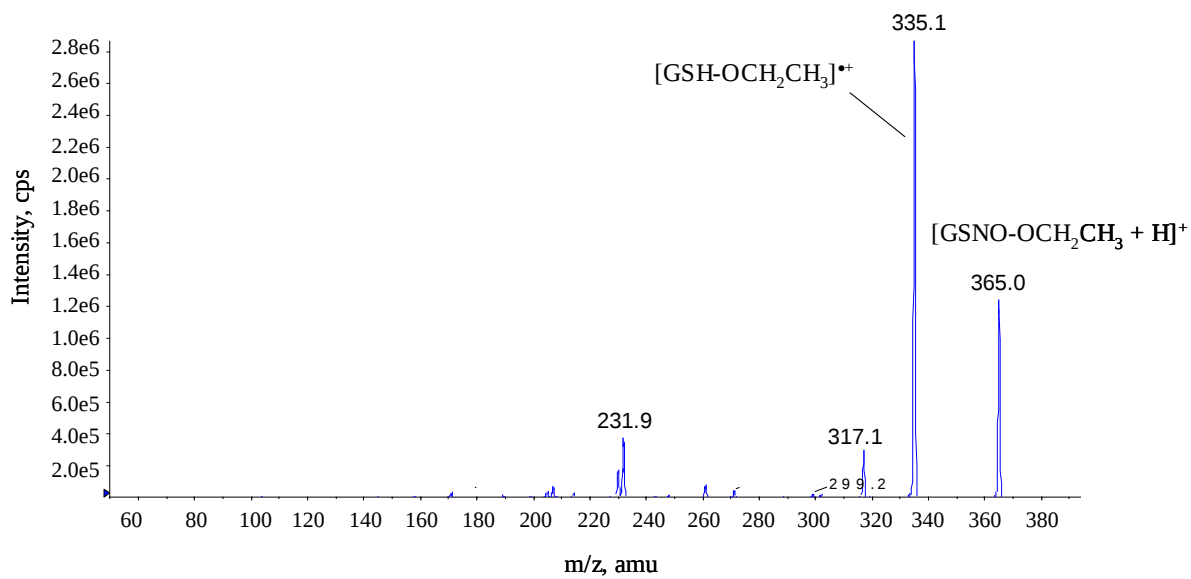


Figure S3: CID of protonated GSNO-OCH<sub>2</sub>CH<sub>3</sub>

Tables of total energies and cartesian coordinates of the optimized structures shown in  
Figures 4-7 at the B3LYP/6-31++G(d,p) level of theory

| N-terminal- $\alpha$ -C-radical ion, 1 | E <sub>t</sub> = -1404.991243 |           |           |
|----------------------------------------|-------------------------------|-----------|-----------|
| 7                                      | 0.431631                      | -0.671484 | 0.383238  |
| 1                                      | 0.505717                      | -0.601408 | 1.387277  |
| 6                                      | 1.344653                      | -0.097564 | -0.438378 |
| 6                                      | 2.464440                      | 0.716445  | 0.154594  |
| 6                                      | 1.234200                      | -0.304904 | -1.843305 |
| 1                                      | 2.388319                      | 0.656448  | 1.243301  |
| 1                                      | 3.425448                      | 0.252704  | -0.099934 |
| 6                                      | 2.486948                      | 2.231701  | -0.236602 |
| 8                                      | 0.218223                      | -1.103019 | -2.219969 |
| 1                                      | 1.517748                      | 2.532593  | -0.652501 |
| 1                                      | 2.643775                      | 2.841299  | 0.656305  |
| 6                                      | 3.546093                      | 2.588013  | -1.253277 |
| 8                                      | 3.664622                      | 1.939839  | -2.358437 |
| 8                                      | 1.996436                      | 0.193709  | -2.714993 |
| 7                                      | 4.364303                      | 3.584485  | -1.014947 |
| 1                                      | 4.371053                      | 4.080792  | -0.115439 |
| 6                                      | 5.448912                      | 4.044321  | -1.892116 |
| 6                                      | 4.883449                      | 4.844445  | -3.093624 |
| 6                                      | 6.342461                      | 4.890755  | -0.945266 |
| 1                                      | 4.029714                      | 4.311594  | -3.515014 |
| 8                                      | 5.926453                      | 5.159958  | 0.188879  |
| 7                                      | 7.530469                      | 5.284060  | -1.418229 |
| 6                                      | 8.442641                      | 6.086081  | -0.619435 |
| 6                                      | 9.735284                      | 6.262134  | -1.393023 |
| 1                                      | 8.018715                      | 7.070977  | -0.390766 |
| 1                                      | 8.649304                      | 5.601151  | 0.340467  |
| 8                                      | 9.929744                      | 5.813053  | -2.502341 |
| 8                                      | 10.625076                     | 6.979640  | -0.692750 |
| 1                                      | 11.434812                     | 7.073971  | -1.224873 |
| 1                                      | 7.811284                      | 5.084924  | -2.376701 |
| 1                                      | -0.295269                     | -1.264029 | 0.003746  |
| 1                                      | 0.222430                      | -1.185051 | -3.188749 |
| 16                                     | 6.105648                      | 5.159669  | -4.426640 |
| 1                                      | 4.537027                      | 5.826978  | -2.761672 |
| 1                                      | 2.939028                      | 1.155877  | -2.488635 |
| 1                                      | 6.084674                      | 3.917279  | -4.952134 |
| 1                                      | 5.997486                      | 3.171666  | -2.259317 |

| middle- $\alpha$ -C-radical ion, 2 | E <sub>t</sub> = -1404.9789491 |           |           |
|------------------------------------|--------------------------------|-----------|-----------|
| 7                                  | -4.249893                      | 1.501461  | 0.063568  |
| 1                                  | -4.400569                      | 2.328185  | -0.516197 |
| 6                                  | -4.745797                      | 0.245191  | -0.598164 |
| 1                                  | -5.524791                      | 0.521222  | -1.316928 |
| 6                                  | -3.633566                      | -0.505537 | -1.359484 |

|                                               |           |                               |           |
|-----------------------------------------------|-----------|-------------------------------|-----------|
| 6                                             | -5.432513 | -0.572883                     | 0.501905  |
| 1                                             | -4.132013 | -1.320502                     | -1.890762 |
| 1                                             | -3.229262 | 0.161254                      | -2.129351 |
| 6                                             | -2.483152 | -1.115101                     | -0.524658 |
| 8                                             | -5.598736 | -0.147494                     | 1.625218  |
| 1                                             | -2.879444 | -1.613528                     | 0.371274  |
| 1                                             | -2.013957 | -1.903661                     | -1.119994 |
| 6                                             | -1.430410 | -0.114771                     | -0.071019 |
| 8                                             | -1.746631 | 1.030634                      | 0.341255  |
| 8                                             | -5.832563 | -1.763626                     | 0.056476  |
| 1                                             | -6.306302 | -2.233363                     | 0.767595  |
| 7                                             | -0.150603 | -0.540646                     | -0.116852 |
| 1                                             | 0.049388  | -1.496542                     | -0.441968 |
| 6                                             | 1.038817  | 0.061710                      | 0.244250  |
| 6                                             | 1.159584  | 1.455843                      | 0.735233  |
| 6                                             | 2.165788  | -0.870319                     | -0.021667 |
| 1                                             | 1.983373  | 1.522562                      | 1.449478  |
| 1                                             | 0.238844  | 1.782181                      | 1.212566  |
| 16                                            | 1.535631  | 2.613597                      | -0.696013 |
| 8                                             | 1.910195  | -2.027275                     | -0.403874 |
| 7                                             | 3.422083  | -0.421602                     | 0.181647  |
| 6                                             | 4.574258  | -1.268124                     | -0.059316 |
| 6                                             | 5.826514  | -0.464598                     | 0.231015  |
| 1                                             | 4.549892  | -2.159024                     | 0.577888  |
| 1                                             | 4.602944  | -1.625204                     | -1.096295 |
| 8                                             | 5.821792  | 0.702606                      | 0.563841  |
| 8                                             | 6.932278  | -1.203751                     | 0.067416  |
| 1                                             | 7.707765  | -0.646441                     | 0.256040  |
| 1                                             | 3.626307  | 0.556806                      | 0.356956  |
| 1                                             | -4.743714 | 1.616927                      | 0.960320  |
| 1                                             | -3.168261 | 1.386778                      | 0.253851  |
| 1                                             | 1.790788  | 3.693081                      | 0.071975  |
| C-terminal- $\alpha$ -C-radical ion, <b>3</b> |           | E <sub>t</sub> = -1404.981649 |           |
| 7                                             | 4.093768  | 1.235800                      | 0.619148  |
| 1                                             | 4.323767  | 1.135167                      | 1.617642  |
| 6                                             | 4.687827  | 0.071526                      | -0.119052 |
| 6                                             | 3.687566  | -1.100595                     | -0.236468 |
| 6                                             | 5.941528  | -0.348567                     | 0.656471  |
| 1                                             | 4.254045  | -1.943098                     | -0.642472 |
| 1                                             | 3.358548  | -1.401351                     | 0.765616  |
| 6                                             | 2.470125  | -0.868154                     | -1.159354 |
| 8                                             | 6.172447  | 0.045359                      | 1.779285  |
| 1                                             | 2.787493  | -0.370353                     | -2.085859 |
| 1                                             | 2.076717  | -1.843216                     | -1.460923 |
| 6                                             | 1.349136  | -0.033355                     | -0.553945 |
| 8                                             | 1.591796  | 0.978439                      | 0.157831  |
| 8                                             | 6.696327  | -1.192002                     | -0.046347 |
| 1                                             | 7.471659  | -1.455861                     | 0.482956  |
| 7                                             | 0.101516  | -0.398595                     | -0.833407 |
| 1                                             | -0.104972 | -1.266303                     | -1.329775 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 6  | -1.092823 | 0.278489  | -0.327025 |
| 6  | -1.366919 | 1.584015  | -1.119464 |
| 6  | -2.217322 | -0.772481 | -0.456046 |
| 1  | -1.764338 | 1.349745  | -2.110858 |
| 1  | -0.427082 | 2.122268  | -1.251135 |
| 16 | -2.592397 | 2.703286  | -0.332245 |
| 8  | -2.019980 | -1.824323 | -1.063850 |
| 7  | -3.410645 | -0.466350 | 0.135838  |
| 6  | -4.503955 | -1.290029 | 0.124131  |
| 6  | -5.680081 | -0.797065 | 0.810298  |
| 8  | -5.717882 | 0.288672  | 1.380075  |
| 8  | -6.718086 | -1.658808 | 0.753987  |
| 1  | -7.463260 | -1.258483 | 1.233290  |
| 1  | -3.542177 | 0.448141  | 0.574978  |
| 1  | 4.498282  | 2.124425  | 0.316294  |
| 1  | 4.979566  | 0.410437  | -1.117474 |
| 1  | -1.784052 | 3.142393  | 0.654760  |
| 1  | -0.928961 | 0.529541  | 0.726526  |
| 1  | 2.999064  | 1.232503  | 0.460398  |
| 1  | -4.435886 | -2.245921 | -0.374218 |

| S-centred radical ion, <b>4</b> | E <sub>t</sub> = -1404.9824036 |           |           |
|---------------------------------|--------------------------------|-----------|-----------|
| 7                               | 4.085776                       | -0.427116 | 1.820505  |
| 1                               | 4.244547                       | -1.059578 | 2.605669  |
| 6                               | 4.648462                       | -0.966599 | 0.535832  |
| 1                               | 5.444041                       | -1.678940 | 0.779288  |
| 6                               | 3.587280                       | -1.700692 | -0.310988 |
| 6                               | 5.317722                       | 0.217489  | -0.170827 |
| 1                               | 4.128700                       | -2.158737 | -1.142777 |
| 1                               | 3.181573                       | -2.526961 | 0.283546  |
| 6                               | 2.439282                       | -0.852741 | -0.900933 |
| 8                               | 5.420131                       | 1.312187  | 0.340542  |
| 1                               | 2.827091                       | 0.077167  | -1.338410 |
| 1                               | 1.996346                       | -1.407606 | -1.733181 |
| 6                               | 1.344934                       | -0.467178 | 0.085160  |
| 8                               | 1.605098                       | -0.200549 | 1.292049  |
| 8                               | 5.778998                       | -0.120994 | -1.374944 |
| 1                               | 6.236415                       | 0.642729  | -1.772663 |
| 7                               | 0.107215                       | -0.395970 | -0.385112 |
| 1                               | -0.118815                      | -0.635935 | -1.351731 |
| 6                               | -1.061486                      | 0.012378  | 0.382772  |
| 1                               | -1.075881                      | -0.542564 | 1.329155  |
| 6                               | -1.055958                      | 1.523709  | 0.724695  |
| 6                               | -2.273485                      | -0.409694 | -0.481871 |
| 1                               | -0.212878                      | 1.726951  | 1.398119  |
| 1                               | -1.958405                      | 1.788004  | 1.287181  |
| 16                              | -0.865190                      | 2.660971  | -0.669649 |
| 8                               | -2.104126                      | -0.808493 | -1.635006 |
| 7                               | -3.481522                      | -0.298447 | 0.099682  |
| 6                               | -4.708997                      | -0.635969 | -0.599649 |
| 6                               | -5.869314                      | -0.427780 | 0.353717  |

|                          |           |                                |           |
|--------------------------|-----------|--------------------------------|-----------|
| 1                        | -4.846255 | -0.009944                      | -1.488475 |
| 1                        | -4.699169 | -1.676496                      | -0.943919 |
| 8                        | -5.742064 | -0.052168                      | 1.501498  |
| 8                        | -7.041082 | -0.710764                      | -0.228460 |
| 1                        | -7.753929 | -0.563381                      | 0.418032  |
| 1                        | -3.595636 | -0.011179                      | 1.066657  |
| 1                        | 4.530705  | 0.480179                       | 2.019171  |
| 1                        | 2.988032  | -0.279802                      | 1.680298  |
| canonical radical ion, 5 |           | E <sub>t</sub> = -1404.935380  |           |
| 7                        | -2.244404 | -1.225922                      | 0.348144  |
| 1                        | -2.393148 | -1.179265                      | 1.359593  |
| 6                        | -3.516442 | -0.931761                      | -0.334876 |
| 6                        | -3.662250 | 0.575251                       | -0.662248 |
| 6                        | -4.697907 | -1.377578                      | 0.535646  |
| 1                        | -4.677595 | 0.730893                       | -1.037067 |
| 1                        | -3.583931 | 1.158695                       | 0.263784  |
| 6                        | -2.695508 | 1.128068                       | -1.738182 |
| 8                        | -4.605103 | -1.607793                      | 1.721431  |
| 1                        | -2.547946 | 0.379582                       | -2.529786 |
| 1                        | -3.146077 | 1.998971                       | -2.219556 |
| 6                        | -1.319794 | 1.593379                       | -1.297158 |
| 8                        | -0.825032 | 2.662216                       | -1.643774 |
| 8                        | -5.839141 | -1.451591                      | -0.167858 |
| 1                        | -6.561540 | -1.712006                      | 0.431659  |
| 7                        | -0.594407 | 0.746492                       | -0.460418 |
| 1                        | -1.129509 | -0.096115                      | -0.025774 |
| 6                        | 0.748302  | 1.034192                       | -0.124282 |
| 6                        | 0.770015  | 2.092276                       | 1.102812  |
| 6                        | 1.429644  | -0.271314                      | 0.358161  |
| 1                        | 0.293803  | 1.617184                       | 1.961845  |
| 1                        | 0.196964  | 2.952297                       | 0.748852  |
| 16                       | 2.413064  | 2.593455                       | 1.611889  |
| 8                        | 0.889531  | -0.957337                      | 1.220180  |
| 7                        | 2.613120  | -0.541365                      | -0.215776 |
| 6                        | 3.432789  | -1.674735                      | 0.185795  |
| 6                        | 4.720697  | -1.621996                      | -0.616769 |
| 8                        | 4.963887  | -0.756459                      | -1.432632 |
| 8                        | 5.531183  | -2.637734                      | -0.308915 |
| 1                        | 6.342755  | -2.570090                      | -0.843245 |
| 1                        | 3.014157  | 0.044772                       | -0.942499 |
| 1                        | -1.939334 | -2.179578                      | 0.163457  |
| 1                        | -3.556062 | -1.494270                      | -1.273700 |
| 1                        | 2.652378  | 3.460801                       | 0.602511  |
| 1                        | 1.248690  | 1.516587                       | -0.968592 |
| 1                        | 2.917049  | -2.622973                      | -0.003018 |
| 1                        | 3.660304  | -1.640306                      | 1.256814  |
| carboxy radical ion, 6   |           | E <sub>t</sub> = -1404.9418434 |           |
| 7                        | 4.214611  | 0.994977                       | 1.237252  |
| 1                        | 4.445935  | 1.119508                       | 2.223638  |

|                        |           |                                |           |
|------------------------|-----------|--------------------------------|-----------|
| 6                      | 4.744230  | -0.300447                      | 0.688396  |
| 1                      | 5.585902  | -0.620477                      | 1.311864  |
| 6                      | 3.686636  | -1.424942                      | 0.695220  |
| 6                      | 5.319057  | 0.024257                       | -0.695425 |
| 1                      | 4.214254  | -2.335401                      | 0.399325  |
| 1                      | 3.356720  | -1.583703                      | 1.728035  |
| 6                      | 2.464700  | -1.259409                      | -0.235516 |
| 8                      | 5.387084  | 1.155732                       | -1.125992 |
| 1                      | 2.777524  | -0.905720                      | -1.227244 |
| 1                      | 2.022129  | -2.246452                      | -0.398937 |
| 6                      | 1.395182  | -0.301212                      | 0.272595  |
| 8                      | 1.696145  | 0.753007                       | 0.893984  |
| 8                      | 5.742511  | -1.071681                      | -1.324879 |
| 1                      | 6.145106  | -0.821305                      | -2.176959 |
| 7                      | 0.128569  | -0.609676                      | 0.009678  |
| 1                      | -0.127586 | -1.488618                      | -0.440290 |
| 6                      | -1.024575 | 0.203054                       | 0.398290  |
| 1                      | -0.862104 | 0.588374                       | 1.409299  |
| 6                      | -1.193286 | 1.400802                       | -0.575779 |
| 6                      | -2.221036 | -0.768303                      | 0.367421  |
| 1                      | -1.429485 | 1.045497                       | -1.581397 |
| 1                      | -0.239292 | 1.930171                       | -0.614732 |
| 16                     | -2.432579 | 2.654091                       | -0.054355 |
| 8                      | -2.133250 | -1.839948                      | -0.229717 |
| 7                      | -3.336331 | -0.367548                      | 1.029314  |
| 6                      | -4.585977 | -1.088920                      | 0.880308  |
| 6                      | -5.315027 | -0.632497                      | -0.372311 |
| 1                      | -4.386692 | -2.160936                      | 0.806172  |
| 1                      | -5.226252 | -0.917766                      | 1.750250  |
| 8                      | -4.906143 | 0.302650                       | -1.103186 |
| 8                      | -6.399097 | -1.149603                      | -0.765202 |
| 1                      | -3.366820 | 0.589645                       | 1.366341  |
| 1                      | 4.617198  | 1.771196                       | 0.692521  |
| 1                      | 3.110798  | 0.993800                       | 1.116682  |
| 1                      | -3.481441 | 2.136902                       | -0.727853 |
| carboxy radical ion, 7 |           | E <sub>t</sub> = -1404.9327557 |           |
| 7                      | 3.716525  | -0.653334                      | 1.890439  |
| 1                      | 3.704017  | -1.271602                      | 2.702965  |
| 6                      | 4.328753  | -1.312303                      | 0.685178  |
| 1                      | 5.001842  | -2.104172                      | 1.030516  |
| 6                      | 3.281818  | -1.932017                      | -0.261450 |
| 6                      | 5.199983  | -0.245996                      | 0.014772  |
| 1                      | 3.851878  | -2.485116                      | -1.014880 |
| 1                      | 2.704460  | -2.680943                      | 0.292119  |
| 6                      | 2.338684  | -0.965232                      | -1.008831 |
| 8                      | 5.427953  | 0.852149                       | 0.550325  |
| 1                      | 2.907580  | -0.131821                      | -1.442517 |
| 1                      | 1.905850  | -1.500821                      | -1.859354 |
| 6                      | 1.221595  | -0.357668                      | -0.172509 |
| 8                      | 1.372709  | -0.096354                      | 1.049017  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | 5.719241  | -0.478434 | -1.123511 |
| 7  | 0.082077  | -0.082967 | -0.808149 |
| 1  | -0.080209 | -0.424710 | -1.753126 |
| 6  | -1.087563 | 0.535869  | -0.197856 |
| 1  | -1.013708 | 0.414913  | 0.885762  |
| 6  | -1.208764 | 2.037196  | -0.564225 |
| 6  | -2.312458 | -0.211632 | -0.777838 |
| 1  | -2.122396 | 2.449613  | -0.128502 |
| 1  | -1.283492 | 2.142027  | -1.650416 |
| 16 | 0.217039  | 3.083486  | -0.082427 |
| 8  | -2.235750 | -0.727026 | -1.893311 |
| 7  | -3.424436 | -0.206548 | -0.020639 |
| 6  | -4.670266 | -0.807897 | -0.465091 |
| 6  | -5.696341 | -0.636790 | 0.638609  |
| 1  | -5.034698 | -0.336510 | -1.384646 |
| 1  | -4.542092 | -1.873934 | -0.685097 |
| 8  | -5.460677 | -0.097137 | 1.700752  |
| 8  | -6.880756 | -1.154022 | 0.293014  |
| 1  | -3.439019 | 0.184453  | 0.916439  |
| 1  | 4.261134  | 0.191246  | 2.122300  |
| 1  | 2.679855  | -0.359467 | 1.624001  |
| 1  | -0.000848 | 3.058905  | 1.249438  |
| 1  | -7.506343 | -1.022487 | 1.027435  |

| TS-1 | E <sub>T</sub> = -1404.9124399 |           |           |
|------|--------------------------------|-----------|-----------|
| 7    | 4.439653                       | -0.658660 | -0.979780 |
| 6    | 3.566760                       | -0.014599 | -0.139599 |
| 6    | 3.392127                       | 1.479822  | -0.389377 |
| 6    | 3.576678                       | -0.641623 | 1.230209  |
| 1    | 4.309457                       | 1.986175  | -0.060402 |
| 1    | 3.337173                       | 1.617999  | -1.476062 |
| 6    | 2.181570                       | 2.178561  | 0.280991  |
| 8    | 3.665865                       | -1.848847 | 1.371715  |
| 1    | 2.378117                       | 2.364337  | 1.336032  |
| 1    | 2.026018                       | 3.143742  | -0.212930 |
| 6    | 0.933759                       | 1.317310  | 0.211134  |
| 8    | 0.519863                       | 0.689262  | 1.180077  |
| 8    | 3.476890                       | 0.244179  | 2.221657  |
| 1    | 3.425815                       | -0.232325 | 3.070270  |
| 7    | 0.406655                       | 1.123042  | -1.050940 |
| 6    | -0.743338                      | 0.249451  | -1.236821 |
| 1    | -0.911065                      | 0.186609  | -2.318306 |
| 6    | -0.459646                      | -1.167061 | -0.698968 |
| 6    | -2.030594                      | 0.915665  | -0.647969 |
| 16   | 1.224212                       | -1.738047 | -1.256051 |
| 8    | -2.084849                      | 2.136149  | -0.590903 |
| 7    | -3.048468                      | 0.097648  | -0.306218 |
| 6    | -4.311554                      | 0.613625  | 0.192796  |
| 6    | -5.196214                      | -0.568951 | 0.534857  |
| 1    | -4.163485                      | 1.234025  | 1.083983  |
| 1    | -4.809608                      | 1.243564  | -0.552939 |

|             |                                      |           |           |
|-------------|--------------------------------------|-----------|-----------|
| 8           | -4.853468                            | -1.727914 | 0.403361  |
| 8           | -6.389329                            | -0.178007 | 0.995144  |
| 1           | -6.920253                            | -0.967804 | 1.200754  |
| 1           | -2.985480                            | -0.913633 | -0.330473 |
| 1           | 1.424029                             | -2.698512 | -0.324805 |
| 1           | 0.489074                             | 1.888265  | -1.708812 |
| 1           | 4.679906                             | -0.280739 | -1.886062 |
| 1           | 4.805221                             | -1.569632 | -0.725262 |
| 1           | 2.229026                             | -0.723595 | -0.577130 |
| 1           | -0.472600                            | -1.195787 | 0.388333  |
| 1           | -1.150687                            | -1.899925 | -1.122726 |
|             |                                      |           |           |
| <b>TS-2</b> | <b>E<sub>t</sub> = -1404.9352399</b> |           |           |
| 7           | -3.104926                            | 0.888837  | 0.095966  |
| 6           | -3.694699                            | -0.452989 | -0.086570 |
| 1           | -4.776127                            | -0.372343 | -0.271732 |
| 6           | -3.101267                            | -1.222955 | -1.292471 |
| 6           | -3.563323                            | -1.210977 | 1.232931  |
| 1           | -3.780762                            | -2.053913 | -1.500253 |
| 1           | -3.149011                            | -0.566156 | -2.169226 |
| 6           | -1.688040                            | -1.833717 | -1.154439 |
| 8           | -3.099547                            | -0.732096 | 2.246085  |
| 1           | -1.580252                            | -2.337920 | -0.184453 |
| 1           | -1.569672                            | -2.620069 | -1.903985 |
| 6           | -0.461381                            | -0.953484 | -1.330635 |
| 8           | 0.565978                             | -1.367717 | -1.862407 |
| 8           | -4.042438                            | -2.461596 | 1.139159  |
| 1           | -3.981620                            | -2.885574 | 2.013924  |
| 7           | -0.508378                            | 0.331581  | -0.818974 |
| 1           | -1.393478                            | 0.661153  | -0.367599 |
| 6           | 0.597921                             | 1.222736  | -1.021936 |
| 1           | 1.091214                             | 0.939104  | -1.958852 |
| 6           | 0.121356                             | 2.695566  | -1.161868 |
| 6           | 1.665668                             | 1.072923  | 0.110431  |
| 1           | -0.630257                            | 2.767150  | -1.949174 |
| 1           | 0.988036                             | 3.306775  | -1.439356 |
| 16          | -0.566049                            | 3.389609  | 0.375232  |
| 8           | 1.682330                             | 1.825287  | 1.110986  |
| 7           | 2.543369                             | 0.093481  | -0.060734 |
| 6           | 3.600241                             | -0.187482 | 0.903381  |
| 6           | 4.442490                             | -1.331794 | 0.366663  |
| 1           | 4.228337                             | 0.695441  | 1.059836  |
| 1           | 3.180923                             | -0.461432 | 1.878145  |
| 8           | 4.220195                             | -1.893546 | -0.683174 |
| 8           | 5.443131                             | -1.625770 | 1.204516  |
| 1           | 5.960668                             | -2.361318 | 0.830835  |
| 1           | 2.461492                             | -0.542839 | -0.857117 |
| 1           | 0.599322                             | 2.919989  | 1.050408  |
| 1           | -3.169398                            | 1.159471  | 1.077343  |
| 1           | -3.604089                            | 1.577997  | -0.460506 |

| TS3  | E <sub>t</sub> = -1404.9301697 |           |           |
|------|--------------------------------|-----------|-----------|
| 7    | 4.217168                       | 0.998968  | 1.286784  |
| 1    | 4.465245                       | 1.074047  | 2.274183  |
| 6    | 4.780185                       | -0.242563 | 0.651944  |
| 1    | 5.648121                       | -0.564488 | 1.237150  |
| 6    | 3.764910                       | -1.404835 | 0.617765  |
| 6    | 5.307529                       | 0.182747  | -0.723647 |
| 1    | 4.318984                       | -2.277498 | 0.262440  |
| 1    | 3.462837                       | -1.631324 | 1.646424  |
| 6    | 2.518542                       | -1.235940 | -0.279615 |
| 8    | 5.319479                       | 1.338654  | -1.089768 |
| 1    | 2.797696                       | -0.818091 | -1.256349 |
| 1    | 2.109461                       | -2.228964 | -0.487797 |
| 6    | 1.425249                       | -0.347342 | 0.298661  |
| 8    | 1.697353                       | 0.681377  | 0.971991  |
| 8    | 5.758146                       | -0.857697 | -1.423833 |
| 1    | 6.129646                       | -0.544170 | -2.269185 |
| 7    | 0.164734                       | -0.689020 | 0.041140  |
| 1    | -0.066873                      | -1.532967 | -0.482758 |
| 6    | -1.007210                      | 0.063338  | 0.479125  |
| 1    | -0.849072                      | 0.422045  | 1.499835  |
| 6    | -1.260224                      | 1.277254  | -0.463508 |
| 6    | -2.187284                      | -0.916952 | 0.382557  |
| 1    | -1.376390                      | 0.927890  | -1.493002 |
| 1    | -0.381882                      | 1.928620  | -0.414795 |
| 16   | -2.670095                      | 2.339727  | 0.002802  |
| 8    | -2.122592                      | -1.885908 | -0.371121 |
| 7    | -3.284971                      | -0.583610 | 1.105097  |
| 6    | -4.592725                      | -1.108412 | 0.754906  |
| 6    | -5.241380                      | -0.393735 | -0.427593 |
| 1    | -4.506353                      | -2.165937 | 0.494658  |
| 1    | -5.266178                      | -1.027704 | 1.612751  |
| 8    | -4.785866                      | 0.708368  | -0.941111 |
| 8    | -6.260455                      | -0.845855 | -0.956609 |
| 1    | -3.255946                      | 0.281418  | 1.632009  |
| 1    | 4.580240                       | 1.819540  | 0.780347  |
| 1    | 3.115513                       | 0.965681  | 1.187885  |
| 1    | -3.776129                      | 1.499040  | -0.559729 |
| TS-4 | E <sub>t</sub> = -1404.933162  |           |           |
| 1    | 2.843779                       | -0.418934 | 1.962103  |
| 7    | 3.879023                       | -0.204684 | 1.883298  |
| 1    | 4.394511                       | -0.598145 | 2.672287  |
| 6    | 4.340185                       | -0.756351 | 0.550057  |
| 1    | 5.420075                       | -0.912601 | 0.615707  |
| 6    | 3.629474                       | -2.091668 | 0.234743  |
| 6    | 4.066561                       | 0.345385  | -0.500975 |
| 1    | 4.285558                       | -2.662891 | -0.426736 |
| 1    | 3.545759                       | -2.672500 | 1.160227  |
| 6    | 2.258245                       | -1.984872 | -0.463195 |
| 8    | 3.543506                       | 1.427391  | -0.103323 |

|             |                                      |           |           |
|-------------|--------------------------------------|-----------|-----------|
| 1           | 2.398817                             | -1.679104 | -1.504682 |
| 1           | 1.804973                             | -2.984010 | -0.491675 |
| 6           | 1.261106                             | -1.048106 | 0.204959  |
| 8           | 1.336254                             | -0.724154 | 1.407403  |
| 8           | 4.365520                             | 0.095556  | -1.685705 |
| 7           | 0.283566                             | -0.568135 | -0.591522 |
| 1           | 0.171197                             | -0.924885 | -1.537728 |
| 6           | -0.788183                            | 0.294394  | -0.137784 |
| 1           | -0.822900                            | 0.260257  | 0.953357  |
| 6           | -0.610400                            | 1.766569  | -0.627485 |
| 6           | -2.093619                            | -0.238942 | -0.786687 |
| 1           | -1.512827                            | 2.334365  | -0.387022 |
| 1           | -0.470290                            | 1.775968  | -1.712330 |
| 16          | 0.747737                             | 2.694477  | 0.158248  |
| 8           | -2.046677                            | -0.716111 | -1.918371 |
| 7           | -3.215401                            | -0.101831 | -0.059248 |
| 6           | -4.516682                            | -0.525536 | -0.551591 |
| 6           | -5.537336                            | -0.265851 | 0.540546  |
| 1           | -4.795830                            | 0.022336  | -1.458389 |
| 1           | -4.516940                            | -1.590441 | -0.810508 |
| 8           | -5.255857                            | 0.200931  | 1.625657  |
| 8           | -6.768628                            | -0.616110 | 0.155092  |
| 1           | -3.202327                            | 0.236522  | 0.898686  |
| 1           | 3.975585                             | 0.820112  | 1.859692  |
| 1           | 1.827219                             | 2.130834  | -0.457552 |
| 1           | -7.389524                            | -0.436122 | 0.883335  |
|             |                                      |           |           |
| <b>TS-5</b> | <b>E<sub>t</sub> = -1404.9470289</b> |           |           |
| 7           | -3.327664                            | 1.027618  | -1.363540 |
| 1           | -2.540158                            | 1.643174  | -1.515903 |
| 6           | -3.398604                            | 0.250039  | -0.215210 |
| 1           | -2.433334                            | -0.718406 | -0.185029 |
| 6           | -3.192793                            | 0.959991  | 1.129011  |
| 6           | -4.577814                            | -0.692723 | -0.298907 |
| 1           | -4.123446                            | 1.468440  | 1.407568  |
| 1           | -3.015486                            | 0.196835  | 1.890824  |
| 6           | -2.071679                            | 2.030559  | 1.154279  |
| 8           | -5.167114                            | -0.927234 | -1.331578 |
| 1           | -2.371198                            | 2.924270  | 0.603443  |
| 1           | -1.902214                            | 2.330590  | 2.194767  |
| 6           | -0.773789                            | 1.562323  | 0.543909  |
| 8           | -0.394928                            | 2.026139  | -0.561414 |
| 8           | -4.846637                            | -1.278740 | 0.883048  |
| 1           | -5.575704                            | -1.910067 | 0.749676  |
| 7           | -0.052080                            | 0.616425  | 1.185927  |
| 1           | -0.465904                            | 0.233934  | 2.027889  |
| 6           | 0.857615                             | -0.321006 | 0.499706  |
| 1           | 1.191149                             | -1.021195 | 1.268514  |
| 6           | 0.128289                             | -1.138367 | -0.612993 |
| 6           | 2.079463                             | 0.385240  | -0.070869 |
| 1           | 0.811992                             | -1.907450 | -0.986743 |

|                              |           |           |           |
|------------------------------|-----------|-----------|-----------|
| 1                            | -0.128691 | -0.495826 | -1.459651 |
| 16                           | -1.357257 | -1.979963 | 0.027123  |
| 8                            | 1.960935  | 1.433441  | -0.802819 |
| 7                            | 3.272761  | -0.127869 | 0.117401  |
| 6                            | 4.505187  | 0.407550  | -0.458549 |
| 6                            | 5.640870  | -0.482876 | 0.026036  |
| 1                            | 4.460097  | 0.404234  | -1.552404 |
| 1                            | 4.669396  | 1.440734  | -0.135991 |
| 8                            | 5.459956  | -1.436020 | 0.754811  |
| 8                            | 6.814397  | -0.075082 | -0.450166 |
| 1                            | 7.520068  | -0.662460 | -0.123115 |
| 1                            | 3.409771  | -0.954747 | 0.700560  |
| 1                            | -3.765841 | 0.637864  | -2.191797 |
| 1                            | 0.931158  | 1.751856  | -0.818630 |
| <b>TS-6</b>                  |           |           |           |
| E <sub>t</sub> = -1404.93225 |           |           |           |
| 7                            | -4.255566 | 1.505683  | -0.252429 |
| 1                            | -4.441848 | 2.210093  | -0.967624 |
| 6                            | -4.778206 | 0.149435  | -0.638887 |
| 1                            | -5.598125 | 0.288279  | -1.351661 |
| 6                            | -3.704217 | -0.734015 | -1.308365 |
| 6                            | -5.394587 | -0.447765 | 0.631509  |
| 1                            | -4.227664 | -1.627334 | -1.658863 |
| 1                            | -3.341728 | -0.219010 | -2.205047 |
| 6                            | -2.511598 | -1.193495 | -0.438541 |
| 8                            | -5.498729 | 0.178779  | 1.664351  |
| 1                            | -2.858065 | -1.527234 | 0.549162  |
| 1                            | -2.065821 | -2.074882 | -0.908770 |
| 6                            | -1.441640 | -0.132917 | -0.215116 |
| 8                            | -1.741573 | 1.071308  | -0.027162 |
| 8                            | -5.810595 | -1.699232 | 0.438271  |
| 1                            | -6.240701 | -2.026975 | 1.249681  |
| 7                            | -0.171509 | -0.563436 | -0.208074 |
| 1                            | 0.044947  | -1.540622 | -0.433954 |
| 6                            | 1.028619  | 0.170399  | -0.028910 |
| 1                            | 1.287083  | 1.083716  | -1.109746 |
| 6                            | 1.097719  | 1.364095  | 0.903685  |
| 6                            | 2.184841  | -0.821660 | -0.110065 |
| 1                            | 1.861376  | 1.275278  | 1.677821  |
| 1                            | 0.138002  | 1.633881  | 1.337838  |
| 16                           | 1.585906  | 2.517367  | -0.474633 |
| 8                            | 1.931258  | -2.007437 | -0.360457 |
| 7                            | 3.424849  | -0.344928 | 0.084302  |
| 6                            | 4.587515  | -1.211059 | 0.000272  |
| 6                            | 5.829008  | -0.376464 | 0.246909  |
| 1                            | 4.532545  | -2.016965 | 0.740053  |
| 1                            | 4.660183  | -1.690802 | -0.983268 |
| 8                            | 5.814456  | 0.819813  | 0.445711  |
| 8                            | 6.937130  | -1.130100 | 0.211457  |
| 1                            | 7.707183  | -0.555388 | 0.367467  |
| 1                            | 3.609088  | 0.652785  | 0.163456  |

|             |                                      |           |           |
|-------------|--------------------------------------|-----------|-----------|
| 1           | -4.700455                            | 1.789844  | 0.632152  |
| 1           | -3.165215                            | 1.421866  | -0.103476 |
| <b>TS-7</b> | <b>E<sub>t</sub> = -1404.9381296</b> |           |           |
| 7           | 4.165644                             | 0.298403  | 1.764348  |
| 1           | 4.436333                             | -0.130405 | 2.650315  |
| 6           | 4.798633                             | -0.386430 | 0.584814  |
| 1           | 5.702040                             | -0.900609 | 0.929759  |
| 6           | 3.868126                             | -1.433207 | -0.063349 |
| 6           | 5.259383                             | 0.729174  | -0.360653 |
| 1           | 4.471967                             | -1.948327 | -0.814923 |
| 1           | 3.612674                             | -2.184461 | 0.692284  |
| 6           | 2.586859                             | -0.916597 | -0.755743 |
| 8           | 5.182621                             | 1.904111  | -0.070913 |
| 1           | 2.803095                             | -0.028360 | -1.364713 |
| 1           | 2.245338                             | -1.681597 | -1.459299 |
| 6           | 1.450808                             | -0.551496 | 0.189504  |
| 8           | 1.668291                             | -0.004535 | 1.303058  |
| 8           | 5.762215                             | 0.240790  | -1.494053 |
| 1           | 6.087171                             | 0.974697  | -2.047817 |
| 7           | 0.211309                             | -0.810275 | -0.219165 |
| 1           | 0.035552                             | -1.297896 | -1.095187 |
| 6           | -0.988620                            | -0.493886 | 0.542685  |
| 1           | -0.828440                            | -0.768511 | 1.592880  |
| 6           | -1.390494                            | 1.015993  | 0.488510  |
| 6           | -2.126784                            | -1.304774 | -0.087972 |
| 1           | -0.492863                            | 1.626191  | 0.624095  |
| 1           | -2.045678                            | 1.239758  | 1.335534  |
| 16          | -2.180791                            | 1.581172  | -1.071903 |
| 8           | -1.963892                            | -1.965743 | -1.094835 |
| 7           | -3.387058                            | -1.032503 | 0.445369  |
| 6           | -4.293456                            | -0.385182 | -0.422979 |
| 6           | -5.428160                            | 0.243447  | 0.306482  |
| 1           | -3.521134                            | 0.701437  | -0.870440 |
| 1           | -4.496617                            | -0.888087 | -1.365564 |
| 8           | -5.404540                            | 0.447355  | 1.507053  |
| 8           | -6.425949                            | 0.597997  | -0.515348 |
| 1           | -7.112446                            | 1.048753  | 0.007313  |
| 1           | -3.420779                            | -0.636380 | 1.383849  |
| 1           | 4.453823                             | 1.287602  | 1.762226  |
| 1           | 3.065611                             | 0.236017  | 1.648787  |
| <b>TS-8</b> | <b>E<sub>t</sub> = -1404.9456121</b> |           |           |
| 7           | -5.324369                            | -0.620754 | 0.365137  |
| 1           | -5.687913                            | -1.558401 | 0.456623  |
| 6           | -4.173083                            | -0.376546 | -0.316185 |
| 6           | -3.300685                            | -1.532880 | -0.722105 |
| 6           | -3.832262                            | 0.971018  | -0.657660 |
| 1           | -3.948551                            | -2.394204 | -0.921078 |
| 1           | -2.813896                            | -1.297093 | -1.673431 |
| 6           | -2.242680                            | -2.008627 | 0.307764  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | -4.790226 | 1.877398  | -0.352446 |
| 1  | -2.657392 | -2.027813 | 1.323417  |
| 1  | -1.955677 | -3.043833 | 0.088634  |
| 6  | -0.957303 | -1.238678 | 0.379809  |
| 8  | 0.018697  | -1.731192 | 1.077180  |
| 8  | -2.754345 | 1.318859  | -1.186436 |
| 7  | -0.708670 | -0.094646 | -0.211053 |
| 1  | -1.447553 | 0.455243  | -0.717350 |
| 6  | 0.628069  | 0.433774  | 0.092656  |
| 1  | 1.224328  | 0.469408  | -0.822355 |
| 6  | 0.566880  | 1.829934  | 0.741347  |
| 6  | 1.199955  | -0.621513 | 1.064557  |
| 1  | -0.104180 | 2.467457  | 0.161511  |
| 8  | 1.801496  | -0.477878 | 2.080005  |
| 7  | 2.366958  | -1.811699 | -0.093404 |
| 6  | 3.768445  | -1.381720 | 0.013345  |
| 6  | 4.076687  | -0.395099 | -1.096362 |
| 1  | 3.921472  | -0.901298 | 0.987434  |
| 1  | 4.469629  | -2.221128 | -0.053626 |
| 8  | 3.268244  | -0.059944 | -1.941701 |
| 8  | 5.337273  | 0.036939  | -1.035313 |
| 1  | 5.496962  | 0.659662  | -1.766709 |
| 1  | -5.956651 | 0.142217  | 0.568973  |
| 1  | -4.478974 | 2.757539  | -0.621371 |
| 16 | 2.215101  | 2.628956  | 0.870660  |
| 1  | 2.221546  | 3.150223  | -0.373648 |
| 1  | 0.174395  | 1.761844  | 1.758368  |
| 1  | 2.086498  | -1.867775 | -1.073609 |
| 1  | 2.223653  | -2.717087 | 0.349578  |

| TS-9 | E <sub>t</sub> = -1404.9313675 |           |           |
|------|--------------------------------|-----------|-----------|
| 7    | 5.673597                       | -0.540532 | -1.104163 |
| 1    | 5.929522                       | -1.457607 | -1.445996 |
| 6    | 4.752857                       | -0.424268 | -0.111809 |
| 6    | 3.993481                       | -1.636951 | 0.352904  |
| 6    | 4.540267                       | 0.873473  | 0.343643  |
| 1    | 4.620615                       | -2.514831 | 0.164468  |
| 1    | 3.847556                       | -1.571427 | 1.431605  |
| 6    | 2.641106                       | -1.836080 | -0.367089 |
| 8    | 3.795493                       | 0.503940  | 2.396935  |
| 1    | 2.788771                       | -1.907902 | -1.451929 |
| 1    | 2.217036                       | -2.794511 | -0.048843 |
| 6    | 1.644066                       | -0.712003 | -0.089576 |
| 8    | 2.021187                       | 0.377571  | 0.398058  |
| 8    | 4.631324                       | 2.028631  | 0.290148  |
| 7    | 0.374980                       | -0.953156 | -0.422631 |
| 1    | 0.061753                       | -1.872734 | -0.741097 |
| 6    | -0.729391                      | -0.016003 | -0.227912 |
| 6    | -0.690522                      | 1.103586  | -1.299323 |
| 6    | -2.003483                      | -0.895002 | -0.304759 |
| 1    | 0.337127                       | 1.452817  | -1.408849 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | -1.913555 | -2.067340 | -0.686239 |
| 7  | -3.160880 | -0.319363 | 0.056195  |
| 6  | -4.417523 | -1.045229 | 0.007746  |
| 6  | -5.506564 | -0.180370 | 0.610508  |
| 1  | -4.693757 | -1.309316 | -1.020299 |
| 1  | -4.344933 | -1.986433 | 0.563084  |
| 8  | -5.331718 | 0.941425  | 1.036441  |
| 8  | -6.688923 | -0.815512 | 0.605838  |
| 1  | -7.357276 | -0.223594 | 0.993489  |
| 1  | -3.203823 | 0.663728  | 0.314638  |
| 1  | 6.198181  | 0.247339  | -1.463166 |
| 1  | 2.866212  | 0.646521  | 2.134611  |
| 16 | -1.770637 | 2.546061  | -0.941948 |
| 1  | -1.020403 | 0.712726  | -2.265881 |
| 1  | -0.991600 | 3.086977  | 0.017503  |
| 1  | -0.641598 | 0.435772  | 0.765659  |
| 1  | 4.046708  | 1.210197  | 3.010928  |

| TS-10 | E <sub>t</sub> = -1404.9164264 |           |           |
|-------|--------------------------------|-----------|-----------|
| 7     | 5.361789                       | -0.497170 | -0.516104 |
| 1     | 5.721609                       | -1.352274 | -0.914094 |
| 6     | 4.220067                       | -0.499964 | 0.226168  |
| 6     | 3.348010                       | -1.724694 | 0.224031  |
| 6     | 3.882228                       | 0.654771  | 0.999614  |
| 1     | 4.004421                       | -2.602848 | 0.179197  |
| 1     | 2.827004                       | -1.791667 | 1.183780  |
| 6     | 2.341508                       | -1.863950 | -0.946441 |
| 8     | 4.835738                       | 1.625682  | 0.989854  |
| 1     | 2.810768                       | -1.575980 | -1.894717 |
| 1     | 2.074373                       | -2.920009 | -1.063591 |
| 6     | 1.005287                       | -1.132042 | -0.903636 |
| 8     | 0.166585                       | -1.386638 | -1.792174 |
| 8     | 2.817476                       | 0.798858  | 1.632029  |
| 7     | 0.759511                       | -0.259991 | 0.101224  |
| 1     | 1.514994                       | -0.018753 | 0.760194  |
| 6     | -0.385460                      | 0.658511  | 0.157969  |
| 1     | -0.248992                      | 1.242688  | 1.070160  |
| 6     | -0.404420                      | 1.626433  | -1.052786 |
| 6     | -1.731185                      | -0.049043 | 0.358125  |
| 1     | 0.523086                       | 2.203392  | -1.038004 |
| 8     | -2.492134                      | 0.244346  | 1.305596  |
| 7     | -2.118720                      | -0.959059 | -0.549640 |
| 6     | -3.374326                      | -1.641285 | -0.329124 |
| 6     | -4.387798                      | -0.651794 | 0.200428  |
| 8     | -5.159135                      | 0.125524  | -0.163372 |
| 8     | -4.610227                      | -1.106204 | 1.942885  |
| 1     | -1.424946                      | -1.247386 | -1.274372 |
| 1     | 5.996383                       | 0.287386  | -0.453257 |
| 1     | 4.522919                       | 2.356638  | 1.546997  |
| 16    | -1.850055                      | 2.751531  | -1.122862 |
| 1     | -1.574516                      | 3.450496  | -0.002031 |

|       |           |                                 |           |
|-------|-----------|---------------------------------|-----------|
| 1     | -0.434438 | 1.062877                        | -1.986986 |
| 1     | -3.297586 | -2.469620                       | 0.381413  |
| 1     | -3.774005 | -2.006604                       | -1.280332 |
| 1     | -3.806196 | -0.636757                       | 2.273853  |
| 1     | -5.401963 | -0.666738                       | 2.304590  |
|       |           |                                 |           |
| TS-11 |           | E <sub>t</sub> = -1404. 9304493 |           |
| 7     | 4.966541  | -0.589610                       | -1.610369 |
| 1     | 5.128680  | -1.556010                       | -1.853568 |
| 6     | 4.275188  | -0.252951                       | -0.492319 |
| 6     | 3.659863  | -1.354107                       | 0.333783  |
| 6     | 4.267680  | 1.120468                        | -0.086144 |
| 1     | 4.306784  | -2.232543                       | 0.229814  |
| 1     | 3.695988  | -1.066495                       | 1.387029  |
| 6     | 2.213596  | -1.814279                       | -0.003636 |
| 8     | 5.101752  | 1.910722                        | -0.802229 |
| 1     | 2.031530  | -1.829104                       | -1.082937 |
| 1     | 2.096549  | -2.841092                       | 0.364604  |
| 6     | 1.126725  | -1.009783                       | 0.695364  |
| 8     | 3.554776  | 1.609428                        | 0.828948  |
| 7     | -0.189525 | -1.442452                       | 0.555422  |
| 6     | -1.200015 | -0.408473                       | 0.809239  |
| 6     | -0.559068 | 1.032799                        | 0.718866  |
| 6     | -2.311113 | -0.612634                       | -0.249869 |
| 1     | -1.204936 | 1.725848                        | 0.178304  |
| 8     | -2.058479 | -1.211200                       | -1.294822 |
| 7     | -3.508167 | -0.077498                       | 0.046401  |
| 6     | -4.645315 | -0.165845                       | -0.854862 |
| 6     | -5.833449 | 0.487951                        | -0.174571 |
| 1     | -4.441361 | 0.337460                        | -1.806346 |
| 1     | -4.884505 | -1.208860                       | -1.091708 |
| 8     | -5.787722 | 0.972965                        | 0.937810  |
| 8     | -6.921811 | 0.458239                        | -0.950793 |
| 1     | -7.658615 | 0.881665                        | -0.475345 |
| 1     | -3.704842 | 0.345232                        | 0.949287  |
| 1     | 5.473297  | 0.115689                        | -2.129051 |
| 1     | 5.023208  | 2.820522                        | -0.469831 |
| 16    | 1.001686  | 0.841147                        | -0.214075 |
| 1     | -0.339675 | 1.438235                        | 1.706713  |
| 1     | -1.628969 | -0.513103                       | 1.811845  |
| 8     | 1.453110  | -0.698304                       | 2.003878  |
| 1     | -0.388990 | -1.872943                       | -0.353048 |
| 1     | 0.808136  | -1.112724                       | 2.597485  |
| 1     | 2.081247  | 1.403124                        | 0.564338  |
|       |           |                                 |           |
| TS-12 |           | E <sub>t</sub> = -1404.9472631  |           |
| 7     | -4.845447 | 0.561875                        | -1.611277 |
| 1     | -4.842909 | 1.458212                        | -2.075513 |
| 6     | -4.299265 | 0.400667                        | -0.382606 |
| 6     | -3.612692 | 1.556055                        | 0.295165  |
| 6     | -4.457520 | -0.848162                       | 0.290542  |

|                        |           |                                |           |
|------------------------|-----------|--------------------------------|-----------|
| 1                      | -4.097574 | 2.484263                       | -0.028539 |
| 1                      | -3.804275 | 1.482065                       | 1.369191  |
| 6                      | -2.093670 | 1.751715                       | 0.056286  |
| 8                      | -5.248723 | -1.736694                      | -0.334159 |
| 1                      | -1.911074 | 2.036191                       | -0.985120 |
| 1                      | -1.779327 | 2.597654                       | 0.679829  |
| 6                      | -1.147400 | 0.585574                       | 0.338362  |
| 8                      | -3.921649 | -1.143095                      | 1.395923  |
| 7                      | 0.139551  | 0.941912                       | 0.616822  |
| 6                      | 1.160898  | -0.053185                      | 0.310193  |
| 6                      | 0.676809  | -0.837825                      | -0.930981 |
| 6                      | 2.476907  | 0.711626                       | 0.058400  |
| 1                      | 0.985004  | -0.358675                      | -1.863451 |
| 8                      | 2.452593  | 1.924590                       | -0.151048 |
| 7                      | 3.598028  | -0.031823                      | 0.062760  |
| 6                      | 4.910683  | 0.543009                       | -0.175883 |
| 6                      | 5.942113  | -0.559858                      | -0.035363 |
| 1                      | 4.978008  | 0.984444                       | -1.176520 |
| 1                      | 5.129676  | 1.344394                       | 0.539035  |
| 8                      | 5.667216  | -1.709520                      | 0.242246  |
| 8                      | 7.181282  | -0.104324                      | -0.254331 |
| 1                      | 7.808195  | -0.842037                      | -0.150918 |
| 1                      | 3.590480  | -1.019737                      | 0.298588  |
| 1                      | -5.358411 | -0.193090                      | -2.047527 |
| 1                      | -5.273004 | -2.557967                      | 0.185836  |
| 16                     | -1.168423 | -0.812556                      | -0.835167 |
| 1                      | 1.017493  | -1.874358                      | -0.922451 |
| 1                      | 1.274914  | -0.742223                      | 1.155542  |
| 8                      | -1.718475 | -0.153369                      | 1.762717  |
| 1                      | 0.446897  | 1.904661                       | 0.478316  |
| 1                      | -1.633548 | 0.452321                       | 2.518758  |
| 1                      | -2.719845 | -0.577367                      | 1.674003  |
| Intermediate <b>10</b> |           | E <sub>t</sub> = -1404.9550865 |           |
| 7                      | -4.943811 | 0.859649                       | -1.228186 |
| 1                      | -4.939741 | 1.838203                       | -1.481111 |
| 6                      | -4.310884 | 0.426810                       | -0.123005 |
| 6                      | -3.600909 | 1.414352                       | 0.768035  |
| 6                      | -4.407433 | -0.950328                      | 0.199733  |
| 1                      | -4.147037 | 2.362565                       | 0.712723  |
| 1                      | -3.695166 | 1.074688                       | 1.802902  |
| 6                      | -2.112980 | 1.716862                       | 0.463483  |
| 8                      | -5.233852 | -1.687679                      | -0.531607 |
| 1                      | -2.011198 | 2.218075                       | -0.502995 |
| 1                      | -1.776831 | 2.418849                       | 1.236365  |
| 6                      | -1.165045 | 0.505991                       | 0.483561  |
| 8                      | -3.785039 | -1.550165                      | 1.171375  |
| 7                      | 0.182947  | 0.890677                       | 0.699737  |
| 6                      | 1.137203  | -0.059243                      | 0.125263  |
| 6                      | 0.587301  | -0.556617                      | -1.240488 |
| 6                      | 2.467183  | 0.692045                       | -0.066491 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 1  | 0.890959  | 0.103726  | -2.056119 |
| 8  | 2.457293  | 1.891703  | -0.340729 |
| 7  | 3.587918  | -0.047753 | 0.040127  |
| 6  | 4.909519  | 0.517097  | -0.162495 |
| 6  | 5.935847  | -0.574316 | 0.068100  |
| 1  | 5.021306  | 0.918577  | -1.176067 |
| 1  | 5.097377  | 1.348036  | 0.527366  |
| 8  | 5.655555  | -1.712927 | 0.383262  |
| 8  | 7.183413  | -0.123397 | -0.118168 |
| 1  | 7.805022  | -0.854972 | 0.043231  |
| 1  | 3.563235  | -1.023846 | 0.316996  |
| 1  | -5.435345 | 0.217828  | -1.838269 |
| 1  | -5.171308 | -2.624924 | -0.275900 |
| 16 | -1.247749 | -0.506396 | -1.094862 |
| 1  | 0.905662  | -1.577569 | -1.458623 |
| 1  | 1.258490  | -0.912506 | 0.800254  |
| 8  | -1.552912 | -0.410166 | 1.561959  |
| 1  | 0.407040  | 1.828041  | 0.360005  |
| 1  | -1.129615 | -0.105658 | 2.382351  |
| 1  | -2.902717 | -1.099643 | 1.440035  |