

Supporting Information

**Collision-Induced Dissociation of Homodimeric and Heterodimeric Radical Cations of  
9-Methylguanine and 9-Methyl-8-oxoguanine: Correlation between Intra-Base Pair Proton  
Transfer Originating from the N1-H at a Watson-Crick Edge and Non-statistical Dissociation**

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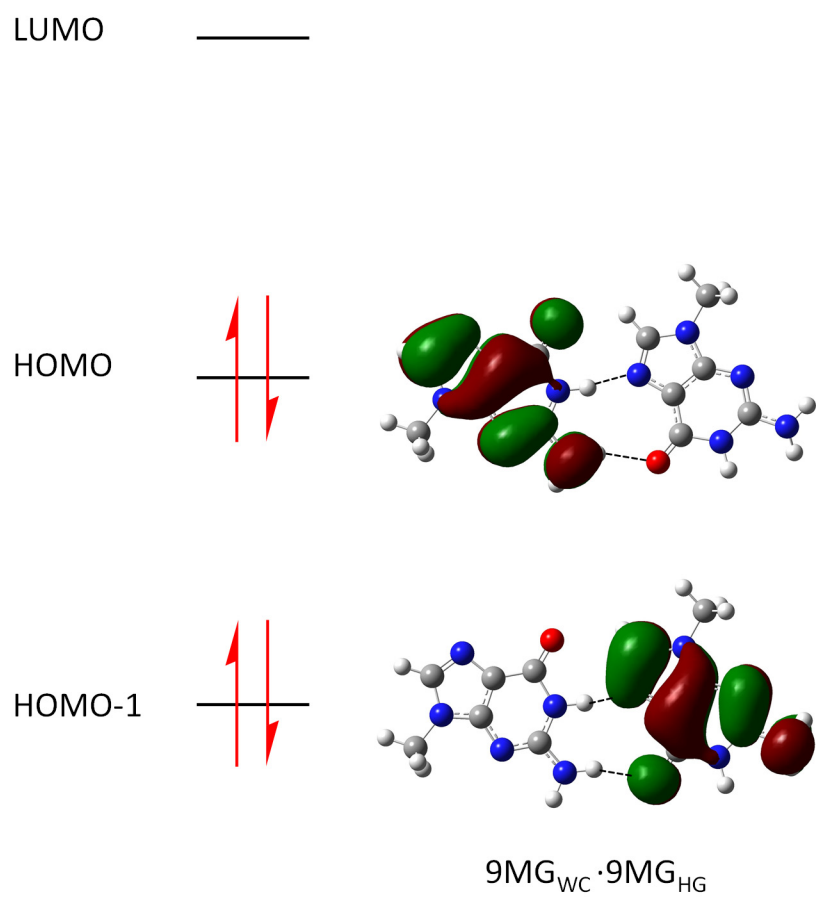
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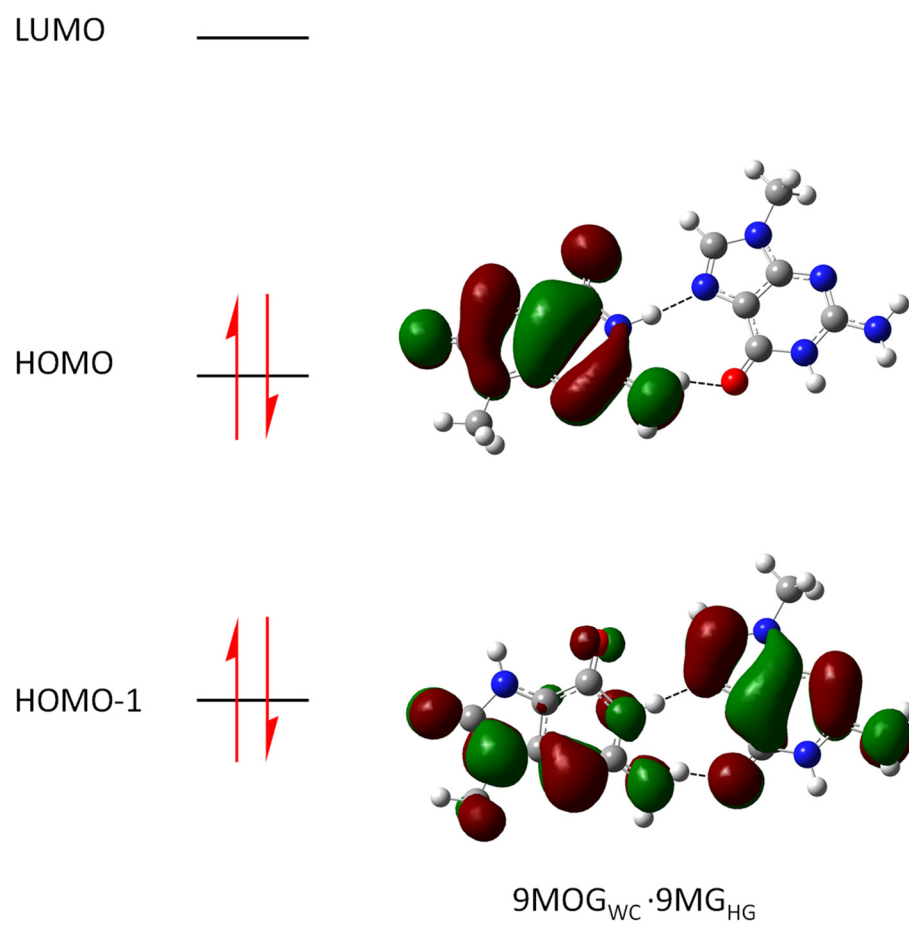
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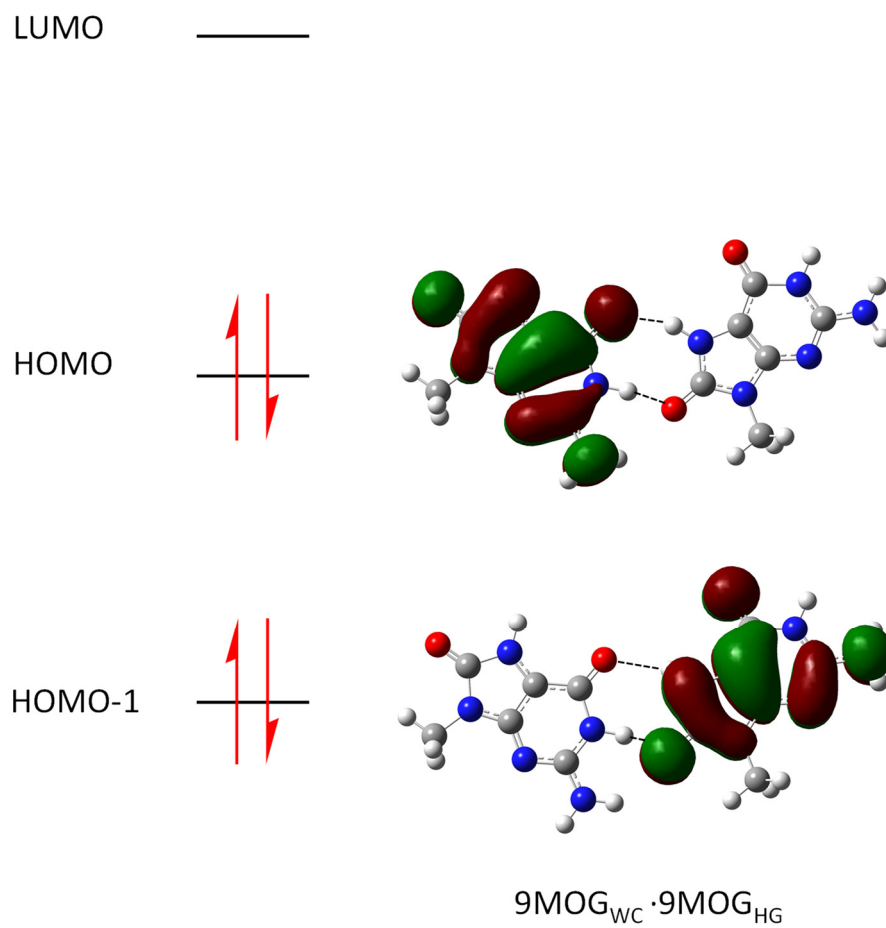
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**Figure S1.** The HOMO of neutral  $9MG \cdot 9MG$  calculated at the  $\omega B97XD/6-311++G(d,p)$  level of theory.



**Figure S2.** The HOMO of neutral 9MOG·9MG calculated at the  $\omega$ B97XD/6-311++G(d,p) level of theory.



**Figure S3.** The HOMO of neutral 9MOG·9MOG calculated at the  $\omega$ B97XD/6-311++G(d,p) level of theory.

**Cartesian coordinates for the structures  
in Scheme 2, optimized at  $\omega$ B97XD/  
6-311++G(d,p).**

**[9MG·9MG]<sup>+</sup>\_1**

C1 2.548446 -1.486703 -0.010590  
 C2 2.401748 -0.076923 -0.008133  
 H3 4.068529 -2.846906 0.026469  
 C4 4.962484 -0.972728 -0.000829  
 C5 1.708585 1.933187 0.008579  
 N6 3.900629 -1.850306 -0.006975  
 N7 1.269184 0.701801 -0.003744  
 N8 3.075088 2.005971 0.014970  
 N9 4.820297 0.327602 -0.000590  
 C10 3.532489 0.718726 0.002920  
 N11 6.200814 -1.512064 0.038119  
 H12 6.972820 -0.872097 -0.048138  
 H13 6.367602 -2.477964 -0.183305  
 O14 1.677327 -2.353175 -0.011310  
 H15 1.078285 2.811036 0.015135  
 C16 3.897931 3.205766 0.010457  
 H17 4.656807 3.128449 0.788132  
 H18 4.384020 3.325542 -0.958088  
 H19 3.261459 4.066664 0.208840  
 C20 -3.998058 -0.414998 0.001201  
 C21 -5.706849 0.933178 -0.007117  
 C22 -3.603772 0.959850 -0.007512  
 H23 -6.739040 1.255926 -0.009631  
 N24 -4.663976 1.763804 -0.012509  
 C25 -6.256500 -1.539035 0.024489  
 H26 -6.168361 -2.051950 0.982064  
 H27 -5.984803 -2.219564 -0.781460  
 H28 -7.280338 -1.197028 -0.116393  
 N29 -5.371482 -0.381524 -0.000216  
 N30 -3.237899 -1.473326 0.006203  
 O31 -1.651117 2.341550 -0.012873  
 C32 -2.171448 1.257516 -0.009405  
 N33 -1.406739 0.076296 -0.005689  
 H34 -0.359938 0.244013 -0.005911  
 N35 -1.075320 -2.205808 0.003979  
 H36 -0.041385 -2.133510 -0.001594  
 H37 -1.493328 -3.123770 0.009850  
 C38 -1.899419 -1.181665 0.001382

Zero-point correction= 0.293463 (Hartree/Particle)  
 Thermal correction to Energy= 0.314809  
 Thermal correction to Enthalpy= 0.315753  
 Thermal correction to Gibbs Free Energy= 0.241210  
 Sum of electronic and zero-point Energies= -1163.174910  
 Sum of electronic and thermal Energies= -1163.153564  
 Sum of electronic and thermal Enthalpies= -1163.152620  
 Sum of electronic and thermal Free Energies= -1163.227163

**[9MG·9MG]<sup>+</sup>\_2**

C1 2.576736 -1.531717 -0.001735  
 C2 2.369458 -0.122114 0.001791

H3 4.180182 -2.795066 -0.010428  
 C4 4.963944 -0.871566 -0.007735  
 C5 1.570027 1.895943 0.013724  
 N6 3.954493 -1.808900 -0.007385  
 N7 1.219845 0.628521 0.009277  
 N8 2.915188 2.010828 0.010823  
 N9 4.746376 0.423815 -0.003421  
 C10 3.443340 0.738278 0.001691  
 N11 6.226826 -1.328880 -0.012585  
 H12 6.970431 -0.651208 -0.015321  
 H13 6.460214 -2.305553 -0.018634  
 O14 1.751420 -2.426041 -0.000317  
 H15 0.860038 2.710021 0.019185  
 C16 3.688668 3.247667 -0.000465  
 H17 4.426578 3.216036 0.799579  
 H18 4.194443 3.356731 -0.959328  
 H19 3.009717 4.083607 0.156845  
 C20 -3.987927 -0.398406 -0.001420  
 C21 -5.574472 1.092906 -0.017557  
 C22 -3.474689 0.934329 -0.004924  
 H23 -6.574780 1.503786 -0.026118  
 N24 -4.465300 1.829091 -0.014965  
 C25 -6.337349 -1.320810 0.006014  
 H26 -6.300188 -1.844387 0.961479  
 H27 -6.123565 -2.021536 -0.800406  
 H28 -7.327275 -0.890763 -0.137644  
 N29 -5.356175 -0.246792 -0.011192  
 N30 -3.311952 -1.508996 0.005579  
 O31 -1.433079 2.156867 0.003673  
 C32 -2.017853 1.087606 0.002347  
 N33 -1.325962 -0.110293 0.008228  
 H34 0.188045 0.258898 0.010560  
 N35 -1.214316 -2.400725 0.011516  
 H36 -0.196267 -2.377118 0.010171  
 H37 -1.695424 -3.284815 0.011471  
 C38 -1.943558 -1.288603 0.008374

Zero-point correction= 0.292569 (Hartree/Particle)  
 Thermal correction to Energy= 0.314123  
 Thermal correction to Enthalpy= 0.315068  
 Thermal correction to Gibbs Free Energy= 0.240029  
 Sum of electronic and zero-point Energies= -1163.169909  
 Sum of electronic and thermal Energies= -1163.148355  
 Sum of electronic and thermal Enthalpies= -1163.147410  
 Sum of electronic and thermal Free Energies= -1163.222449

**[9MG·9MG]<sup>+</sup>\_3**

C1 -2.106139 -1.007774 -0.116871  
 C2 -2.584568 0.325494 -0.038411  
 H3 -2.876118 -2.894072 -0.138902  
 C4 -4.500823 -1.602469 -0.046961  
 N5 -3.165004 -1.924931 -0.116897  
 N6 -1.902489 1.521315 -0.011897  
 N7 -4.101557 1.895890 0.104171  
 N8 -4.938133 -0.370825 0.027649  
 C9 -3.949096 0.541222 0.033590

N10 -5.379445 -2.626700 -0.028672  
 H11 -6.356776 -2.388927 -0.054057  
 H12 -5.114479 -3.565309 -0.269758  
 O13 -0.951474 -1.415616 -0.175951  
 C14 4.087257 0.416010 -0.021265  
 C15 -5.364751 2.608050 0.215327  
 H16 -5.806308 2.442216 1.198344  
 H17 -5.181753 3.671893 0.071829  
 H18 -6.051397 2.252004 -0.551802  
 N19 5.449063 0.590569 -0.003146  
 N20 5.069484 -1.628589 0.181353  
 C21 5.976684 -0.654622 0.118284  
 H22 7.045028 -0.816681 0.160962  
 N23 3.176398 1.342707 -0.118893  
 C24 1.895236 0.857985 -0.100464  
 C25 3.901624 -0.995807 0.097585  
 C26 6.152880 1.861857 -0.105112  
 H27 5.791353 2.541302 0.665962  
 H28 7.216902 1.682168 0.038483  
 H29 5.984943 2.301672 -1.088017  
 C30 2.532035 -1.511608 0.103442  
 O31 2.188520 -2.655298 0.185138  
 N32 1.592589 -0.455145 -0.007472  
 H33 0.596434 -0.756922 -0.048365  
 N34 0.938623 1.758039 -0.180233  
 H35 -0.083861 1.570915 -0.129720  
 H36 1.244875 2.716410 -0.251838  
 C37 -2.840599 2.428150 0.074559  
 H38 -2.680353 3.495426 0.119424

Zero-point correction= 0.293786 (Hartree/Particle)  
 Thermal correction to Energy= 0.315264  
 Thermal correction to Enthalpy= 0.316209  
 Thermal correction to Gibbs Free Energy= 0.240140  
 Sum of electronic and zero-point Energies= -1163.168707  
 Sum of electronic and thermal Energies= -1163.147228  
 Sum of electronic and thermal Enthalpies= -1163.146284  
 Sum of electronic and thermal Free Energies= -1163.222353

#### [9MG·9MG]<sup>+</sup>\_4

C1 2.027167 0.855309 -0.016707  
 C2 3.487902 0.918035 0.007105  
 H3 0.519751 -0.633197 -0.045584  
 C4 2.359737 -1.563508 -0.021946  
 N5 1.582329 -0.463617 -0.031874  
 N6 4.322721 1.950270 0.027926  
 N7 5.526582 0.037220 0.038265  
 N8 3.722180 -1.539772 -0.001308  
 C9 4.203193 -0.326926 0.011849  
 N10 1.759512 -2.739514 -0.032784  
 H11 2.322224 -3.575889 -0.026444  
 H12 0.745748 -2.803531 -0.045313  
 O13 1.244527 1.777915 -0.023681  
 C14 -4.208885 0.139635 0.008953  
 C15 6.666536 -0.873220 0.034985  
 H16 6.734888 -1.376905 -0.928939

H17 7.572538 -0.296984 0.213667  
 H18 6.541168 -1.610531 0.826733  
 N19 -5.397416 -0.515411 0.032471  
 N20 -3.813428 -2.108262 0.003357  
 C21 -5.088420 -1.862382 0.029597  
 H22 -5.869520 -2.609359 0.045418  
 N23 -4.036899 1.474537 0.007707  
 C24 -2.779852 1.830191 -0.023293  
 C25 -3.235588 -0.858818 -0.010198  
 C26 -6.713847 0.096356 0.080473  
 H27 -6.801360 0.843089 -0.708343  
 H28 -7.464256 -0.678336 -0.070775  
 H29 -6.875215 0.574226 1.047544  
 C30 -1.887881 -0.458896 -0.037068  
 O31 -0.867018 -1.176969 -0.054594  
 N32 -1.741499 0.928290 -0.042950  
 H33 -0.788080 1.285136 -0.071161  
 N34 -2.443235 3.138395 -0.063326  
 H35 -1.496769 3.449542 0.069676  
 H36 -3.187339 3.807207 0.038146  
 C37 5.536523 1.392415 0.045275  
 H38 6.460711 1.953875 0.065047

Zero-point correction= 0.292915 (Hartree/Particle)  
 Thermal correction to Energy= 0.314551  
 Thermal correction to Enthalpy= 0.315496  
 Thermal correction to Gibbs Free Energy= 0.239159  
 Sum of electronic and zero-point Energies= -1163.161301  
 Sum of electronic and thermal Energies= -1163.139665  
 Sum of electronic and thermal Enthalpies= -1163.138721  
 Sum of electronic and thermal Free Energies= -1163.215057

#### [9MG·9MG]<sup>+</sup>\_5

C1 1.867291 0.607355 0.001675  
 C2 3.303721 0.872801 0.003984  
 H3 -0.034533 -1.107560 0.003377  
 C4 2.458623 -1.678202 -0.004493  
 N5 1.526902 -0.721610 -0.002087  
 N6 3.998337 2.009426 0.010598  
 N7 5.441065 0.269408 0.007207  
 N8 3.829038 -1.514742 -0.003809  
 C9 4.171635 -0.261330 0.000688  
 N10 2.064479 -2.949436 -0.007995  
 H11 2.761700 -3.676213 -0.009979  
 H12 1.086562 -3.194471 -0.008672  
 O13 1.015216 1.492101 0.002762  
 C14 -4.146450 0.236304 -0.002454  
 C15 6.687223 -0.485388 -0.009225  
 H16 6.801220 -0.993228 -0.966851  
 H17 7.514412 0.206461 0.139944  
 H18 6.676040 -1.219897 0.795053  
 N19 -5.394435 -0.290181 -0.004359  
 N20 -3.990131 -2.050237 0.006567  
 C21 -5.228272 -1.665340 0.003584  
 H22 -6.085384 -2.324419 0.004126  
 N23 -3.824706 1.533989 -0.007208

C24 -2.528861 1.747587 -0.007949  
 C25 -3.280823 -0.869533 0.002914  
 C26 -6.642520 0.455950 0.010161  
 H27 -6.621825 1.218053 -0.768119  
 H28 -7.461979 -0.234813 -0.182239  
 H29 -6.787648 0.932841 0.980074  
 C30 -1.924213 -0.588644 0.002175  
 O31 -0.987528 -1.480367 0.006397  
 N32 -1.598352 0.734959 -0.003049  
 H33 -0.591241 0.998879 -0.001546  
 N34 -2.039759 2.998621 -0.013676  
 H35 -1.051240 3.188473 -0.011364  
 H36 -2.693221 3.762631 -0.014448  
 C37 5.273065 1.614450 0.011483  
 H38 6.116048 2.291949 0.016799

Zero-point correction= 0.293073 (Hartree/Particle)  
 Thermal correction to Energy= 0.314362  
 Thermal correction to Enthalpy= 0.315306  
 Thermal correction to Gibbs Free Energy= 0.240376  
 Sum of electronic and zero-point Energies= -1163.160086  
 Sum of electronic and thermal Energies= -1163.138797  
 Sum of electronic and thermal Enthalpies= -1163.137853  
 Sum of electronic and thermal Free Energies= -1163.212783

#### [9MG·9MG]<sup>+</sup>\_6

C1 1.695825 -1.112916 -0.233518  
 C2 3.134432 -0.903011 -0.393230  
 H3 -0.726475 -0.311594 0.009104  
 C4 1.702673 0.898956 0.985779  
 C5 5.199260 -0.927644 -0.798973  
 N6 1.032311 -0.111815 0.446217  
 N7 4.077677 -1.620940 -1.001018  
 N8 3.051852 1.176955 0.886518  
 C9 3.687596 0.270373 0.205163  
 N10 1.024522 1.798691 1.713950  
 H11 1.541524 2.524107 2.184403  
 H12 0.082808 1.598701 2.007141  
 O13 1.105186 -2.097205 -0.657649  
 H14 6.171458 -1.229755 -1.164237  
 C15 -2.641941 0.557474 -0.287226  
 C16 -3.605912 2.450573 -0.736820  
 C17 -3.994894 0.485004 -0.064884  
 H18 -3.691169 3.481773 -1.048041  
 N19 -4.582863 1.688982 -0.349419  
 N20 -1.746815 -0.478279 -0.128315  
 O21 -5.721085 -1.062986 0.576359  
 C22 -4.591100 -0.767780 0.331135  
 N23 -3.573665 -1.807336 0.387582  
 H24 -3.954919 -2.722219 0.592918  
 N25 -1.421109 -2.708620 0.333563  
 H26 -1.767482 -3.619266 0.584712  
 H27 -0.453945 -2.609472 -0.007727  
 C28 -2.248619 -1.683536 0.198818  
 N29 -2.376767 1.811754 -0.724314  
 N30 5.031004 0.212919 -0.084017

C31 -1.107191 2.334319 -1.203594  
 H32 -0.399993 2.464883 -0.383246  
 H33 -0.686140 1.659101 -1.950456  
 H34 -1.288871 3.300992 -1.670237  
 C35 6.038752 1.187101 0.313013  
 H36 5.862485 2.134191 -0.196620  
 H37 5.991101 1.338128 1.390904  
 H38 7.020511 0.802305 0.042480

Zero-point correction= 0.293350 (Hartree/Particle)  
 Thermal correction to Energy= 0.314776  
 Thermal correction to Enthalpy= 0.315720  
 Thermal correction to Gibbs Free Energy= 0.240634  
 Sum of electronic and zero-point Energies= -1163.140380  
 Sum of electronic and thermal Energies= -1163.118954  
 Sum of electronic and thermal Enthalpies= -1163.118010  
 Sum of electronic and thermal Free Energies= -1163.193096

#### [9MG·9MG]<sup>+</sup>\_7

C1 1.816475 -1.142120 -0.022033  
 C2 3.205013 -0.972718 -0.259153  
 H3 0.242162 0.007646 0.614677  
 C4 1.949413 1.123980 0.941259  
 C5 5.234426 -1.127550 -0.805035  
 N6 1.256964 -0.002225 0.578789  
 N7 4.127525 -1.809906 -0.833794  
 N8 3.216621 1.291579 0.729897  
 C9 3.794010 0.230960 0.112519  
 N10 1.187266 2.126906 1.517555  
 H11 1.766986 2.903413 1.807801  
 H12 0.584143 1.817978 2.268625  
 O13 1.096329 -2.107974 -0.279764  
 H14 6.189868 -1.469801 -1.177036  
 C15 -2.753773 0.533350 -0.276537  
 C16 -3.823104 2.382844 -0.684627  
 C17 -4.171715 0.382195 -0.145930  
 H18 -3.985318 3.418182 -0.951798  
 N19 -4.801469 1.524435 -0.390863  
 N20 -1.824223 -0.367727 -0.098718  
 O21 -5.830791 -1.257625 0.405003  
 C22 -4.696850 -0.930839 0.224608  
 N23 -3.631362 -1.867454 0.349636  
 H24 -3.937810 -2.808631 0.565329  
 N25 -1.420951 -2.580151 0.274145  
 H26 -1.701307 -3.532144 0.457933  
 H27 -0.397279 -2.371766 0.070159  
 C28 -2.301736 -1.620444 0.177766  
 N29 -2.576329 1.847639 -0.625276  
 N30 5.099804 0.124287 -0.241263  
 C31 -1.308146 2.492777 -0.954050  
 H32 -0.638796 2.480864 -0.092138  
 H33 -0.843785 1.972401 -1.791887  
 H34 -1.512176 3.523946 -1.237192  
 C35 6.134833 1.123738 -0.039017  
 H36 5.855005 2.056725 -0.528178  
 H37 6.281932 1.303640 1.026240

H38 7.062074 0.753616 -0.473816

Sum of electronic and thermal Free Energies= -1163.187466

Zero-point correction= 0.293951 (Hartree/Particle)  
 Thermal correction to Energy= 0.314971  
 Thermal correction to Enthalpy= 0.315915  
 Thermal correction to Gibbs Free Energy= 0.241929  
 Sum of electronic and zero-point Energies= -1163.139771  
 Sum of electronic and thermal Energies= -1163.118750  
 Sum of electronic and thermal Enthalpies= -1163.117806  
 Sum of electronic and thermal Free Energies= -1163.191793

**[9MG·9MG]<sup>+</sup>\_8**

C1 1.844778 -1.129718 -0.243717  
 C2 3.214233 -0.907972 -0.361941  
 H3 0.123034 -0.139975 0.297647  
 C4 1.749301 0.994716 0.911498  
 C5 5.286178 -0.933156 -0.721170  
 N6 1.150926 -0.119921 0.375997  
 N7 4.225712 -1.655101 -0.915373  
 N8 3.025496 1.239492 0.830116  
 C9 3.711842 0.286282 0.174589  
 N10 0.902428 1.889830 1.509031  
 H11 1.386113 2.639919 1.981872  
 H12 0.132402 1.506346 2.037431  
 O13 1.225214 -2.163486 -0.671117  
 H14 6.288105 -1.201022 -1.026642  
 C15 -2.726279 0.542579 -0.283451  
 C16 -3.926736 2.317185 -0.684003  
 C17 -4.119699 0.312097 -0.080165  
 H18 -4.161499 3.333598 -0.969041  
 N19 -4.830465 1.412359 -0.322989  
 N20 -1.737119 -0.298103 -0.130028  
 O21 -5.662734 -1.391671 0.591881  
 C22 -4.551302 -1.019612 0.350498  
 N23 -3.439264 -1.884033 0.447537  
 H24 -3.681354 -2.834459 0.697019  
 N25 -1.167878 -2.470192 0.245914  
 H26 -1.470005 -3.409531 0.482750  
 H27 0.249657 -2.260399 -0.317268  
 C28 -2.112199 -1.594287 0.195436  
 N29 -2.645964 1.858619 -0.670886  
 N30 5.043919 0.258623 -0.058739  
 C31 -1.443338 2.563075 -1.093449  
 H32 -0.699832 2.547431 -0.295792  
 H33 -1.036373 2.093120 -1.989611  
 H34 -1.707089 3.595532 -1.316876  
 C35 6.010601 1.289037 0.290383  
 H36 6.055226 2.050750 -0.488921  
 H37 5.713098 1.749758 1.231120  
 H38 6.989852 0.827814 0.409089

Zero-point correction= 0.293291 (Hartree/Particle)  
 Thermal correction to Energy= 0.314031  
 Thermal correction to Enthalpy= 0.314975  
 Thermal correction to Gibbs Free Energy= 0.242135  
 Sum of electronic and zero-point Energies= -1163.136311  
 Sum of electronic and thermal Energies= -1163.115571  
 Sum of electronic and thermal Enthalpies= -1163.114627

**[9MG·9MG]<sup>+</sup>\_9**

C1 4.121488 -1.650374 -0.373892  
 C2 4.257601 -0.260343 0.062440  
 H3 2.606758 -2.910290 -0.894145  
 C4 1.661738 -1.129374 -0.451271  
 N5 2.763760 -1.953563 -0.605166  
 N6 5.344511 0.437628 0.390023  
 N7 3.534151 1.770025 0.569216  
 N8 1.841417 0.196982 -0.085060  
 C9 3.079473 0.539100 0.157633  
 N10 0.449227 -1.530646 -0.633252  
 H11 -0.961769 -0.630097 -0.275782  
 H12 0.394412 -2.502850 -0.921757  
 O13 4.985688 -2.463990 -0.530033  
 C14 -3.067968 -0.544963 0.143698  
 C15 2.725613 2.953412 0.812478  
 H16 1.831989 2.670915 1.368950  
 H17 3.304580 3.659323 1.405617  
 H18 2.446486 3.423248 -0.132143  
 N19 -3.366372 -1.800405 0.551437  
 C20 -4.741995 -1.808334 0.707282  
 H21 -5.256937 -2.702467 1.027933  
 N22 -1.821237 -0.028387 -0.136977  
 C23 -1.758285 1.262597 -0.479956  
 C24 -4.253790 0.147966 0.078153  
 C25 -2.455677 -2.915902 0.746476  
 H26 -1.553321 -2.573960 1.255070  
 H27 -2.946827 -3.659292 1.372226  
 H28 -2.194743 -3.372252 -0.210348  
 C29 -4.255327 1.536989 -0.304487  
 O30 -5.139768 2.328121 -0.430086  
 N31 -0.571831 1.812158 -0.740307  
 H32 -0.515407 2.739259 -1.124772  
 H33 0.290645 1.288837 -0.559400  
 C34 4.884181 1.645989 0.690610  
 H35 5.504067 2.472464 1.010457  
 N36 -5.294778 -0.665482 0.437185  
 N37 -2.888469 1.983774 -0.547640  
 H38 -2.832268 2.968948 -0.772143

Zero-point correction= 0.292619 (Hartree/Particle)  
 Thermal correction to Energy= 0.314189  
 Thermal correction to Enthalpy= 0.315133  
 Thermal correction to Gibbs Free Energy= 0.238770  
 Sum of electronic and zero-point Energies= -1163.126913  
 Sum of electronic and thermal Energies= -1163.105343  
 Sum of electronic and thermal Enthalpies= -1163.104399  
 Sum of electronic and thermal Free Energies= -1163.180762

**[9MG·9MG]<sup>+</sup>\_10**

C1 -4.103401 1.550504 -0.612212  
 C2 -4.234049 0.227421 -0.004492  
 H3 -2.574939 2.768134 -1.244615  
 C4 -1.659729 1.056423 -0.555549



|     |           |           |           |
|-----|-----------|-----------|-----------|
| N5  | -2.727933 | 1.850311  | -0.844055 |
| N6  | -5.311299 | -0.443434 | 0.381283  |
| N7  | -3.477886 | -1.702560 | 0.785591  |
| N8  | -1.804092 | -0.193747 | -0.028206 |
| C9  | -3.040411 | -0.529526 | 0.229284  |
| N10 | -0.436675 | 1.468714  | -0.780388 |
| H11 | 0.398202  | 0.870953  | -0.483950 |
| H12 | -0.266803 | 2.373093  | -1.194281 |
| O13 | -4.959644 | 2.330024  | -0.899990 |
| C14 | 2.969729  | 0.506632  | 0.228863  |
| C15 | -2.641113 | -2.824477 | 1.201070  |
| H16 | -1.757811 | -2.439725 | 1.708910  |
| H17 | -3.210572 | -3.450073 | 1.885863  |
| H18 | -2.341930 | -3.410858 | 0.332004  |
| N19 | 3.178367  | 1.731084  | 0.789540  |
| C20 | 4.549489  | 1.858759  | 0.907384  |
| H21 | 4.991412  | 2.749334  | 1.331273  |
| N22 | 1.751343  | -0.041782 | -0.077303 |
| C23 | 1.838709  | -1.273134 | -0.533370 |
| C24 | 4.223598  | -0.040198 | 0.042553  |
| C25 | 2.177504  | 2.697969  | 1.185155  |
| H26 | 1.326157  | 2.184257  | 1.634219  |
| H27 | 2.605985  | 3.370865  | 1.927010  |
| H28 | 1.843639  | 3.293527  | 0.330683  |
| C29 | 4.338672  | -1.367448 | -0.502332 |
| O30 | 5.295765  | -2.046511 | -0.750952 |
| N31 | 0.700655  | -1.978343 | -0.786577 |
| H32 | 0.716456  | -2.702918 | -1.484627 |
| H33 | -0.173453 | -1.494064 | -0.636192 |
| C34 | -4.830849 | -1.595762 | 0.854113  |
| H35 | -5.445293 | -2.385969 | 1.264036  |
| N36 | 5.198737  | 0.822041  | 0.472997  |
| N37 | 3.020640  | -1.902116 | -0.737365 |
| H38 | 3.028082  | -2.868804 | -1.034242 |

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.292600 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.314113                    |
| Thermal correction to Enthalpy=              | 0.315057                    |
| Thermal correction to Gibbs Free Energy=     | 0.239090                    |
| Sum of electronic and zero-point Energies=   | -1163.123703                |
| Sum of electronic and thermal Energies=      | -1163.102191                |
| Sum of electronic and thermal Enthalpies=    | -1163.101246                |
| Sum of electronic and thermal Free Energies= | -1163.177214                |

**Cartesian coordinates for the structures  
in Scheme 3, optimized at  $\omega$ B97XD/  
6-311++G(d,p).**

**[9MOG·9MG]<sup>+</sup>\_1**

|     |           |           |           |
|-----|-----------|-----------|-----------|
| C1  | 1.899472  | 1.124569  | 0.004986  |
| C2  | 3.302433  | 0.779486  | 0.006323  |
| H3  | 0.056756  | 0.179627  | -0.004599 |
| C4  | 1.569990  | -1.293020 | -0.005870 |
| C5  | 5.557915  | 0.696742  | 0.008598  |
| N6  | 1.099982  | -0.017299 | -0.000310 |
| N7  | 4.413473  | 1.529222  | 0.011561  |
| N8  | 5.053948  | -0.614274 | 0.003023  |
| N9  | 2.891158  | -1.613750 | -0.007902 |
| C10 | 3.698584  | -0.590074 | -0.000830 |
| N11 | 0.709999  | -2.288081 | -0.010023 |
| H12 | 1.096901  | -3.219353 | -0.014543 |
| H13 | -0.318751 | -2.181607 | -0.006133 |
| O14 | 1.448934  | 2.248442  | 0.007716  |
| C15 | -3.816543 | 0.770314  | -0.003731 |
| C16 | 5.895009  | -1.802352 | -0.014643 |
| H17 | 5.794859  | -2.315321 | -0.971271 |
| H18 | 6.925048  | -1.479603 | 0.125641  |
| H19 | 5.599064  | -2.469229 | 0.794381  |
| O20 | 6.696561  | 1.046381  | 0.012132  |
| H21 | 4.464749  | 2.538519  | 0.017339  |
| N22 | -3.321233 | 2.043897  | -0.002190 |
| N23 | -1.554727 | 0.686800  | -0.012351 |
| C24 | -1.957961 | 1.930796  | -0.008913 |
| H25 | -1.302574 | 2.789977  | -0.008335 |
| N26 | -5.115459 | 0.418368  | -0.002054 |
| C27 | -5.296378 | -0.877545 | 0.008423  |
| C28 | -2.710026 | -0.058345 | -0.009951 |
| C29 | -4.109440 | 3.266671  | -0.015370 |
| H30 | -4.864892 | 3.220337  | 0.768027  |
| H31 | -3.446932 | 4.111047  | 0.168275  |
| H32 | -4.598652 | 3.388714  | -0.982048 |
| C33 | -2.898431 | -1.463960 | -0.001771 |
| O34 | -2.053908 | -2.354887 | 0.001673  |
| N35 | -4.261330 | -1.786436 | 0.007409  |
| H36 | -4.458782 | -2.777420 | 0.046829  |
| N37 | -6.549744 | -1.378935 | 0.052160  |
| H38 | -6.746033 | -2.343487 | -0.149721 |
| H39 | -7.303661 | -0.717969 | -0.034775 |

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.298773 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.321262                    |
| Thermal correction to Enthalpy=              | 0.322206                    |
| Thermal correction to Gibbs Free Energy=     | 0.245099                    |
| Sum of electronic and zero-point Energies=   | -1238.435628                |
| Sum of electronic and thermal Energies=      | -1238.413139                |
| Sum of electronic and thermal Enthalpies=    | -1238.412195                |
| Sum of electronic and thermal Free Energies= | -1238.489302                |

**[9MOG·9MG]<sup>+</sup>\_2**

|    |           |          |           |
|----|-----------|----------|-----------|
| C1 | -1.758599 | 0.944447 | -0.009300 |
|----|-----------|----------|-----------|

|     |           |           |           |
|-----|-----------|-----------|-----------|
| C2  | -3.189670 | 0.726766  | -0.006258 |
| H3  | 0.484685  | 0.208697  | -0.004825 |
| C4  | -1.611753 | -1.417153 | 0.000161  |
| C5  | -5.446928 | 0.824047  | -0.002499 |
| N6  | -1.023672 | -0.212861 | -0.006935 |
| N7  | -4.241567 | 1.561338  | -0.008440 |
| N8  | -5.052663 | -0.520077 | 0.001652  |
| N9  | -2.961006 | -1.678596 | 0.006358  |
| C10 | -3.693462 | -0.604746 | 0.001828  |
| N11 | -0.834781 | -2.496325 | 0.002094  |
| H12 | -1.279057 | -3.399480 | 0.007976  |
| H13 | 0.180569  | -2.431398 | -0.002647 |
| O14 | -1.248562 | 2.060989  | -0.013222 |
| C15 | 3.719098  | 0.795204  | 0.002977  |
| C16 | -5.984197 | -1.635779 | 0.020047  |
| H17 | -5.922894 | -2.159711 | 0.974330  |
| H18 | -6.985739 | -1.231100 | -0.115006 |
| H19 | -5.746182 | -2.323171 | -0.791237 |
| O20 | -6.555807 | 1.266915  | -0.003055 |
| H21 | -4.212430 | 2.570504  | -0.013906 |
| N22 | 3.148674  | 2.049867  | 0.001964  |
| N23 | 1.500771  | 0.611706  | -0.001389 |
| C24 | 1.808390  | 1.890309  | 0.000241  |
| H25 | 1.072450  | 2.680775  | -0.001168 |
| N26 | 5.031668  | 0.524835  | 0.003316  |
| C27 | 5.292761  | -0.763005 | -0.000772 |
| C28 | 2.674733  | -0.100439 | 0.000230  |
| C29 | 3.881676  | 3.311170  | 0.019266  |
| H30 | 4.616303  | 3.309474  | -0.784376 |
| H31 | 3.175257  | 4.125906  | -0.128088 |
| H32 | 4.388445  | 3.428787  | 0.976579  |
| C33 | 2.928769  | -1.502832 | -0.004001 |
| O34 | 2.133646  | -2.423145 | -0.007389 |
| N35 | 4.315127  | -1.733396 | -0.003858 |
| H36 | 4.573811  | -2.711493 | -0.006643 |
| N37 | 6.570085  | -1.177019 | -0.002008 |
| H38 | 6.836563  | -2.145319 | -0.004119 |
| H39 | 7.290646  | -0.474783 | 0.001660  |

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.297994 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.320631                    |
| Thermal correction to Enthalpy=              | 0.321575                    |
| Thermal correction to Gibbs Free Energy=     | 0.244203                    |
| Sum of electronic and zero-point Energies=   | -1238.431412                |
| Sum of electronic and thermal Energies=      | -1238.408775                |
| Sum of electronic and thermal Enthalpies=    | -1238.407831                |
| Sum of electronic and thermal Free Energies= | -1238.485203                |

**[9MOG·9MG]<sup>+</sup>\_3**

|    |           |           |           |
|----|-----------|-----------|-----------|
| C1 | -2.401074 | -1.012193 | -0.127710 |
| C2 | -2.905408 | 0.309487  | -0.029621 |
| H3 | -3.133518 | -2.912966 | -0.179915 |
| C4 | -4.783251 | -1.654989 | -0.073350 |
| N5 | -3.440894 | -1.949971 | -0.145740 |
| N6 | -2.246897 | 1.517695  | 0.016252  |
| N7 | -4.453247 | 1.847227  | 0.135488  |

N8 -5.244977 -0.434031 0.020879  
 C9 -4.274355 0.497387 0.043866  
 N10 -5.640829 -2.697644 -0.072639  
 H11 -6.622487 -2.478080 -0.099781  
 H12 -5.357472 -3.623243 -0.341854  
 O13 -1.237442 -1.396898 -0.189360  
 C14 3.775647 0.537827 -0.048103  
 C15 -5.729825 2.533643 0.256846  
 H16 -6.163958 2.353241 1.240605  
 H17 -5.567995 3.601660 0.119201  
 H18 -6.412446 2.169112 -0.509859  
 N19 5.115326 0.743816 -0.048978  
 C20 5.788537 -0.482228 0.090055  
 N21 2.836508 1.436953 -0.152222  
 C22 1.569753 0.944575 -0.116027  
 C23 3.565221 -0.862269 0.096612  
 C24 5.792559 2.025536 -0.175210  
 H25 5.427128 2.709321 0.590423  
 H26 6.857903 1.849155 -0.038140  
 H27 5.611912 2.448207 -1.163601  
 C28 2.224015 -1.399937 0.122747  
 O29 1.941378 -2.566934 0.229583  
 N30 1.271747 -0.376675 0.002474  
 H31 0.278482 -0.693021 -0.041008  
 N32 0.592594 1.822631 -0.204166  
 H33 -0.422133 1.613777 -0.132284  
 H34 0.877409 2.785790 -0.294597  
 C35 -3.202493 2.404281 0.115631  
 H36 -3.062680 3.473584 0.177467  
 N37 4.765497 -1.453850 0.177482  
 H38 4.947575 -2.442687 0.281181  
 O39 6.963881 -0.672872 0.129271

Zero-point correction= 0.298907 (Hartree/Particle)  
 Thermal correction to Energy= 0.321512  
 Thermal correction to Enthalpy= 0.322456  
 Thermal correction to Gibbs Free Energy= 0.243945  
 Sum of electronic and zero-point Energies= -1238.430605  
 Sum of electronic and thermal Energies= -1238.408000  
 Sum of electronic and thermal Enthalpies= -1238.407056  
 Sum of electronic and thermal Free Energies= -1238.485567

#### [9MOG·9MG]<sup>+</sup>\_4

C1 -1.772287 -0.675452 0.049183  
 C2 -3.216419 -0.674094 0.020002  
 H3 -0.203666 0.737978 0.067147  
 C4 -2.024425 1.740286 0.020582  
 C5 -5.430444 -1.111493 -0.025297  
 N6 -1.274094 0.612143 0.051113  
 N7 -4.123651 -1.658428 0.009028  
 N8 -5.242267 0.281569 -0.032029  
 N9 -3.375540 1.758843 -0.009873  
 C10 -3.921658 0.571127 -0.008135  
 N11 -1.375866 2.892110 0.020377  
 H12 -1.905935 3.748957 -0.002431  
 H13 -0.361930 2.919272 0.038500

O14 -1.052903 -1.658028 0.068856  
 C15 4.502641 -0.217482 -0.019343  
 C16 -6.336158 1.243281 -0.078836  
 H17 -6.340512 1.754508 -1.041458  
 H18 -7.266035 0.692878 0.051414  
 H19 -6.215488 1.968613 0.724830  
 O20 -6.455476 -1.715000 -0.042084  
 H21 -3.944771 -2.653344 0.021324  
 N22 5.710316 0.400601 -0.047903  
 N23 4.175861 2.040332 0.010090  
 C24 5.442762 1.756301 -0.026225  
 H25 6.245686 2.479788 -0.041973  
 N26 4.288323 -1.547047 -0.021525  
 C27 3.021909 -1.863116 0.000773  
 C28 3.560604 0.809470 0.015728  
 C29 7.008778 -0.250519 -0.067789  
 H30 7.033892 -0.996321 -0.861785  
 H31 7.773037 0.502365 -0.255081  
 H32 7.204032 -0.736330 0.888984  
 C33 2.200699 0.452039 0.043740  
 O34 1.205088 1.202639 0.072746  
 N35 2.011012 -0.930571 0.033959  
 H36 1.046649 -1.256353 0.029822  
 N37 2.642961 -3.162828 -0.044017  
 H38 1.709987 -3.441971 0.205857  
 H39 3.375991 -3.846096 0.047875

Zero-point correction= 0.298148 (Hartree/Particle)  
 Thermal correction to Energy= 0.320841  
 Thermal correction to Enthalpy= 0.321785  
 Thermal correction to Gibbs Free Energy= 0.242619  
 Sum of electronic and zero-point Energies= -1238.421093  
 Sum of electronic and thermal Energies= -1238.398400  
 Sum of electronic and thermal Enthalpies= -1238.397455  
 Sum of electronic and thermal Free Energies= -1238.476621

#### [9MOG·9MG]<sup>+</sup>\_5

C1 -1.617301 0.427155 -0.007238  
 C2 -3.050101 0.606389 -0.002638  
 H3 0.353971 -1.186713 -0.006246  
 C4 -2.106008 -1.875438 -0.007697  
 C5 -5.200734 1.298596 0.008869  
 N6 -1.210689 -0.871372 -0.009262  
 N7 -3.838870 1.690071 0.002555  
 N8 -5.177156 -0.103258 0.009183  
 N9 -3.468749 -1.773319 -0.004168  
 C10 -3.893048 -0.543715 -0.000343  
 N11 -1.637199 -3.121524 -0.009971  
 H12 -2.292242 -3.886418 -0.009078  
 H13 -0.647491 -3.310855 -0.012332  
 O14 -0.830717 1.382721 -0.008781  
 C15 4.411046 0.321830 0.003667  
 C16 -6.374190 -0.931428 0.003848  
 H17 -6.303371 -1.675457 0.796404  
 H18 -7.227894 -0.279306 0.179364  
 H19 -6.481732 -1.428665 -0.960365

|     |           |           |           |
|-----|-----------|-----------|-----------|
| O20 | -6.148575 | 2.020843  | 0.015214  |
| H21 | -3.545981 | 2.656526  | 0.003147  |
| N22 | 5.678160  | -0.155065 | 0.013589  |
| N23 | 4.343085  | -1.968612 | 0.009078  |
| C24 | 5.565296  | -1.535959 | 0.014103  |
| H25 | 6.447649  | -2.160849 | 0.021061  |
| N26 | 4.037709  | 1.606127  | -0.001062 |
| C27 | 2.735832  | 1.769032  | -0.005497 |
| C28 | 3.588933  | -0.816164 | 0.002455  |
| C29 | 6.897131  | 0.638108  | -0.000645 |
| H30 | 6.840297  | 1.408716  | 0.767383  |
| H31 | 7.740793  | -0.017778 | 0.208445  |
| H32 | 7.032954  | 1.107325  | -0.975611 |
| C33 | 2.222091  | -0.589654 | -0.002292 |
| O34 | 1.323967  | -1.518150 | -0.003099 |
| N35 | 1.843655  | 0.721807  | -0.006358 |
| H36 | 0.829758  | 0.947439  | -0.009146 |
| N37 | 2.200248  | 3.001888  | -0.009838 |
| H38 | 1.205942  | 3.153325  | -0.014365 |
| H39 | 2.824907  | 3.789681  | -0.011105 |

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.298104 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.320574                    |
| Thermal correction to Enthalpy=              | 0.321518                    |
| Thermal correction to Gibbs Free Energy=     | 0.243953                    |
| Sum of electronic and zero-point Energies=   | -1238.420126                |
| Sum of electronic and thermal Energies=      | -1238.397656                |
| Sum of electronic and thermal Enthalpies=    | -1238.396711                |
| Sum of electronic and thermal Free Energies= | -1238.474276                |

**[9MOG·9MG]<sup>+</sup> 6**

|     |           |           |           |
|-----|-----------|-----------|-----------|
| C1  | 3.116824  | -1.847192 | -0.011858 |
| C2  | 2.629561  | -0.483093 | -0.006289 |
| H3  | 4.939195  | -2.794816 | -0.012118 |
| C4  | 5.349154  | -0.769425 | -0.001481 |
| C5  | 1.500416  | 1.360524  | -0.000778 |
| N6  | 4.540027  | -1.864621 | -0.008937 |
| N7  | 1.386352  | -0.018273 | -0.006907 |
| N8  | 2.855930  | 1.723155  | 0.002208  |
| N9  | 4.894845  | 0.484344  | 0.004509  |
| C10 | 3.579447  | 0.583219  | 0.001148  |
| N11 | 6.669826  | -0.952148 | 0.000445  |
| H12 | 7.256958  | -0.133544 | 0.006417  |
| H13 | 7.100782  | -1.860936 | -0.004125 |
| O14 | 2.485704  | -2.868580 | -0.018013 |
| C15 | -4.316874 | -0.062321 | 0.002408  |
| C16 | 3.368108  | 3.083183  | 0.024165  |
| H17 | 4.095433  | 3.213016  | -0.776691 |
| H18 | 2.526726  | 3.756913  | -0.125375 |
| H19 | 3.840079  | 3.290917  | 0.984879  |
| O20 | 0.571262  | 2.155503  | -0.000256 |
| H21 | -0.087923 | -0.886160 | 0.004322  |
| N22 | -5.485296 | -0.745779 | 0.007813  |
| N23 | -3.863340 | -2.307261 | 0.020319  |
| C24 | -5.140705 | -2.087997 | 0.016608  |
| H25 | -5.904713 | -2.852844 | 0.022212  |

|     |           |           |           |
|-----|-----------|-----------|-----------|
| N26 | -4.168330 | 1.267718  | -0.008007 |
| C27 | -2.914196 | 1.649299  | -0.008172 |
| C28 | -3.314241 | -1.044301 | 0.011424  |
| C29 | -6.818993 | -0.167806 | -0.019982 |
| H30 | -7.007638 | 0.299905  | -0.986842 |
| H31 | -7.546016 | -0.960805 | 0.148027  |
| H32 | -6.911302 | 0.579830  | 0.767305  |
| C33 | -2.002829 | -0.591881 | 0.008264  |
| O34 | -0.969337 | -1.363707 | 0.013075  |
| N35 | -1.856648 | 0.766713  | -0.001112 |
| H36 | -0.912942 | 1.181258  | -0.002223 |
| N37 | -2.591764 | 2.953960  | -0.016319 |
| H38 | -1.635357 | 3.267833  | -0.013939 |
| H39 | -3.339552 | 3.625773  | -0.021117 |

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.298536 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.321227                    |
| Thermal correction to Enthalpy=              | 0.322172                    |
| Thermal correction to Gibbs Free Energy=     | 0.243729                    |
| Sum of electronic and zero-point Energies=   | -1238.418825                |
| Sum of electronic and thermal Energies=      | -1238.396134                |
| Sum of electronic and thermal Enthalpies=    | -1238.395190                |
| Sum of electronic and thermal Free Energies= | -1238.473632                |

**[9MOG·9MG]<sup>+</sup> 7**

|     |           |           |           |
|-----|-----------|-----------|-----------|
| C1  | -1.686730 | 0.420744  | 0.000721  |
| C2  | -3.034620 | 0.622091  | -0.003932 |
| H3  | -0.254332 | -1.093188 | 0.009566  |
| C4  | -2.148423 | -1.935039 | 0.014947  |
| C5  | -5.188285 | 1.328893  | -0.017309 |
| N6  | -1.276944 | -0.888581 | 0.009944  |
| N7  | -3.864035 | 1.729820  | -0.014748 |
| N8  | -5.144811 | -0.089247 | -0.008033 |
| N9  | -3.462293 | -1.779697 | 0.012174  |
| C10 | -3.864728 | -0.515454 | 0.001614  |
| N11 | -1.621764 | -3.167679 | 0.023856  |
| H12 | -2.251129 | -3.952042 | 0.026141  |
| H13 | -0.627220 | -3.324930 | 0.022973  |
| O14 | -0.795974 | 1.379848  | -0.003481 |
| C15 | 4.446632  | 0.343272  | -0.002088 |
| C16 | -6.335615 | -0.920788 | 0.002950  |
| H17 | -6.437083 | -1.424675 | 0.964750  |
| H18 | -7.189365 | -0.264768 | -0.158976 |
| H19 | -6.276135 | -1.661076 | -0.794353 |
| O20 | -6.175156 | 2.007581  | -0.027274 |
| H21 | -3.592434 | 2.697584  | -0.023176 |
| N22 | 5.731472  | -0.148739 | -0.018116 |
| N23 | 4.340844  | -1.931208 | -0.023424 |
| C24 | 5.603304  | -1.498185 | -0.028814 |
| H25 | 6.466219  | -2.150094 | -0.042101 |
| N26 | 4.063872  | 1.584755  | 0.011057  |
| C27 | 2.689019  | 1.704792  | 0.019278  |
| C28 | 3.613072  | -0.815729 | -0.007050 |
| C29 | 6.954917  | 0.642592  | -0.004011 |
| H30 | 7.061804  | 1.144455  | 0.957573  |
| H31 | 7.801263  | -0.022495 | -0.166773 |

H32 6.915303 1.383912 -0.801106  
 C33 2.169522 -0.593720 0.003186  
 O34 1.349129 -1.508588 0.001339  
 N35 1.784180 0.722911 0.015121  
 H36 0.167873 1.059565 0.004052  
 N37 2.259591 2.965368 0.032671  
 H38 1.275820 3.180970 0.040506  
 H39 2.936246 3.711307 0.035788

Zero-point correction= 0.297425 (Hartree/Particle)  
 Thermal correction to Energy= 0.320138  
 Thermal correction to Enthalpy= 0.321082  
 Thermal correction to Gibbs Free Energy= 0.242780  
 Sum of electronic and zero-point Energies= -1238.408316  
 Sum of electronic and thermal Energies= -1238.385603  
 Sum of electronic and thermal Enthalpies= -1238.384659  
 Sum of electronic and thermal Free Energies= -1238.462961

### [9MOG·9MG]<sup>+</sup>\_8

C1 3.607236 -1.857501 0.012161  
 C2 2.932476 -0.605459 0.009857  
 H3 5.560960 -2.477143 -0.026553  
 C4 5.626046 -0.409079 0.001857  
 C5 1.450298 1.069373 -0.004789  
 N6 5.010563 -1.629636 0.008099  
 N7 1.579635 -0.279128 0.005693  
 N8 2.717150 1.598665 -0.010428  
 N9 4.969840 0.727703 0.003558  
 C10 3.635673 0.567298 0.000384  
 N11 6.978585 -0.392232 -0.039576  
 H12 7.418414 0.506688 0.064978  
 H13 7.520379 -1.205566 0.194841  
 O14 3.156111 -2.980345 0.013696  
 C15 -4.513083 0.000874 0.001701  
 C16 3.030709 3.015241 -0.011865  
 H17 3.768222 3.222301 -0.786487  
 H18 2.112489 3.561914 -0.217213  
 H19 3.431252 3.316823 0.956808  
 O20 0.390400 1.729931 -0.010300  
 H21 0.800546 -0.929094 0.003420  
 N22 -5.751539 -0.589381 -0.002192  
 N23 -4.229848 -2.260980 -0.016632  
 C24 -5.522583 -1.926635 -0.011922  
 H25 -6.332540 -2.643256 -0.016782  
 N26 -4.249721 1.279558 0.009840  
 C27 -2.913520 1.541601 0.006451  
 C28 -3.590088 -1.098090 -0.008484  
 C29 -7.034003 0.105596 0.020489  
 H30 -7.063079 0.836480 -0.786425  
 H31 -7.826748 -0.626769 -0.120840  
 H32 -7.164522 0.608978 0.978124  
 C33 -2.161361 -0.785143 -0.009452  
 O34 -1.236378 -1.556654 -0.014280  
 N35 -1.952567 0.599943 -0.003111  
 H36 -0.946211 0.946716 -0.006732

N37 -2.536458 2.809296 0.013172  
 H38 -1.553661 3.055315 0.011797  
 H39 -3.242836 3.528034 0.020852

Zero-point correction= 0.298114 (Hartree/Particle)  
 Thermal correction to Energy= 0.320951  
 Thermal correction to Enthalpy= 0.321895  
 Thermal correction to Gibbs Free Energy= 0.242352  
 Sum of electronic and zero-point Energies= -1238.407275  
 Sum of electronic and thermal Energies= -1238.384438  
 Sum of electronic and thermal Enthalpies= -1238.383494  
 Sum of electronic and thermal Free Energies= -1238.463037

### [9MOG·9MG]<sup>+</sup>\_9

C1 1.452395 -1.032423 -0.048598  
 C2 2.864276 -0.763099 -0.200955  
 H3 -0.995017 -0.274357 0.092320  
 C4 1.382141 1.021061 1.077038  
 C5 5.079030 -0.715911 -0.639216  
 N6 0.745262 -0.044934 0.579246  
 N7 2.705329 1.344818 0.965068  
 C8 3.400194 0.447514 0.325613  
 N9 0.650240 1.914421 1.762200  
 H10 1.131473 2.673529 2.217542  
 H11 -0.272040 1.663962 2.077312  
 O12 0.935226 -2.073759 -0.459564  
 C13 -2.921765 0.523980 -0.323832  
 C14 -3.924165 2.367147 -0.882890  
 C15 -4.281693 0.410155 -0.170578  
 H16 -4.027295 3.384782 -1.231162  
 N17 -4.894134 1.582955 -0.524004  
 N18 -2.002618 -0.475522 -0.084707  
 O19 -5.986200 -1.174241 0.439622  
 C20 -4.856001 -0.847546 0.240922  
 N21 -3.807962 -1.848385 0.388387  
 H22 -4.169219 -2.768180 0.607669  
 N23 -1.627670 -2.677486 0.470378  
 H24 -1.959005 -3.587518 0.743091  
 H25 -0.649820 -2.565840 0.165110  
 C26 -2.480614 -1.685279 0.259768  
 N27 -2.676617 1.773120 -0.785733  
 N28 4.728123 0.457179 0.047925  
 C29 -1.399586 2.335334 -1.195102  
 H30 -0.754936 2.514390 -0.333338  
 H31 -0.903579 1.661407 -1.895701  
 H32 -1.587997 3.282692 -1.697339  
 C33 5.679553 1.498459 0.406743  
 H34 5.366603 2.447623 -0.027568  
 H35 5.738555 1.590654 1.491198  
 H36 6.649836 1.210094 0.006367  
 O37 6.153603 -1.042666 -1.036688  
 N38 3.870744 -1.443596 -0.766086  
 H39 3.813960 -2.342261 -1.224659

Zero-point correction= 0.298422 (Hartree/Particle)  
 Thermal correction to Energy= 0.321073  
 Thermal correction to Enthalpy= 0.322017

Thermal correction to Gibbs Free Energy= 0.243390  
 Sum of electronic and zero-point Energies= -1238.402346  
 Sum of electronic and thermal Energies= -1238.379696  
 Sum of electronic and thermal Enthalpies= -1238.378752  
 Sum of electronic and thermal Free Energies= -1238.457378

### [9MOG·9MG]<sup>+</sup>\_10

C1 1.557585 -1.013478 0.106153  
 C2 2.918976 -0.790827 -0.100977  
 H3 -0.084578 0.079955 0.673093  
 C4 1.574327 1.259392 1.022412  
 C5 5.119060 -0.870376 -0.639094  
 N6 0.931273 0.109620 0.672981  
 N7 2.845754 1.461908 0.828804  
 C8 3.483021 0.425725 0.246686  
 N9 0.782871 2.255219 1.561698  
 H10 1.336530 3.049916 1.853118  
 H11 0.150190 1.952480 2.289953  
 O12 0.893490 -2.032495 -0.154178  
 C13 -3.021686 0.485707 -0.321153  
 C14 -4.130119 2.281646 -0.846426  
 C15 -4.438002 0.298220 -0.223723  
 H16 -4.313293 3.297586 -1.168970  
 N17 -5.092042 1.408554 -0.540283  
 N18 -2.072177 -0.378454 -0.076672  
 O19 -6.063014 -1.363644 0.363157  
 C20 -4.935056 -1.011347 0.196037  
 N21 -3.846135 -1.909535 0.391963  
 H22 -4.131930 -2.848936 0.641333  
 N23 -1.614474 -2.560797 0.396210  
 H24 -1.873696 -3.511266 0.615381  
 H25 -0.592282 -2.332847 0.196494  
 C26 -2.520401 -1.632186 0.240415  
 N27 -2.870920 1.786276 -0.726481  
 N28 4.799916 0.386949 -0.072714  
 C29 -1.609038 2.453177 -1.035943  
 H30 -1.007597 2.569148 -0.132730  
 H31 -1.062328 1.862811 -1.771325  
 H32 -1.830993 3.433290 -1.454253  
 C33 5.781266 1.434933 0.135082  
 H34 5.464343 2.351428 -0.362883  
 H35 5.915762 1.624392 1.200688  
 H36 6.718355 1.085376 -0.295831  
 O37 6.199824 -1.222883 -1.027962  
 N38 3.928000 -1.570567 -0.638204  
 H39 3.845062 -2.508891 -0.990135

Zero-point correction= 0.298161 (Hartree/Particle)  
 Thermal correction to Energy= 0.320570  
 Thermal correction to Enthalpy= 0.321514  
 Thermal correction to Gibbs Free Energy= 0.244409  
 Sum of electronic and zero-point Energies= -1238.387930  
 Sum of electronic and thermal Energies= -1238.365520  
 Sum of electronic and thermal Enthalpies= -1238.364576  
 Sum of electronic and thermal Free Energies= -1238.441682

### [9MOG·9MG]<sup>+</sup>\_11

C1 -3.733256 2.005488 -0.391606  
 C2 -3.942861 0.621455 -0.036079  
 H3 -2.153264 3.210974 -0.822156  
 C4 -1.320491 1.347901 -0.451481  
 N5 -2.371305 2.252220 -0.584654  
 N6 -3.355876 -1.493293 0.382344  
 N7 -1.591030 0.023251 -0.153910  
 C8 -2.843226 -0.277561 0.049447  
 N9 -0.088273 1.692580 -0.596576  
 H10 1.255849 0.689371 -0.270746  
 H11 0.025176 2.671490 -0.839811  
 O12 -4.585365 2.849404 -0.510267  
 C13 3.347332 0.457105 0.164302  
 C14 -2.613524 -2.722890 0.591112  
 H15 -1.710635 -2.505773 1.162212  
 H16 -3.247688 -3.406075 1.153907  
 H17 -2.356769 -3.182641 -0.365324  
 N18 3.721988 1.684176 0.595646  
 C19 5.092696 1.598262 0.771312  
 H20 5.660898 2.451511 1.112868  
 N21 2.073854 0.029121 -0.142783  
 C22 1.930852 -1.249470 -0.508990  
 C23 4.485441 -0.311924 0.105757  
 C24 2.886058 2.856053 0.792803  
 H25 1.961779 2.573278 1.298462  
 H26 3.425107 3.562973 1.421353  
 H27 2.658156 3.331483 -0.163251  
 C28 4.401014 -1.691699 -0.300413  
 O29 5.234512 -2.536418 -0.427445  
 N30 0.716876 -1.714163 -0.801482  
 H31 0.604860 -2.642267 -1.171118  
 H32 -0.115368 -1.143079 -0.616441  
 C33 -4.754076 -1.410742 0.512505  
 N34 5.572637 0.425355 0.491752  
 N35 3.012640 -2.042954 -0.571067  
 H36 2.895599 -3.017472 -0.817483  
 N37 -5.065179 -0.063263 0.237544  
 H38 -6.007615 0.302315 0.251421  
 O39 -5.511167 -2.285384 0.797260

Zero-point correction= 0.298200 (Hartree/Particle)  
 Thermal correction to Energy= 0.320730  
 Thermal correction to Enthalpy= 0.321674  
 Thermal correction to Gibbs Free Energy= 0.243683  
 Sum of electronic and zero-point Energies= -1238.387777  
 Sum of electronic and thermal Energies= -1238.365247  
 Sum of electronic and thermal Enthalpies= -1238.364303  
 Sum of electronic and thermal Free Energies= -1238.442293

### [9MOG·9MG]<sup>+</sup>\_12

C1 1.596833 -1.010058 -0.170580  
 C2 2.939044 -0.755765 -0.247146  
 H3 -0.182417 -0.067618 0.293145  
 C4 1.393976 1.117459 0.934503  
 C5 5.184889 -0.707647 -0.535507

N6 0.842214 -0.010364 0.408985  
 N7 2.677037 1.386321 0.886583  
 C8 3.416014 0.453817 0.279912  
 N9 0.531220 2.016522 1.490662  
 H10 0.990529 2.782201 1.962282  
 H11 -0.275088 1.651001 1.974631  
 O12 1.022666 -2.083863 -0.610199  
 C13 -3.022212 0.494093 -0.320329  
 C14 -4.274788 2.213859 -0.794953  
 C15 -4.409223 0.227562 -0.117328  
 H16 -4.539558 3.210367 -1.121265  
 N17 -5.152139 1.294932 -0.406097  
 N18 -2.008276 -0.308584 -0.128590  
 O19 -5.903020 -1.498615 0.606946  
 C20 -4.802051 -1.100416 0.360100  
 N21 -3.663815 -1.924251 0.498092  
 H22 -3.878353 -2.871652 0.782041  
 N23 -1.373381 -2.447331 0.331303  
 H24 -1.652448 -3.384195 0.604069  
 H25 0.062440 -2.217821 -0.251295  
 C26 -2.344004 -1.603942 0.242887  
 N27 -2.980071 1.796954 -0.755841  
 N28 4.750335 0.485442 0.106576  
 C29 -1.797526 2.523561 -1.197066  
 H30 -1.060552 2.565488 -0.394266  
 H31 -1.367297 2.032983 -2.070993  
 H32 -2.092920 3.537170 -1.463139  
 C33 5.660215 1.539786 0.521351  
 H34 5.453475 2.456532 -0.031224  
 H35 5.553507 1.722178 1.590566  
 H36 6.670299 1.197773 0.301658  
 O37 6.312212 -0.981311 -0.826915  
 N38 4.031763 -1.448110 -0.730316  
 H39 4.032306 -2.348664 -1.179436

Zero-point correction= 0.297746 (Hartree/Particle)  
 Thermal correction to Energy= 0.319928  
 Thermal correction to Enthalpy= 0.320872  
 Thermal correction to Gibbs Free Energy= 0.244675  
 Sum of electronic and zero-point Energies= -1238.385339  
 Sum of electronic and thermal Energies= -1238.363157  
 Sum of electronic and thermal Enthalpies= -1238.362212  
 Sum of electronic and thermal Free Energies= -1238.438409

### [9MOG·9MG]<sup>+</sup>\_13

C1 -3.723340 1.908265 -0.654579  
 C2 -3.930261 0.578316 -0.133419  
 H3 -2.129305 3.077661 -1.186672  
 C4 -1.331391 1.267611 -0.577051  
 N5 -2.345490 2.149614 -0.843420  
 N6 -3.306726 -1.452691 0.563250  
 N7 -1.562214 0.011294 -0.128190  
 C8 -2.818962 -0.287245 0.091650  
 N9 -0.084513 1.630305 -0.758823  
 H10 0.709074 0.976854 -0.476315  
 H11 0.140928 2.543342 -1.122696

O12 -4.566123 2.728171 -0.901706  
 C13 3.246740 0.423669 0.268102  
 C14 -2.536631 -2.634091 0.932145  
 H15 -1.635001 -2.321139 1.457046  
 H16 -3.156486 -3.247505 1.583572  
 H17 -2.271629 -3.204525 0.041138  
 N18 3.518912 1.607050 0.887080  
 C19 4.893246 1.646963 1.028459  
 H20 5.379852 2.489971 1.498307  
 N21 2.002986 -0.036422 -0.076228  
 C22 2.023393 -1.251079 -0.583044  
 C23 4.469150 -0.187822 0.072771  
 C24 2.570049 2.607564 1.324570  
 H25 1.686832 2.119978 1.739843  
 H26 3.028861 3.215104 2.103768  
 H27 2.278355 3.264645 0.500324  
 C28 4.512851 -1.495880 -0.525967  
 O29 5.431845 -2.220535 -0.790665  
 N30 0.850070 -1.873081 -0.879903  
 H31 0.831942 -2.590467 -1.584655  
 H32 0.000964 -1.349380 -0.716183  
 C33 -4.713363 -1.383524 0.654427  
 N34 5.486973 0.594580 0.554632  
 N35 3.169733 -1.940174 -0.800006  
 H36 3.125148 -2.892012 -1.138606  
 N37 -5.044218 -0.083531 0.202270  
 H38 -5.994927 0.260101 0.153718  
 O39 -5.460984 -2.226103 1.031671

Zero-point correction= 0.297926 (Hartree/Particle)  
 Thermal correction to Energy= 0.320538  
 Thermal correction to Enthalpy= 0.321482  
 Thermal correction to Gibbs Free Energy= 0.243017  
 Sum of electronic and zero-point Energies= -1238.385311  
 Sum of electronic and thermal Energies= -1238.362699  
 Sum of electronic and thermal Enthalpies= -1238.361755  
 Sum of electronic and thermal Free Energies= -1238.440220

### [9MOG·9MG]<sup>+</sup>\_14

C1 -3.883546 1.931973 -0.305025  
 C2 -3.963344 0.544239 -0.013461  
 H3 -2.386733 3.308861 -0.674143  
 C4 -1.421908 1.522605 -0.462190  
 N5 -2.502515 2.317397 -0.507107  
 N6 -3.211393 -1.510460 0.345897  
 N7 -1.579133 0.220182 -0.194407  
 C8 -2.851676 -0.242968 0.033103  
 N9 -0.197146 2.005478 -0.669067  
 H10 0.627281 1.415228 -0.511516  
 H11 -0.072454 2.947748 -0.996767  
 O12 -4.745688 2.765097 -0.386039  
 C13 3.361669 0.450264 0.169211  
 C14 -2.372629 -2.682559 0.494224  
 H15 -1.507581 -2.452574 1.118451  
 H16 -2.977569 -3.447630 0.979780  
 H17 -2.049871 -3.056493 -0.480200

|     |           |           |           |
|-----|-----------|-----------|-----------|
| N18 | 3.910412  | 1.635409  | 0.599191  |
| C19 | 5.243994  | 1.399145  | 0.738292  |
| H20 | 5.925610  | 2.168440  | 1.074547  |
| N21 | 2.103383  | 0.212527  | -0.093890 |
| C22 | 1.822220  | -1.091584 | -0.476339 |
| C23 | 4.470982  | -0.443230 | 0.082642  |
| C24 | 3.199376  | 2.880322  | 0.838673  |
| H25 | 2.277563  | 2.669862  | 1.381015  |
| H26 | 3.825402  | 3.533195  | 1.444641  |
| H27 | 2.974395  | 3.376126  | -0.107236 |
| C28 | 4.227943  | -1.814080 | -0.367503 |
| O29 | 5.025694  | -2.693278 | -0.519743 |
| N30 | 0.584329  | -1.389422 | -0.684376 |
| H31 | 0.451050  | -2.352351 | -0.978115 |
| H32 | -0.747975 | -0.432034 | -0.336327 |
| C33 | -4.625884 | -1.561238 | 0.506684  |
| N34 | 5.606658  | 0.159295  | 0.432458  |
| N35 | 2.852960  | -2.003909 | -0.618420 |
| H36 | 2.621317  | -2.942690 | -0.916319 |
| N37 | -5.045536 | -0.269416 | 0.277982  |
| H38 | -6.010510 | 0.014865  | 0.321689  |
| O39 | -5.260910 | -2.540251 | 0.784883  |

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.297246 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.319942                    |
| Thermal correction to Enthalpy=              | 0.320887                    |
| Thermal correction to Gibbs Free Energy=     | 0.242271                    |
| Sum of electronic and zero-point Energies=   | -1238.375048                |
| Sum of electronic and thermal Energies=      | -1238.352352                |
| Sum of electronic and thermal Enthalpies=    | -1238.351408                |
| Sum of electronic and thermal Free Energies= | -1238.430024                |



**Cartesian coordinates for the structures  
in Scheme 4, optimized at  $\omega$ B97XD/  
6-311++G(d,p).**

**[9MOG·9MOG]<sup>+</sup>\_1**

|     |           |           |           |
|-----|-----------|-----------|-----------|
| C1  | -1.902956 | -0.527217 | 0.018117  |
| C2  | -3.324209 | -0.783520 | 0.006496  |
| H3  | -0.620589 | 1.147368  | 0.020759  |
| C4  | -2.589235 | 1.804058  | 0.004969  |
| C5  | -5.417397 | -1.621842 | -0.012154 |
| N6  | -1.642717 | 0.835562  | 0.016066  |
| N7  | -5.489026 | -0.215846 | -0.018204 |
| N8  | -3.920260 | 1.578028  | -0.004537 |
| C9  | -4.244223 | 0.309989  | -0.004835 |
| N10 | -2.167076 | 3.059239  | 0.003864  |
| H11 | -2.849769 | 3.800220  | -0.003976 |
| H12 | -1.178596 | 3.275604  | 0.010090  |
| O13 | -1.027737 | -1.367186 | 0.028205  |
| C14 | -6.743118 | 0.526289  | -0.021864 |
| H15 | -6.881124 | 1.028428  | 0.935683  |
| H16 | -6.727139 | 1.260092  | -0.826615 |
| H17 | -7.547277 | -0.189224 | -0.183335 |
| O18 | -6.316014 | -2.401252 | -0.020009 |
| C19 | 3.772453  | -1.920691 | 0.010762  |
| C20 | 3.165801  | -0.635045 | 0.016863  |
| H21 | 5.688931  | -2.645799 | -0.049497 |
| C22 | 5.864525  | -0.583681 | -0.019263 |
| C23 | 1.771980  | 1.111881  | 0.017005  |
| N24 | 5.184987  | -1.770200 | -0.007437 |
| N25 | 1.831137  | -0.241232 | 0.026305  |
| N26 | 3.062508  | 1.576865  | 0.001309  |
| N27 | 5.269888  | 0.586091  | -0.010103 |
| C28 | 3.929000  | 0.500248  | 0.000720  |
| N29 | 7.215202  | -0.639933 | -0.074583 |
| H30 | 7.705204  | 0.233421  | 0.023282  |
| H31 | 7.715022  | -1.482338 | 0.150193  |
| O32 | 3.259107  | -3.017411 | 0.015350  |
| C33 | 3.425418  | 2.982214  | -0.011405 |
| H34 | 3.100358  | 3.464901  | 0.910810  |
| H35 | 4.509019  | 3.042619  | -0.093878 |
| H36 | 2.963726  | 3.477392  | -0.865761 |
| O37 | 0.752586  | 1.832435  | 0.020530  |
| H38 | 1.019694  | -0.849890 | 0.033925  |
| N39 | -4.033126 | -1.918448 | 0.002459  |
| H40 | -3.669849 | -2.862468 | 0.007267  |

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.303104 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.327089                    |
| Thermal correction to Enthalpy=              | 0.328033                    |
| Thermal correction to Gibbs Free Energy=     | 0.246000                    |
| Sum of electronic and zero-point Energies=   | -1313.669403                |
| Sum of electronic and thermal Energies=      | -1313.645417                |
| Sum of electronic and thermal Enthalpies=    | -1313.644473                |
| Sum of electronic and thermal Free Energies= | -1313.726507                |

**[9MOG·9MOG]<sup>+</sup>\_2**

|     |           |           |           |
|-----|-----------|-----------|-----------|
| C1  | -1.772118 | -0.351259 | -0.023045 |
| C2  | -3.082322 | -0.730721 | -0.011150 |
| H3  | -0.584151 | 1.370562  | -0.027036 |
| C4  | -2.560924 | 1.922021  | -0.008474 |
| C5  | -5.111117 | -1.736489 | 0.011033  |
| N6  | -1.549145 | 1.006148  | -0.022468 |
| N7  | -5.268970 | -0.324633 | 0.015261  |
| N8  | -3.838089 | 1.586854  | 0.006120  |
| C9  | -4.061954 | 0.276829  | 0.004105  |
| N10 | -2.208129 | 3.216211  | -0.009679 |
| H11 | -2.939812 | 3.905934  | 0.001366  |
| H12 | -1.244305 | 3.506753  | -0.020658 |
| O13 | -0.777093 | -1.192760 | -0.034967 |
| C14 | -6.564504 | 0.330403  | 0.045001  |
| H15 | -6.711497 | 0.834606  | 1.000747  |
| H16 | -6.631248 | 1.055076  | -0.766055 |
| H17 | -7.320597 | -0.442746 | -0.081609 |
| O18 | -5.994097 | -2.545935 | 0.019389  |
| C19 | 3.269883  | -1.900811 | -0.015849 |
| C20 | 2.861282  | -0.511658 | -0.016331 |
| H21 | 5.034604  | -2.951519 | 0.005453  |
| C22 | 5.558520  | -0.952382 | 0.023049  |
| C23 | 1.836032  | 1.390771  | -0.014939 |
| N24 | 4.688344  | -2.000351 | 0.005265  |
| N25 | 1.645574  | 0.020336  | -0.028143 |
| N26 | 3.208434  | 1.678205  | 0.008854  |
| N27 | 5.176385  | 0.324918  | 0.021632  |
| C28 | 3.869146  | 0.500349  | 0.003836  |
| N29 | 6.866260  | -1.210070 | 0.042507  |
| H30 | 7.499377  | -0.426449 | 0.053651  |
| H31 | 7.245292  | -2.141768 | 0.045468  |
| O32 | 2.579699  | -2.884064 | -0.029770 |
| C33 | 3.783152  | 3.013705  | 0.011829  |
| H34 | 3.124812  | 3.672278  | 0.575508  |
| H35 | 4.761146  | 2.967928  | 0.487865  |
| H36 | 3.887835  | 3.386725  | -1.007745 |
| O37 | 0.953991  | 2.237779  | -0.017255 |
| H38 | 0.129622  | -0.767018 | -0.035287 |
| N39 | -3.744705 | -1.945066 | -0.006511 |
| H40 | -3.333250 | -2.862918 | -0.015105 |

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.302929 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.327009                    |
| Thermal correction to Enthalpy=              | 0.327953                    |
| Thermal correction to Gibbs Free Energy=     | 0.245690                    |
| Sum of electronic and zero-point Energies=   | -1313.669358                |
| Sum of electronic and thermal Energies=      | -1313.645278                |
| Sum of electronic and thermal Enthalpies=    | -1313.644334                |
| Sum of electronic and thermal Free Energies= | -1313.726597                |

**[9MOG·9MOG]<sup>+</sup>\_3**

|    |           |           |           |
|----|-----------|-----------|-----------|
| C1 | -1.912813 | -0.424885 | -0.011335 |
| C2 | -3.349596 | -0.564858 | 0.003161  |
| H3 | 0.143753  | 1.133239  | -0.004852 |
| C4 | -2.336242 | 1.886619  | -0.036714 |

C5 -5.518006 -1.198206 0.035144  
 N6 -1.466448 0.860446 -0.029743  
 N7 -4.167038 -1.626624 0.025747  
 N8 -5.456280 0.202747 0.018343  
 N9 -3.701020 1.823858 -0.024783  
 C10 -4.160995 0.607210 -0.003513  
 N11 -1.835784 3.121115 -0.057674  
 H12 -2.470835 3.902635 -0.062751  
 H13 -0.842216 3.282764 -0.069770  
 O14 -1.156679 -1.405510 -0.006628  
 C15 -6.630651 1.062878 0.010048  
 H16 -6.537493 1.810911 0.796530  
 H17 -6.727904 1.555046 -0.957821  
 H18 -7.501257 0.435732 0.193432  
 O19 -6.484852 -1.894115 0.055497  
 H20 -3.900525 -2.600662 0.036459  
 C21 1.976113 0.429191 0.001369  
 C22 3.330100 0.584446 0.010355  
 H23 0.495427 -1.039455 -0.018302  
 C24 2.359909 -1.940923 -0.029762  
 C25 5.505546 1.220264 0.033924  
 N26 1.521492 -0.867155 -0.018408  
 N27 5.415362 -0.196366 0.013785  
 N28 3.676920 -1.829323 -0.023180  
 C29 4.122587 -0.579179 -0.001908  
 N30 1.795128 -3.157359 -0.049460  
 H31 2.400221 -3.960626 -0.055874  
 H32 0.796935 -3.282591 -0.051952  
 O33 1.120838 1.418060 0.011107  
 C34 6.578680 -1.066099 -0.000477  
 H35 6.491107 -1.812167 0.788794  
 H36 6.668885 -1.562742 -0.967124  
 H37 7.452769 -0.440471 0.172703  
 O38 6.514073 1.865381 0.051441  
 N39 4.195012 1.664207 0.031103  
 H40 3.954903 2.640291 0.047325

Zero-point correction= 0.302528 (Hartree/Particle)  
 Thermal correction to Energy= 0.326391  
 Thermal correction to Enthalpy= 0.327335  
 Thermal correction to Gibbs Free Energy= 0.246450  
 Sum of electronic and zero-point Energies= -1313.668310  
 Sum of electronic and thermal Energies= -1313.644446  
 Sum of electronic and thermal Enthalpies= -1313.643502  
 Sum of electronic and thermal Free Energies= -1313.724387

#### [9MOG·9MOG]<sup>+</sup>\_4

C1 1.941972 -0.284284 0.030514  
 C2 3.299486 -0.544922 0.013035  
 H3 0.673246 1.350119 0.024572  
 C4 2.606854 2.067088 0.007033  
 C5 5.394094 -1.414685 -0.013549  
 N6 1.657111 1.086040 0.027470  
 N7 4.046990 -1.714008 0.008362  
 N8 5.453769 -0.000913 -0.023133  
 N9 3.896742 1.817926 -0.009455

C10 4.201443 0.516077 -0.008758  
 N11 2.175623 3.345584 -0.020181  
 H12 2.873483 4.066937 0.046935  
 H13 1.213578 3.587433 0.139868  
 O14 0.994125 -1.116301 0.047750  
 C15 6.699524 0.741937 -0.056569  
 H16 6.810866 1.256050 -1.012084  
 H17 6.720486 1.469836 0.754273  
 H18 7.506761 0.021653 0.067471  
 O19 6.331061 -2.167275 -0.021230  
 H20 3.701975 -2.657228 0.024979  
 C21 -2.040656 0.660048 0.031114  
 C22 -3.484067 0.625471 0.011195  
 H23 -0.428746 -0.715666 0.042716  
 C24 -2.235745 -1.757019 0.013572  
 C25 -5.707732 1.011493 -0.022449  
 N26 -1.508016 -0.613638 0.031833  
 N27 -5.487214 -0.377287 -0.028650  
 N28 -3.585150 -1.809077 -0.004474  
 C29 -4.160890 -0.635187 -0.006570  
 N30 -1.562583 -2.895623 0.013886  
 H31 -2.074048 -3.763915 0.000906  
 H32 -0.549751 -2.897989 0.024815  
 O33 -1.348755 1.663344 0.044926  
 C34 -6.559945 -1.364174 -0.039924  
 H35 -6.379802 -2.084102 -0.837176  
 H36 -6.603357 -1.877462 0.920639  
 H37 -7.494167 -0.834928 -0.217934  
 O38 -6.746116 1.590946 -0.036836  
 N39 -4.413183 1.588805 0.001943  
 H40 -4.257689 2.587808 0.008060

Zero-point correction= 0.302010 (Hartree/Particle)  
 Thermal correction to Energy= 0.326236  
 Thermal correction to Enthalpy= 0.327180  
 Thermal correction to Gibbs Free Energy= 0.244915  
 Sum of electronic and zero-point Energies= -1313.668228  
 Sum of electronic and thermal Energies= -1313.644002  
 Sum of electronic and thermal Enthalpies= -1313.643058  
 Sum of electronic and thermal Free Energies= -1313.725323

#### [9MOG·9MOG]<sup>+</sup>\_5

C1 2.037809 1.099820 -0.766578  
 C2 2.202416 -0.160698 -0.271258  
 H3 3.052960 2.819867 -1.137954  
 C4 4.385641 1.463600 -0.304186  
 C5 2.094923 -2.282193 0.491623  
 N6 3.179632 1.880742 -0.783898  
 N7 1.371734 -1.250138 -0.072237  
 N8 3.404878 -1.762479 0.695387  
 N9 4.558975 0.266592 0.222391  
 C10 3.476693 -0.504840 0.224318  
 N11 5.424161 2.310909 -0.367638  
 H12 6.310226 1.988952 -0.015729  
 H13 5.366501 3.226593 -0.776576  
 O14 0.985994 1.683001 -1.253289

C15 4.486710 -2.534769 1.279777  
 H16 5.283508 -2.677100 0.549175  
 H17 4.880514 -2.022883 2.157734  
 H18 4.072467 -3.499988 1.566442  
 O19 1.733151 -3.390799 0.769341  
 H20 0.476202 -1.415560 -0.532610  
 C21 -2.155896 -1.204049 -0.841571  
 C22 -2.242368 0.121324 -0.296608  
 H23 -3.384408 -2.807663 -1.155990  
 C24 -4.541559 -1.345144 -0.248944  
 C25 -1.920276 2.139018 0.460581  
 N26 -3.396635 -1.864288 -0.789536  
 N27 -3.280700 1.791660 0.718754  
 N28 -4.619494 -0.134486 0.287462  
 C29 -3.487780 0.554109 0.253681  
 N30 -5.639780 -2.104092 -0.261228  
 H31 -6.479924 -1.717704 0.138132  
 H32 -5.668382 -3.029105 -0.654265  
 O33 -1.176571 -1.762189 -1.296778  
 C34 -4.245676 2.663774 1.364796  
 H35 -5.050949 2.908766 0.671749  
 H36 -4.657230 2.174959 2.247786  
 H37 -3.720153 3.572183 1.654195  
 O38 -1.415531 3.186795 0.759668  
 N39 -1.309172 1.058347 -0.185042  
 H40 0.103318 1.335151 -0.868317

Zero-point correction= 0.302151 (Hartree/Particle)  
 Thermal correction to Energy= 0.326162  
 Thermal correction to Enthalpy= 0.327106  
 Thermal correction to Gibbs Free Energy= 0.246154  
 Sum of electronic and zero-point Energies= -1313.663231  
 Sum of electronic and thermal Energies= -1313.639220  
 Sum of electronic and thermal Enthalpies= -1313.638276  
 Sum of electronic and thermal Free Energies= -1313.719228

#### [9MOG-9MOG]<sup>+</sup>\_6

C1 1.957471 1.162232 -0.426603  
 C2 2.417633 -0.117224 -0.143071  
 H3 2.711039 3.036998 -0.703581  
 C4 4.310107 1.817931 -0.200413  
 C5 2.712684 -2.313952 0.314224  
 N6 2.999551 2.100193 -0.456595  
 N7 1.781067 -1.342448 0.013749  
 N8 3.946581 -1.631921 0.402037  
 N9 4.731017 0.612550 0.105756  
 C10 3.767609 -0.316767 0.117044  
 N11 5.204127 2.827133 -0.299796  
 H12 6.146877 2.619993 -0.014828  
 H13 4.917937 3.790327 -0.306726  
 O14 0.800423 1.571971 -0.660089  
 C15 5.200222 -2.283725 0.725977  
 H16 5.908529 -2.172276 -0.095693  
 H17 5.626532 -1.853165 1.632692  
 H18 4.983608 -3.339029 0.884695  
 O19 2.539347 -3.495444 0.476433

H20 0.845538 -1.570368 -0.293745  
 C21 -2.108825 -1.333044 -0.509596  
 C22 -2.420203 0.035029 -0.185005  
 H23 -3.103552 -3.111442 -0.681817  
 C24 -4.520109 -1.697037 -0.143908  
 C25 -2.459903 2.216157 0.264205  
 N26 -3.267869 -2.135457 -0.466407  
 N27 -3.775240 1.700727 0.406776  
 N28 -4.800375 -0.430929 0.164841  
 C29 -3.767096 0.387163 0.138919  
 N30 -5.516854 -2.576405 -0.135245  
 H31 -6.436590 -2.240958 0.105962  
 H32 -5.397671 -3.551475 -0.354483  
 O33 -1.034524 -1.807337 -0.788757  
 C34 -4.924101 2.509284 0.788638  
 H35 -5.666782 2.496896 -0.008691  
 H36 -5.360571 2.118404 1.707419  
 H37 -4.567964 3.525368 0.948471  
 O38 -2.121490 3.345693 0.432586  
 N39 -1.655239 1.121813 -0.109281  
 H40 -0.597272 1.218599 -0.324375

Zero-point correction= 0.301931 (Hartree/Particle)  
 Thermal correction to Energy= 0.325894  
 Thermal correction to Enthalpy= 0.326838  
 Thermal correction to Gibbs Free Energy= 0.245928  
 Sum of electronic and zero-point Energies= -1313.661857  
 Sum of electronic and thermal Energies= -1313.637895  
 Sum of electronic and thermal Enthalpies= -1313.636951  
 Sum of electronic and thermal Free Energies= -1313.717861

#### [9MOG-9MOG]<sup>+</sup>\_7

C1 1.658317 -1.110735 -0.052692  
 C2 3.043711 -0.747901 -0.243863  
 H3 -0.791786 -0.488127 0.207171  
 C4 1.526015 0.843265 1.233908  
 C5 5.227300 -0.530911 -0.777863  
 N6 0.925710 -0.217859 0.677534  
 N7 2.822407 1.251453 1.090022  
 C8 3.534686 0.450230 0.350662  
 N9 0.784507 1.631119 2.023842  
 H10 1.234418 2.398232 2.497035  
 H11 -0.125051 1.328657 2.328384  
 O12 1.180679 -2.147510 -0.521929  
 C13 -2.737132 0.255868 -0.184882  
 C14 -3.762950 2.215112 -0.648676  
 C15 -4.077435 0.040039 -0.089490  
 N16 -1.792826 -0.722256 0.009932  
 O17 -5.748164 -1.615623 0.287801  
 C18 -4.608531 -1.250544 0.183420  
 N19 -3.537160 -2.214352 0.310304  
 H20 -3.865919 -3.162834 0.441076  
 N21 -1.318900 -2.943199 0.391278  
 H22 -1.610330 -3.890442 0.566282  
 H23 -0.345331 -2.759241 0.101165  
 C24 -2.216099 -1.981167 0.237814

N25 -2.509846 1.551241 -0.513230  
 N26 4.843847 0.563179 0.013565  
 C27 -1.254182 2.192483 -0.854420  
 H28 -0.683439 2.449233 0.039131  
 H29 -0.664009 1.540951 -1.501539  
 H30 -1.500893 3.108993 -1.389796  
 C31 5.749508 1.631184 0.410993  
 H32 5.340108 2.591929 0.100244  
 H33 5.885376 1.620360 1.492501  
 H34 6.703485 1.456315 -0.083150  
 O35 6.297365 -0.759283 -1.249238  
 N36 4.058508 -1.321137 -0.905203  
 H37 4.030872 -2.182858 -1.432146  
 O38 -3.910786 3.367012 -0.952163  
 N39 -4.700032 1.247586 -0.364674  
 H40 -5.692997 1.410095 -0.405167

Zero-point correction= 0.303780 (Hartree/Particle)  
 Thermal correction to Energy= 0.327242  
 Thermal correction to Enthalpy= 0.328187  
 Thermal correction to Gibbs Free Energy= 0.248867  
 Sum of electronic and zero-point Energies= -1313.650420  
 Sum of electronic and thermal Energies= -1313.626958  
 Sum of electronic and thermal Enthalpies= -1313.626013  
 Sum of electronic and thermal Free Energies= -1313.705333

### [9MOG·9MOG]<sup>++</sup>\_8

C1 1.804409 -1.070365 0.071651  
 C2 3.147121 -0.761641 -0.147697  
 H3 0.119011 -0.103589 0.734785  
 C4 1.722931 1.135771 1.136376  
 C5 5.334487 -0.684485 -0.736949  
 N6 1.132259 -0.021153 0.722101  
 N7 2.977926 1.417747 0.931727  
 C8 3.653754 0.458468 0.268370  
 N9 0.896763 2.049225 1.758007  
 H10 1.412048 2.851045 2.095607  
 H11 0.281921 1.667838 2.463464  
 O12 1.190015 -2.105669 -0.240784  
 C13 -2.844388 0.223190 -0.201605  
 C14 -4.034883 2.094530 -0.635215  
 C15 -4.233178 -0.087833 -0.106583  
 N16 -1.859242 -0.619952 -0.016390  
 O17 -5.790223 -1.820505 0.326924  
 C18 -4.659613 -1.431211 0.205965  
 N19 -3.541129 -2.277963 0.347470  
 H20 -3.771953 -3.247526 0.527705  
 N21 -1.279111 -2.800560 0.317198  
 H22 -1.491045 -3.773532 0.477743  
 H23 -0.273423 -2.512050 0.121072  
 C24 -2.227732 -1.906589 0.216193  
 N25 -2.746759 1.532157 -0.515997  
 N26 4.962749 0.512945 -0.081040  
 C27 -1.520888 2.269288 -0.801191  
 H28 -0.926322 2.390990 0.105576  
 H29 -0.946173 1.730760 -1.555157

H30 -1.809191 3.246472 -1.184760  
 C31 5.887627 1.602317 0.167725  
 H32 5.511221 2.523812 -0.277031  
 H33 6.028641 1.744648 1.239744  
 H34 6.835509 1.330207 -0.294265  
 O35 6.422702 -0.950152 -1.172325  
 N36 4.183465 -1.448307 -0.756531  
 H37 4.141848 -2.364878 -1.167872  
 O38 -4.318642 3.215227 -0.911509  
 N39 -4.925339 1.030498 -0.357737  
 H40 -5.931876 1.133501 -0.368953

Zero-point correction= 0.303416 (Hartree/Particle)  
 Thermal correction to Energy= 0.326922  
 Thermal correction to Enthalpy= 0.327866  
 Thermal correction to Gibbs Free Energy= 0.248094  
 Sum of electronic and zero-point Energies= -1313.649436  
 Sum of electronic and thermal Energies= -1313.625929  
 Sum of electronic and thermal Enthalpies= -1313.624985  
 Sum of electronic and thermal Free Energies= -1313.704757

### [9MOG·9MOG]<sup>++</sup>\_9

C1 1.843495 -1.024101 -0.217573  
 C2 3.170358 -0.700864 -0.299177  
 H3 0.029677 -0.202302 0.335496  
 C4 1.561872 1.015947 1.026493  
 C5 5.405893 -0.528599 -0.617772  
 N6 1.052819 -0.101199 0.437543  
 N7 2.830873 1.347596 0.975879  
 C8 3.600353 0.493241 0.297936  
 N9 0.674093 1.835507 1.655716  
 H10 1.102972 2.592864 2.166941  
 H11 -0.121232 1.412678 2.108747  
 O12 1.313929 -2.094902 -0.716071  
 C13 -2.837597 0.229184 -0.200872  
 C14 -4.189504 2.005080 -0.593579  
 C15 -4.188254 -0.172981 -0.005020  
 N16 -1.788908 -0.535286 -0.065766  
 O17 -5.605326 -1.977217 0.575767  
 C18 -4.504676 -1.532294 0.372072  
 N19 -3.335126 -2.293604 0.464482  
 H20 -3.488347 -3.269674 0.683158  
 N21 -1.021790 -2.660697 0.252402  
 H22 -1.242838 -3.626043 0.471055  
 H23 0.371945 -2.309230 -0.340639  
 C24 -2.034586 -1.867927 0.221319  
 N25 -2.860500 1.543381 -0.546367  
 N26 4.928982 0.598475 0.107182  
 C27 -1.724989 2.351253 -0.963546  
 H28 -1.006418 2.450058 -0.149247  
 H29 -1.246603 1.893800 -1.830840  
 H30 -2.106785 3.334690 -1.233268  
 C31 5.794934 1.670128 0.568177  
 H32 5.561850 2.597314 0.043933  
 H33 5.668256 1.812531 1.641145  
 H34 6.819641 1.373765 0.349913

O35 6.539357 -0.729706 -0.943871  
 N36 4.285339 -1.309265 -0.841900  
 H37 4.318520 -2.175874 -1.352124  
 O38 -4.571854 3.097012 -0.876928  
 N39 -4.975585 0.890390 -0.233334  
 H40 -5.984658 0.918426 -0.177061

Zero-point correction= 0.302917 (Hartree/Particle)  
 Thermal correction to Energy= 0.326242  
 Thermal correction to Enthalpy= 0.327186  
 Thermal correction to Gibbs Free Energy= 0.248454  
 Sum of electronic and zero-point Energies= -1313.646644  
 Sum of electronic and thermal Energies= -1313.623320  
 Sum of electronic and thermal Enthalpies= -1313.622376  
 Sum of electronic and thermal Free Energies= -1313.701108

### [9MOG·9MOG]<sup>+</sup>\_10

C1 -3.871346 2.056908 -0.514947  
 C2 -4.146201 0.715148 -0.059816  
 H3 -2.223432 3.149765 -1.047913  
 C4 -1.527537 1.259477 -0.574563  
 N5 -2.488543 2.219433 -0.747445  
 N6 -3.635055 -1.387558 0.500875  
 N7 -1.822922 -0.002631 -0.184210  
 C8 -3.087906 -0.232198 0.071517  
 N9 -0.268072 1.552102 -0.794189  
 H10 0.490033 0.851141 -0.566137  
 H11 0.006566 2.475286 -1.092735  
 O12 -4.666940 2.941280 -0.681828  
 C13 3.053314 0.162797 0.068418  
 C14 -2.937125 -2.638283 0.769353  
 H15 -1.990829 -2.420252 1.262867  
 H16 -3.568242 -3.241418 1.419627  
 H17 -2.759691 -3.176259 -0.162796  
 N18 3.413437 1.417036 0.477998  
 C19 4.816289 1.476988 0.653002  
 N20 1.782095 -0.251306 -0.201513  
 C21 1.691048 -1.525588 -0.525052  
 C22 4.190958 -0.590518 -0.027310  
 C23 2.563587 2.551033 0.745637  
 H24 1.681368 2.238213 1.307366  
 H25 3.141567 3.256963 1.341930  
 H26 2.268730 3.053068 -0.181747  
 C27 4.135096 -1.958376 -0.399849  
 O28 5.019224 -2.772692 -0.521609  
 N29 0.466542 -2.083306 -0.732614  
 H30 0.389103 -2.875919 -1.347831  
 H31 -0.329613 -1.461546 -0.674312  
 C32 -5.029771 -1.231973 0.653165  
 N33 2.772246 -2.334479 -0.626874  
 H34 2.649988 -3.320255 -0.817010  
 N35 -5.288702 0.109940 0.286080  
 H36 -6.215056 0.517665 0.296470  
 O37 -5.817060 -2.044773 1.014598  
 O38 5.438520 2.444155 1.012652  
 N39 5.260249 0.216957 0.329109

H40 6.228191 -0.056045 0.363879

Zero-point correction= 0.303044 (Hartree/Particle)  
 Thermal correction to Energy= 0.326769  
 Thermal correction to Enthalpy= 0.327713  
 Thermal correction to Gibbs Free Energy= 0.247261  
 Sum of electronic and zero-point Energies= -1313.637092  
 Sum of electronic and thermal Energies= -1313.613367  
 Sum of electronic and thermal Enthalpies= -1313.612423  
 Sum of electronic and thermal Free Energies= -1313.692875

### [9MOG·9MOG]<sup>+</sup>\_11

C1 -3.855215 2.115081 -0.393832  
 C2 -4.146376 0.750942 -0.018380  
 H3 -2.208509 3.213034 -0.864611  
 C4 -1.491379 1.303939 -0.489859  
 N5 -2.483379 2.272636 -0.612487  
 N6 -3.687548 -1.391544 0.417652  
 N7 -1.840325 0.003183 -0.168890  
 C8 -3.105146 -0.215084 0.060306  
 N9 -0.242550 1.563880 -0.665933  
 H10 1.034715 0.514540 -0.352740  
 H11 -0.065111 2.530670 -0.918677  
 O12 -4.654281 3.009468 -0.508553  
 C13 3.116787 0.184475 0.040986  
 C14 -3.021001 -2.663189 0.628231  
 H15 -2.099789 -2.498549 1.187612  
 H16 -3.689201 -3.301753 1.203935  
 H17 -2.805287 -3.145010 -0.327612  
 N18 3.551719 1.420546 0.384202  
 C19 4.962323 1.375390 0.577388  
 N20 1.822698 -0.191342 -0.222953  
 C21 1.588774 -1.477118 -0.518381  
 C22 4.175578 -0.672898 0.005935  
 C23 2.789987 2.644049 0.531858  
 H24 1.897729 2.464541 1.133743  
 H25 3.434517 3.359670 1.041351  
 H26 2.514818 3.051367 -0.443768  
 C27 4.013956 -2.047291 -0.312857  
 O28 4.824198 -2.931619 -0.390159  
 N29 0.342962 -1.875433 -0.767337  
 H30 0.163792 -2.816686 -1.072042  
 H31 -0.449869 -1.244068 -0.595811  
 C32 -5.075087 -1.218677 0.570871  
 N33 2.617520 -2.339368 -0.553482  
 H34 2.442755 -3.317122 -0.747585  
 N35 -5.304758 0.142513 0.284178  
 H36 -6.221791 0.567444 0.309713  
 O37 -5.880462 -2.040313 0.879778  
 O38 5.653106 2.306345 0.887175  
 N39 5.301843 0.063310 0.334901  
 H40 6.244274 -0.285511 0.397997

Zero-point correction= 0.302772 (Hartree/Particle)  
 Thermal correction to Energy= 0.326471  
 Thermal correction to Enthalpy= 0.327415  
 Thermal correction to Gibbs Free Energy= 0.247122  
 Sum of electronic and zero-point Energies= -1313.636326

|  |              |
|--|--------------|
| Sum of electronic and thermal Energies=      | -1313.612626 |
| Sum of electronic and thermal Enthalpies=    | -1313.611682 |
| Sum of electronic and thermal Free Energies= | -1313.691975 |

**Cartesian coordinates for the structures  
in Figure 2, optimized at  $\omega$ B97XD/  
6-311++G(d,p).**

**9MG<sup>+</sup>-9MG**

|     |           |           |           |
|-----|-----------|-----------|-----------|
| C1  | 2.548446  | -1.486703 | -0.010590 |
| C2  | 2.401748  | -0.076923 | -0.008133 |
| H3  | 4.068529  | -2.846906 | 0.026469  |
| C4  | 4.962484  | -0.972728 | -0.000829 |
| C5  | 1.708585  | 1.933187  | 0.008579  |
| N6  | 3.900629  | -1.850306 | -0.006975 |
| N7  | 1.269184  | 0.701801  | -0.003744 |
| N8  | 3.075088  | 2.005971  | 0.014970  |
| N9  | 4.820297  | 0.327602  | -0.000590 |
| C10 | 3.532489  | 0.718726  | 0.002920  |
| N11 | 6.200814  | -1.512064 | 0.038119  |
| H12 | 6.972820  | -0.872097 | -0.048138 |
| H13 | 6.367602  | -2.477964 | -0.183305 |
| O14 | 1.677327  | -2.353175 | -0.011310 |
| H15 | 1.078285  | 2.811036  | 0.015135  |
| C16 | 3.897931  | 3.205766  | 0.010457  |
| H17 | 4.656807  | 3.128449  | 0.788132  |
| H18 | 4.384020  | 3.325542  | -0.958088 |
| H19 | 3.261459  | 4.066664  | 0.208840  |
| C20 | -3.998058 | -0.414998 | 0.001201  |
| C21 | -5.706849 | 0.933178  | -0.007117 |
| C22 | -3.603772 | 0.959850  | -0.007512 |
| H23 | -6.739040 | 1.255926  | -0.009631 |
| N24 | -4.663976 | 1.763804  | -0.012509 |
| C25 | -6.256500 | -1.539035 | 0.024489  |
| H26 | -6.168361 | -2.051950 | 0.982064  |
| H27 | -5.984803 | -2.219564 | -0.781460 |
| H28 | -7.280338 | -1.197028 | -0.116393 |
| N29 | -5.371482 | -0.381524 | -0.000216 |
| N30 | -3.237899 | -1.473326 | 0.006203  |
| O31 | -1.651117 | 2.341550  | -0.012873 |
| C32 | -2.171448 | 1.257516  | -0.009405 |
| N33 | -1.406739 | 0.076296  | -0.005689 |
| H34 | -0.359938 | 0.244013  | -0.005911 |
| N35 | -1.075320 | -2.205808 | 0.003979  |
| H36 | -0.041385 | -2.133510 | -0.001594 |
| H37 | -1.493328 | -3.123770 | 0.009850  |
| C38 | -1.899419 | -1.181665 | 0.001382  |

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.293463 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.314809                    |
| Thermal correction to Enthalpy=              | 0.315753                    |
| Thermal correction to Gibbs Free Energy=     | 0.241210                    |
| Sum of electronic and zero-point Energies=   | -1163.174910                |
| Sum of electronic and thermal Energies=      | -1163.153564                |
| Sum of electronic and thermal Enthalpies=    | -1163.152620                |
| Sum of electronic and thermal Free Energies= | -1163.227163                |

**TS-G-PT1**

|    |          |           |           |
|----|----------|-----------|-----------|
| C1 | 2.561174 | -1.531461 | -0.002386 |
| C2 | 2.338855 | -0.126749 | 0.001567  |

|     |           |           |           |
|-----|-----------|-----------|-----------|
| H3  | 4.165681  | -2.791086 | -0.010179 |
| C4  | 4.943065  | -0.864616 | -0.007138 |
| C5  | 1.532597  | 1.873384  | 0.013623  |
| N6  | 3.937385  | -1.805681 | -0.007536 |
| N7  | 1.177028  | 0.608947  | 0.008705  |
| N8  | 2.880876  | 2.003169  | 0.011554  |
| N9  | 4.719114  | 0.428073  | -0.002570 |
| C10 | 3.413210  | 0.736770  | 0.002233  |
| N11 | 6.208651  | -1.318231 | -0.010888 |
| H12 | 6.949581  | -0.637865 | -0.014803 |
| H13 | 6.445142  | -2.293954 | -0.021071 |
| O14 | 1.742815  | -2.437269 | -0.001620 |
| H15 | 0.828852  | 2.692891  | 0.018978  |
| C16 | 3.644048  | 3.245000  | 0.000425  |
| H17 | 4.383866  | 3.220220  | 0.799128  |
| H18 | 4.147918  | 3.361347  | -0.958786 |
| H19 | 2.958631  | 4.075384  | 0.159895  |
| C20 | -3.947354 | -0.409148 | -0.000975 |
| C21 | -5.577635 | 1.033243  | -0.016711 |
| C22 | -3.475123 | 0.938160  | -0.005469 |
| H23 | -6.589816 | 1.414043  | -0.024702 |
| N24 | -4.490611 | 1.802724  | -0.015181 |
| C25 | -6.267541 | -1.402775 | 0.008113  |
| H26 | -6.214528 | -1.923456 | 0.964304  |
| H27 | -6.032304 | -2.096925 | -0.797903 |
| H28 | -7.269649 | -1.002372 | -0.136265 |
| N29 | -5.318646 | -0.299112 | -0.009835 |
| N30 | -3.238971 | -1.499859 | 0.006065  |
| O31 | -1.470657 | 2.220741  | 0.001255  |
| C32 | -2.025453 | 1.140816  | 0.000626  |
| N33 | -1.300204 | -0.045857 | 0.006423  |
| H34 | 0.026537  | 0.222880  | 0.008787  |
| N35 | -1.123807 | -2.339387 | 0.011075  |
| H36 | -0.101114 | -2.309488 | 0.008802  |
| H37 | -1.591508 | -3.231396 | 0.012011  |
| C38 | -1.879886 | -1.251207 | 0.007766  |

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.289064 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.310394                    |
| Thermal correction to Enthalpy=              | 0.311338                    |
| Thermal correction to Gibbs Free Energy=     | 0.236806                    |
| Sum of electronic and zero-point Energies=   | -1163.172733                |
| Sum of electronic and thermal Energies=      | -1163.151403                |
| Sum of electronic and thermal Enthalpies=    | -1163.150459                |
| Sum of electronic and thermal Free Energies= | -1163.224992                |

**[9MG - H<sub>N1</sub>]<sup>-</sup> · [9MG + H<sub>N7</sub>]<sup>+</sup>**

|    |          |           |           |
|----|----------|-----------|-----------|
| C1 | 2.576736 | -1.531717 | -0.001735 |
| C2 | 2.369458 | -0.122114 | 0.001791  |
| H3 | 4.180182 | -2.795066 | -0.010428 |
| C4 | 4.963944 | -0.871566 | -0.007735 |
| C5 | 1.570027 | 1.895943  | 0.013724  |
| N6 | 3.954493 | -1.808900 | -0.007385 |
| N7 | 1.219845 | 0.628521  | 0.009277  |
| N8 | 2.915188 | 2.010828  | 0.010823  |
| N9 | 4.746376 | 0.423815  | -0.003421 |

C10 3.443340 0.738278 0.001691  
 N11 6.226826 -1.328880 -0.012585  
 H12 6.970431 -0.651208 -0.015321  
 H13 6.460214 -2.305553 -0.018634  
 O14 1.751420 -2.426041 -0.000317  
 H15 0.860038 2.710021 0.019185  
 C16 3.688668 3.247667 -0.000465  
 H17 4.426578 3.216036 0.799579  
 H18 4.194443 3.356731 -0.959328  
 H19 3.009717 4.083607 0.156845  
 C20 -3.987927 -0.398406 -0.001420  
 C21 -5.574472 1.092906 -0.017557  
 C22 -3.474689 0.934329 -0.004924  
 H23 -6.574780 1.503786 -0.026118  
 N24 -4.465300 1.829091 -0.014965  
 C25 -6.337349 -1.320810 0.006014  
 H26 -6.300188 -1.844387 0.961479  
 H27 -6.123565 -2.021536 -0.800406  
 H28 -7.327275 -0.890763 -0.137644  
 N29 -5.356175 -0.246792 -0.011192  
 N30 -3.311952 -1.508996 0.005579  
 O31 -1.433079 2.156867 0.003673  
 C32 -2.017853 1.087606 0.002347  
 N33 -1.325962 -0.110293 0.008228  
 H34 0.188045 0.258898 0.010560  
 N35 -1.214316 -2.400725 0.011516  
 H36 -0.196267 -2.377118 0.010171  
 H37 -1.695424 -3.284815 0.011471  
 C38 -1.943558 -1.288603 0.008374

Zero-point correction= 0.292569 (Hartree/Particle)  
 Thermal correction to Energy= 0.314123  
 Thermal correction to Enthalpy= 0.315068  
 Thermal correction to Gibbs Free Energy= 0.240029  
 Sum of electronic and zero-point Energies= -1163.169909  
 Sum of electronic and thermal Energies= -1163.148355  
 Sum of electronic and thermal Enthalpies= -1163.147410  
 Sum of electronic and thermal Free Energies= -1163.222449

**9MG<sup>+</sup>**

N1 1.947625 -0.353540 -0.005643  
 C2 2.315095 0.953144 -0.004812  
 H3 3.354398 1.253134 -0.007230  
 N4 1.288855 1.810559 -0.002588  
 C5 0.215752 1.034053 -0.000509  
 C6 -1.204737 1.375218 0.002035  
 O7 -1.721565 2.449543 0.004616  
 N8 -1.997021 0.181551 0.001626  
 H9 -2.995489 0.355940 0.003518  
 C10 -1.527133 -1.088852 -0.000929  
 N11 -2.375063 -2.104886 -0.002525  
 H12 -3.376555 -1.991117 -0.002734  
 H13 -1.993311 -3.039347 -0.003959  
 N14 -0.209624 -1.396550 -0.001778  
 C15 0.578553 -0.353825 -0.001595  
 C16 2.810103 -1.532777 0.009063

H17 2.713488 -2.046256 0.965146  
 H18 2.521148 -2.200388 -0.801328  
 H19 3.839639 -1.210018 -0.133490

Zero-point correction= 0.145836 (Hartree/Particle)  
 Thermal correction to Energy= 0.155778  
 Thermal correction to Enthalpy= 0.156722  
 Thermal correction to Gibbs Free Energy= 0.109820  
 Sum of electronic and zero-point Energies= -581.413801  
 Sum of electronic and thermal Energies= -581.403859  
 Sum of electronic and thermal Enthalpies= -581.402914  
 Sum of electronic and thermal Free Energies= -581.449817

**9MG**

C1 1.130096 1.404442 0.000941  
 C2 -0.252698 1.012964 -0.010446  
 C3 1.530184 -1.060342 0.000917  
 C4 -2.362990 0.899747 -0.009227  
 N5 1.956347 0.237894 0.006668  
 N6 -1.398399 1.772546 -0.011644  
 N7 -1.921609 -0.405452 -0.008764  
 N8 0.275563 -1.407021 -0.013354  
 C9 -0.560680 -0.337509 -0.006202  
 N10 2.501798 -2.026940 0.060743  
 H11 2.152115 -2.957997 -0.101375  
 H12 3.391475 -1.830400 -0.368417  
 O13 1.649037 2.495465 0.013387  
 H14 -3.419408 1.128931 -0.010761  
 C15 -2.715825 -1.615621 0.020456  
 H16 -2.383688 -2.296607 -0.763681  
 H17 -2.619669 -2.114460 0.986559  
 H18 -3.760216 -1.354298 -0.148486  
 H19 2.942676 0.441847 0.084891

Zero-point correction= 0.146257 (Hartree/Particle)  
 Thermal correction to Energy= 0.156150  
 Thermal correction to Enthalpy= 0.157094  
 Thermal correction to Gibbs Free Energy= 0.111048  
 Sum of electronic and zero-point Energies= -581.690897  
 Sum of electronic and thermal Energies= -581.681004  
 Sum of electronic and thermal Enthalpies= -581.680060  
 Sum of electronic and thermal Free Energies= -581.726106

**[9MG - HN1]\***

N1 1.928242 -0.363151 -0.007921  
 C2 2.286445 0.949585 -0.005452  
 H3 3.326154 1.247685 -0.008150  
 N4 1.265940 1.794537 -0.002739  
 C5 0.176100 1.007984 -0.000813  
 C6 -1.267246 1.316908 0.002496  
 O7 -1.692959 2.453394 0.006123  
 N8 -2.088910 0.201723 0.001746  
 C9 -1.586604 -1.001875 -0.000957  
 N10 -2.427655 -2.056675 -0.002576  
 H11 -3.417949 -1.886764 -0.001956  
 H12 -2.059107 -2.990156 -0.004450  
 N13 -0.241291 -1.397178 -0.002337



C14 0.549283 -0.366739 -0.002590  
 C15 2.782395 -1.533943 0.011145  
 H16 2.693279 -2.050928 0.967760  
 H17 2.489873 -2.213272 -0.789731  
 H18 3.814902 -1.220028 -0.138651

Zero-point correction= 0.131989 (Hartree/Particle)  
 Thermal correction to Energy= 0.142073  
 Thermal correction to Enthalpy= 0.143017  
 Thermal correction to Gibbs Free Energy= 0.095651  
 Sum of electronic and zero-point Energies= -581.041053  
 Sum of electronic and thermal Energies= -581.030969  
 Sum of electronic and thermal Enthalpies= -581.030025  
 Sum of electronic and thermal Free Energies= -581.077392

### [9MG + HN7]<sup>+</sup>

C1 1.153343 1.398909 0.001821  
 C2 -0.217647 0.964052 0.000918  
 H3 2.979880 0.480054 0.002068  
 C4 1.581215 -1.052193 -0.000718  
 C5 -2.404039 0.785336 -0.004167  
 N6 1.991747 0.259404 0.001351  
 N7 -1.406576 1.659263 -0.001278  
 N8 -1.909173 -0.457417 -0.004582  
 N9 0.311520 -1.411744 -0.000968  
 C10 -0.526602 -0.372927 -0.000586  
 N11 2.526343 -1.999404 -0.002363  
 H12 2.230141 -2.961506 -0.003605  
 H13 3.510672 -1.796241 -0.002883  
 O14 1.585610 2.520603 0.002807  
 H15 -3.453410 1.032967 -0.006438  
 C16 -2.668556 -1.707071 0.006628  
 H17 -2.322552 -2.336480 -0.811447  
 H18 -2.506895 -2.217311 0.955168  
 H19 -3.725139 -1.479773 -0.120954  
 H20 -1.500888 2.666111 -0.002863

Zero-point correction= 0.159532 (Hartree/Particle)  
 Thermal correction to Energy= 0.169755  
 Thermal correction to Enthalpy= 0.170699  
 Thermal correction to Gibbs Free Energy= 0.123954  
 Sum of electronic and zero-point Energies= -582.064167  
 Sum of electronic and thermal Energies= -582.053943  
 Sum of electronic and thermal Enthalpies= -582.052999  
 Sum of electronic and thermal Free Energies= -582.099744

**Cartesian coordinates for the structures  
in Figure 4, optimized at  $\omega$ B97XD/  
6-311++G(d,p).**

**9MOG<sup>+</sup>·9MG**

|     |           |           |           |
|-----|-----------|-----------|-----------|
| C1  | 1.899472  | 1.124569  | 0.004986  |
| C2  | 3.302433  | 0.779486  | 0.006323  |
| H3  | 0.056756  | 0.179627  | -0.004599 |
| C4  | 1.569990  | -1.293020 | -0.005870 |
| C5  | 5.557915  | 0.696742  | 0.008598  |
| N6  | 1.099982  | -0.017299 | -0.000310 |
| N7  | 4.413473  | 1.529222  | 0.011561  |
| N8  | 5.053948  | -0.614274 | 0.003023  |
| N9  | 2.891158  | -1.613750 | -0.007902 |
| C10 | 3.698584  | -0.590074 | -0.000830 |
| N11 | 0.709999  | -2.288081 | -0.010023 |
| H12 | 1.096901  | -3.219353 | -0.014543 |
| H13 | -0.318751 | -2.181607 | -0.006133 |
| O14 | 1.448934  | 2.248442  | 0.007716  |
| C15 | -3.816543 | 0.770314  | -0.003731 |
| C16 | 5.895009  | -1.802352 | -0.014643 |
| H17 | 5.794859  | -2.315321 | -0.971271 |
| H18 | 6.925048  | -1.479603 | 0.125641  |
| H19 | 5.599064  | -2.469229 | 0.794381  |
| O20 | 6.696561  | 1.046381  | 0.012132  |
| H21 | 4.464749  | 2.538519  | 0.017339  |
| N22 | -3.321233 | 2.043897  | -0.002190 |
| N23 | -1.554727 | 0.686800  | -0.012351 |
| C24 | -1.957961 | 1.930796  | -0.008913 |
| H25 | -1.302574 | 2.789977  | -0.008335 |
| N26 | -5.115459 | 0.418368  | -0.002054 |
| C27 | -5.296378 | -0.877545 | 0.008423  |
| C28 | -2.710026 | -0.058345 | -0.009951 |
| C29 | -4.109440 | 3.266671  | -0.015370 |
| H30 | -4.864892 | 3.220337  | 0.768027  |
| H31 | -3.446932 | 4.111047  | 0.168275  |
| H32 | -4.598652 | 3.388714  | -0.982048 |
| C33 | -2.898431 | -1.463960 | -0.001771 |
| O34 | -2.053908 | -2.354887 | 0.001673  |
| N35 | -4.261330 | -1.786436 | 0.007409  |
| H36 | -4.458782 | -2.777420 | 0.046829  |
| N37 | -6.549744 | -1.378935 | 0.052160  |
| H38 | -6.746033 | -2.343487 | -0.149721 |
| H39 | -7.303661 | -0.717969 | -0.034775 |

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.298773 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.321262                    |
| Thermal correction to Enthalpy=              | 0.322206                    |
| Thermal correction to Gibbs Free Energy=     | 0.245099                    |
| Sum of electronic and zero-point Energies=   | -1238.435628                |
| Sum of electronic and thermal Energies=      | -1238.413139                |
| Sum of electronic and thermal Enthalpies=    | -1238.412195                |
| Sum of electronic and thermal Free Energies= | -1238.489302                |

**TS-G-PT1**

|    |           |          |           |
|----|-----------|----------|-----------|
| C1 | -1.765038 | 1.006896 | -0.009664 |
|----|-----------|----------|-----------|

|     |           |           |           |
|-----|-----------|-----------|-----------|
| C2  | -3.186583 | 0.741750  | -0.006854 |
| H3  | 0.308193  | 0.165368  | -0.004329 |
| C4  | -1.546441 | -1.369637 | 0.001262  |
| C5  | -5.444746 | 0.770712  | -0.003406 |
| N6  | -0.997848 | -0.138783 | -0.006453 |
| N7  | -4.261648 | 1.544960  | -0.009557 |
| N8  | -5.008457 | -0.561800 | 0.001478  |
| N9  | -2.885842 | -1.657019 | 0.007225  |
| C10 | -3.649541 | -0.604171 | 0.001893  |
| N11 | -0.744056 | -2.423770 | 0.003991  |
| H12 | -1.175534 | -3.333843 | 0.010383  |
| H13 | 0.275936  | -2.354358 | -0.001262 |
| O14 | -1.284980 | 2.131099  | -0.014032 |
| C15 | 3.687583  | 0.791410  | 0.002996  |
| C16 | -5.905920 | -1.706062 | 0.020600  |
| H17 | -5.829175 | -2.225768 | 0.975961  |
| H18 | -6.919223 | -1.332527 | -0.116128 |
| H19 | -5.645920 | -2.386531 | -0.789655 |
| O20 | -6.565923 | 1.178377  | -0.004326 |
| H21 | -4.262889 | 2.554887  | -0.015584 |
| N22 | 3.114043  | 2.039786  | 0.002473  |
| N23 | 1.455934  | 0.589848  | -0.000762 |
| C24 | 1.770650  | 1.865085  | 0.001244  |
| H25 | 1.041823  | 2.662257  | 0.000147  |
| N26 | 5.002913  | 0.526100  | 0.002969  |
| C27 | 5.269506  | -0.758807 | -0.001548 |
| C28 | 2.641975  | -0.106591 | 0.000291  |
| C29 | 3.836899  | 3.305347  | 0.020630  |
| H30 | 4.573955  | 3.310702  | -0.780977 |
| H31 | 3.124683  | 4.114720  | -0.129328 |
| H32 | 4.340878  | 3.430041  | 0.978748  |
| C33 | 2.910712  | -1.503509 | -0.004307 |
| O34 | 2.122800  | -2.435234 | -0.007670 |
| N35 | 4.295201  | -1.732219 | -0.004633 |
| H36 | 4.555736  | -2.709634 | -0.007816 |
| N37 | 6.549255  | -1.170035 | -0.003396 |
| H38 | 6.818013  | -2.137504 | -0.004834 |
| H39 | 7.267555  | -0.465752 | 0.000734  |

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.294341 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.316763                    |
| Thermal correction to Enthalpy=              | 0.317707                    |
| Thermal correction to Gibbs Free Energy=     | 0.240956                    |
| Sum of electronic and zero-point Energies=   | -1238.434135                |
| Sum of electronic and thermal Energies=      | -1238.411713                |
| Sum of electronic and thermal Enthalpies=    | -1238.410768                |
| Sum of electronic and thermal Free Energies= | -1238.487519                |

**[9MOG - H<sub>N1</sub>]<sup>-</sup> · [9MG + H<sub>N7</sub>]<sup>+</sup>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| C1 | -1.758599 | 0.944447  | -0.009300 |
| C2 | -3.189670 | 0.726766  | -0.006258 |
| H3 | 0.484685  | 0.208697  | -0.004825 |
| C4 | -1.611753 | -1.417153 | 0.000161  |
| C5 | -5.446928 | 0.824047  | -0.002499 |
| N6 | -1.023672 | -0.212861 | -0.006935 |
| N7 | -4.241567 | 1.561338  | -0.008440 |

N8 -5.052663 -0.520077 0.001652  
 N9 -2.961006 -1.678596 0.006358  
 C10 -3.693462 -0.604746 0.001828  
 N11 -0.834781 -2.496325 0.002094  
 H12 -1.279057 -3.399480 0.007976  
 H13 0.180569 -2.431398 -0.002647  
 O14 -1.248562 2.060989 -0.013222  
 C15 3.719098 0.795204 0.002977  
 C16 -5.984197 -1.635779 0.020047  
 H17 -5.922894 -2.159711 0.974330  
 H18 -6.985739 -1.231100 -0.115006  
 H19 -5.746182 -2.323171 -0.791237  
 O20 -6.555807 1.266915 -0.003055  
 H21 -4.212430 2.570504 -0.013906  
 N22 3.148674 2.049867 0.001964  
 N23 1.500771 0.611706 -0.001389  
 C24 1.808390 1.890309 0.000241  
 H25 1.072450 2.680775 -0.001168  
 N26 5.031668 0.524835 0.003316  
 C27 5.292761 -0.763005 -0.000772  
 C28 2.674733 -0.100439 0.000230  
 C29 3.881676 3.311170 0.019266  
 H30 4.616303 3.309474 -0.784376  
 H31 3.175257 4.125906 -0.128088  
 H32 4.388445 3.428787 0.976579  
 C33 2.928769 -1.502832 -0.004001  
 O34 2.133646 -2.423145 -0.007389  
 N35 4.315127 -1.733396 -0.003858  
 H36 4.573811 -2.711493 -0.006643  
 N37 6.570085 -1.177019 -0.002008  
 H38 6.836563 -2.145319 -0.004119  
 H39 7.290646 -0.474783 0.001660

Zero-point correction= 0.297994 (Hartree/Particle)  
 Thermal correction to Energy= 0.320631  
 Thermal correction to Enthalpy= 0.321575  
 Thermal correction to Gibbs Free Energy= 0.244203  
 Sum of electronic and zero-point Energies= -1238.431412  
 Sum of electronic and thermal Energies= -1238.408775  
 Sum of electronic and thermal Enthalpies= -1238.407831  
 Sum of electronic and thermal Free Energies= -1238.485203

**9MOG<sup>++</sup>**

C1 1.261357 1.483533 0.000736  
 C2 -0.057794 0.899485 0.001156  
 H3 3.199490 0.810088 -0.000111  
 C4 1.993296 -0.873416 -0.000485  
 C5 -2.262870 0.436519 -0.000792  
 N6 2.246226 0.466654 -0.000134  
 N7 -1.275271 1.452014 0.001061  
 N8 -1.538239 -0.775901 -0.002779  
 N9 0.759287 -1.396544 0.000514  
 C10 -0.217381 -0.519264 0.000353  
 N11 3.015074 -1.717509 -0.001510  
 H12 2.810123 -2.705534 -0.001119  
 H13 3.978410 -1.423233 -0.002503

O14 1.539890 2.651554 0.001102  
 C15 -2.171771 -2.090312 0.003496  
 H16 -1.996783 -2.581349 0.960530  
 H17 -3.239346 -1.940277 -0.145675  
 H18 -1.761963 -2.692477 -0.806228  
 O19 -3.441203 0.582572 -0.002657  
 H20 -1.497986 2.439504 0.000701

Zero-point correction= 0.151234 (Hartree/Particle)  
 Thermal correction to Energy= 0.162256  
 Thermal correction to Enthalpy= 0.163200  
 Thermal correction to Gibbs Free Energy= 0.113871  
 Sum of electronic and zero-point Energies= -656.675467  
 Sum of electronic and thermal Energies= -656.664444  
 Sum of electronic and thermal Enthalpies= -656.663500  
 Sum of electronic and thermal Free Energies= -656.712830

**9MG**

C1 1.130096 1.404442 0.000941  
 C2 -0.252698 1.012964 -0.010446  
 C3 1.530184 -1.060342 0.000917  
 C4 -2.362990 0.899747 -0.009227  
 N5 1.956347 0.237894 0.006668  
 N6 -1.398399 1.772546 -0.011644  
 N7 -1.921609 -0.405452 -0.008764  
 N8 0.275563 -1.407021 -0.013354  
 C9 -0.560680 -0.337509 -0.006202  
 N10 2.501798 -2.026940 0.060743  
 H11 2.152115 -2.957997 -0.101375  
 H12 3.391475 -1.830400 -0.368417  
 O13 1.649037 2.495465 0.013387  
 H14 -3.419408 1.128931 -0.010761  
 C15 -2.715825 -1.615621 0.020456  
 H16 -2.383688 -2.296607 -0.763681  
 H17 -2.619669 -2.114460 0.986559  
 H18 -3.760216 -1.354298 -0.148486  
 H19 2.942676 0.441847 0.084891

Zero-point correction= 0.146257 (Hartree/Particle)  
 Thermal correction to Energy= 0.156150  
 Thermal correction to Enthalpy= 0.157094  
 Thermal correction to Gibbs Free Energy= 0.111048  
 Sum of electronic and zero-point Energies= -581.690897  
 Sum of electronic and thermal Energies= -581.681004  
 Sum of electronic and thermal Enthalpies= -581.680060  
 Sum of electronic and thermal Free Energies= -581.726106

**[9MOG - H<sub>N1</sub>]<sup>\*</sup>**

C1 1.338047 1.439829 0.001018  
 C2 -0.004850 0.870869 0.000984  
 C3 2.039509 -0.779548 -0.000425  
 C4 -2.224101 0.433668 -0.001156  
 N5 2.337289 0.500571 0.000062  
 N6 -1.232684 1.429075 0.000110  
 N7 -1.527833 -0.776258 -0.002859  
 N8 0.790742 -1.397710 0.000821  
 C9 -0.177332 -0.535734 0.000542  
 N10 3.055884 -1.662560 -0.002201

H11 2.860867 -2.647331 -0.001796  
 H12 3.999215 -1.316372 -0.002972  
 O13 1.506547 2.649790 0.001763  
 C14 -2.163241 -2.077726 0.003834  
 H15 -1.974017 -2.587647 0.949755  
 H16 -3.233767 -1.924432 -0.123408  
 H17 -1.773406 -2.681765 -0.815984  
 O18 -3.413637 0.597730 -0.002501  
 H19 -1.434151 2.417411 -0.000014

Zero-point correction= 0.137707 (Hartree/Particle)  
 Thermal correction to Energy= 0.148816  
 Thermal correction to Enthalpy= 0.149760  
 Thermal correction to Gibbs Free Energy= 0.100002  
 Sum of electronic and zero-point Energies= -656.308079  
 Sum of electronic and thermal Energies= -656.296971  
 Sum of electronic and thermal Enthalpies= -656.296027  
 Sum of electronic and thermal Free Energies= -656.345784

**[9MG + H<sub>N7</sub>]<sup>+</sup>**

C1 1.153343 1.398909 0.001821  
 C2 -0.217647 0.964052 0.000918  
 H3 2.979880 0.480054 0.002068  
 C4 1.581215 -1.052193 -0.000718  
 C5 -2.404039 0.785336 -0.004167  
 N6 1.991747 0.259404 0.001351  
 N7 -1.406576 1.659263 -0.001278  
 N8 -1.909173 -0.457417 -0.004582  
 N9 0.311520 -1.411744 -0.000968  
 C10 -0.526602 -0.372927 -0.000586  
 N11 2.526343 -1.999404 -0.002363  
 H12 2.230141 -2.961506 -0.003605  
 H13 3.510672 -1.796241 -0.002883  
 O14 1.585610 2.520603 0.002807  
 H15 -3.453410 1.032967 -0.006438  
 C16 -2.668556 -1.707071 0.006628  
 H17 -2.322552 -2.336480 -0.811447  
 H18 -2.506895 -2.217311 0.955168  
 H19 -3.725139 -1.479773 -0.120954  
 H20 -1.500888 2.666111 -0.002863

Zero-point correction= 0.159532 (Hartree/Particle)  
 Thermal correction to Energy= 0.169755  
 Thermal correction to Enthalpy= 0.170699  
 Thermal correction to Gibbs Free Energy= 0.123954  
 Sum of electronic and zero-point Energies= -582.064167  
 Sum of electronic and thermal Energies= -582.053943  
 Sum of electronic and thermal Enthalpies= -582.052999  
 Sum of electronic and thermal Free Energies= -582.099744

**Cartesian coordinates for the structures  
in Figure 6, optimized at  $\omega$ B97XD/  
6-311++G(d,p).**

**${}^9\text{MOG}_{\text{WC}}^+ \cdot {}^9\text{MOG}_{\text{HG}}$**

|     |           |           |           |
|-----|-----------|-----------|-----------|
| C1  | -1.902956 | -0.527217 | 0.018117  |
| C2  | -3.324209 | -0.783520 | 0.006496  |
| H3  | -0.620589 | 1.147368  | 0.020759  |
| C4  | -2.589235 | 1.804058  | 0.004969  |
| C5  | -5.417397 | -1.621842 | -0.012154 |
| N6  | -1.642717 | 0.835562  | 0.016066  |
| N7  | -5.489026 | -0.215846 | -0.018204 |
| N8  | -3.920260 | 1.578028  | -0.004537 |
| C9  | -4.244223 | 0.309989  | -0.004835 |
| N10 | -2.167076 | 3.059239  | 0.003864  |
| H11 | -2.849769 | 3.800220  | -0.003976 |
| H12 | -1.178596 | 3.275604  | 0.010090  |
| O13 | -1.027737 | -1.367186 | 0.028205  |
| C14 | -6.743118 | 0.526289  | -0.021864 |
| H15 | -6.881124 | 1.028428  | 0.935683  |
| H16 | -6.727139 | 1.260092  | -0.826615 |
| H17 | -7.547277 | -0.189224 | -0.183335 |
| O18 | -6.316014 | -2.401252 | -0.020009 |
| C19 | 3.772453  | -1.920691 | 0.010762  |
| C20 | 3.165801  | -0.635045 | 0.016863  |
| H21 | 5.688931  | -2.645799 | -0.049497 |
| C22 | 5.864525  | -0.583681 | -0.019263 |
| C23 | 1.771980  | 1.111881  | 0.017005  |
| N24 | 5.184987  | -1.770200 | -0.007437 |
| N25 | 1.831137  | -0.241232 | 0.026305  |
| N26 | 3.062508  | 1.576865  | 0.001309  |
| N27 | 5.269888  | 0.586091  | -0.010103 |
| C28 | 3.929000  | 0.500248  | 0.000720  |
| N29 | 7.215202  | -0.639933 | -0.074583 |
| H30 | 7.705204  | 0.233421  | 0.023282  |
| H31 | 7.715022  | -1.482338 | 0.150193  |
| O32 | 3.259107  | -3.017411 | 0.015350  |
| C33 | 3.425418  | 2.982214  | -0.011405 |
| H34 | 3.100358  | 3.464901  | 0.910810  |
| H35 | 4.509019  | 3.042619  | -0.093878 |
| H36 | 2.963726  | 3.477392  | -0.865761 |
| O37 | 0.752586  | 1.832435  | 0.020530  |
| H38 | 1.019694  | -0.849890 | 0.033925  |
| N39 | -4.033126 | -1.918448 | 0.002459  |
| H40 | -3.669849 | -2.862468 | 0.007267  |

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.303104 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.327089                    |
| Thermal correction to Enthalpy=              | 0.328033                    |
| Thermal correction to Gibbs Free Energy=     | 0.246000                    |
| Sum of electronic and zero-point Energies=   | -1313.669403                |
| Sum of electronic and thermal Energies=      | -1313.645417                |
| Sum of electronic and thermal Enthalpies=    | -1313.644473                |
| Sum of electronic and thermal Free Energies= | -1313.726507                |

**TS-OG\_HT'**

|     |           |           |           |
|-----|-----------|-----------|-----------|
| C1  | -1.719045 | -0.144234 | 0.014228  |
| C2  | -2.999617 | -0.657179 | 0.013420  |
| H3  | -0.768407 | 1.692025  | 0.001805  |
| C4  | -2.802470 | 2.036265  | -0.011547 |
| C5  | -4.892012 | -1.903767 | 0.011458  |
| N6  | -1.685732 | 1.249207  | 0.002687  |
| N7  | -5.216552 | -0.524610 | -0.002521 |
| N8  | -4.024615 | 1.552431  | -0.015146 |
| C9  | -4.083730 | 0.217421  | -0.002891 |
| N10 | -2.615754 | 3.370604  | -0.029044 |
| H11 | -3.429472 | 3.960265  | -0.018475 |
| H12 | -1.706746 | 3.795376  | 0.013686  |
| O13 | -0.645954 | -0.817728 | 0.024328  |
| C14 | -6.577081 | -0.025517 | -0.029198 |
| H15 | -6.741454 | 0.660510  | 0.801719  |
| H16 | -6.774389 | 0.489509  | -0.970089 |
| H17 | -7.240938 | -0.883277 | 0.063057  |
| O18 | -5.672933 | -2.817135 | 0.014477  |
| C19 | 3.185018  | -1.904804 | -0.010736 |
| C20 | 2.836409  | -0.500215 | -0.001871 |
| H21 | 4.906483  | -3.022649 | -0.020325 |
| C22 | 5.508073  | -1.045316 | -0.009755 |
| C23 | 1.883166  | 1.482818  | 0.008607  |
| N24 | 4.599431  | -2.058330 | -0.014420 |
| N25 | 1.653878  | 0.109830  | 0.002675  |
| N26 | 3.271785  | 1.684665  | 0.006537  |
| N27 | 5.172198  | 0.249527  | -0.000711 |
| C28 | 3.876971  | 0.477525  | 0.001805  |
| N29 | 6.803532  | -1.344041 | -0.014068 |
| H30 | 7.464879  | -0.583935 | -0.009855 |
| H31 | 7.158481  | -2.285518 | -0.020832 |
| O32 | 2.454741  | -2.855887 | -0.015000 |
| C33 | 3.924077  | 2.984880  | 0.023537  |
| H34 | 3.156154  | 3.743460  | -0.112060 |
| H35 | 4.427363  | 3.138147  | 0.978034  |
| H36 | 4.648631  | 3.041309  | -0.787627 |
| O37 | 1.038856  | 2.350141  | 0.012315  |
| H38 | 0.537757  | -0.336730 | 0.010908  |
| N39 | -3.513019 | -1.944674 | 0.021873  |
| H40 | -2.990641 | -2.803136 | 0.033725  |

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.298885 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.322942                    |
| Thermal correction to Enthalpy=              | 0.323887                    |
| Thermal correction to Gibbs Free Energy=     | 0.241745                    |
| Sum of electronic and zero-point Energies=   | -1313.631091                |
| Sum of electronic and thermal Energies=      | -1313.607033                |
| Sum of electronic and thermal Enthalpies=    | -1313.606089                |
| Sum of electronic and thermal Free Energies= | -1313.688230                |

**${}^9\text{MOG} + \text{H}_{\text{O6}}^+ \cdot {}^9\text{MOG} - \text{H}_{\text{N7}}^{\bullet} \text{HG}$**

|    |           |           |           |
|----|-----------|-----------|-----------|
| C1 | -1.772118 | -0.351259 | -0.023045 |
| C2 | -3.082322 | -0.730721 | -0.011150 |
| H3 | -0.584151 | 1.370562  | -0.027036 |
| C4 | -2.560924 | 1.922021  | -0.008474 |

C5 -5.111117 -1.736489 0.011033  
 N6 -1.549145 1.006148 -0.022468  
 N7 -5.268970 -0.324633 0.015261  
 N8 -3.838089 1.586854 0.006120  
 C9 -4.061954 0.276829 0.004105  
 N10 -2.208129 3.216211 -0.009679  
 H11 -2.939812 3.905934 0.001366  
 H12 -1.244305 3.506753 -0.020658  
 O13 -0.777093 -1.192760 -0.034967  
 C14 -6.564504 0.330403 0.045001  
 H15 -6.711497 0.834606 1.000747  
 H16 -6.631248 1.055076 -0.766055  
 H17 -7.320597 -0.442746 -0.081609  
 O18 -5.994097 -2.545935 0.019389  
 C19 3.269883 -1.900811 -0.015849  
 C20 2.861282 -0.511658 -0.016331  
 H21 5.034604 -2.951519 0.005453  
 C22 5.558520 -0.952382 0.023049  
 C23 1.836032 1.390771 -0.014939  
 N24 4.688344 -2.000351 0.005265  
 N25 1.645574 0.020336 -0.028143  
 N26 3.208434 1.678205 0.008854  
 N27 5.176385 0.324918 0.021632  
 C28 3.869146 0.500349 0.003836  
 N29 6.866260 -1.210070 0.042507  
 H30 7.499377 -0.426449 0.053651  
 H31 7.245292 -2.141768 0.045468  
 O32 2.579699 -2.884064 -0.029770  
 C33 3.783152 3.013705 0.011829  
 H34 3.124812 3.672278 0.575508  
 H35 4.761146 2.967928 0.487865  
 H36 3.887835 3.386725 -1.007745  
 O37 0.953991 2.237779 -0.017255  
 H38 0.129622 -0.767018 -0.035287  
 N39 -3.744705 -1.945066 -0.006511  
 H40 -3.333250 -2.862918 -0.015105

Zero-point correction= 0.302929 (Hartree/Particle)  
 Thermal correction to Energy= 0.327009  
 Thermal correction to Enthalpy= 0.327953  
 Thermal correction to Gibbs Free Energy= 0.245690  
 Sum of electronic and zero-point Energies= -1313.669358  
 Sum of electronic and thermal Energies= -1313.645278  
 Sum of electronic and thermal Enthalpies= -1313.644334  
 Sum of electronic and thermal Free Energies= -1313.726597

### 9MOG<sub>WC</sub><sup>+</sup>-9MOG<sub>WC</sub>

C1 1.941972 -0.284284 0.030514  
 C2 3.299486 -0.544922 0.013035  
 H3 0.673246 1.350119 0.024572  
 C4 2.606854 2.067088 0.007033  
 C5 5.394094 -1.414685 -0.013549  
 N6 1.657111 1.086040 0.027470  
 N7 4.046990 -1.714008 0.008362  
 N8 5.453769 -0.000913 -0.023133  
 N9 3.896742 1.817926 -0.009455

C10 4.201443 0.516077 -0.008758  
 N11 2.175623 3.345584 -0.020181  
 H12 2.873483 4.066937 0.046935  
 H13 1.213578 3.587433 0.139868  
 O14 0.994125 -1.116301 0.047750  
 C15 6.699524 0.741937 -0.056569  
 H16 6.810866 1.256050 -1.012084  
 H17 6.720486 1.469836 0.754273  
 H18 7.506761 0.021653 0.067471  
 O19 6.331061 -2.167275 -0.021230  
 H20 3.701975 -2.657228 0.024979  
 C21 -2.040656 0.660048 0.031114  
 C22 -3.484067 0.625471 0.011195  
 H23 -0.428746 -0.715666 0.042716  
 C24 -2.235745 -1.757019 0.013572  
 C25 -5.707732 1.011493 -0.022449  
 N26 -1.508016 -0.613638 0.031833  
 N27 -5.487214 -0.377287 -0.028650  
 N28 -3.585150 -1.809077 -0.004474  
 C29 -4.160890 -0.635187 -0.006570  
 N30 -1.562583 -2.895623 0.013886  
 H31 -2.074048 -3.763915 0.000906  
 H32 -0.549751 -2.897989 0.024815  
 O33 -1.348755 1.663344 0.044926  
 C34 -6.559945 -1.364174 -0.039924  
 H35 -6.379802 -2.084102 -0.837176  
 H36 -6.603357 -1.877462 0.920639  
 H37 -7.494167 -0.834928 -0.217934  
 O38 -6.746116 1.590946 -0.036836  
 N39 -4.413183 1.588805 0.001943  
 H40 -4.257689 2.587808 0.008060

Zero-point correction= 0.302010 (Hartree/Particle)  
 Thermal correction to Energy= 0.326236  
 Thermal correction to Enthalpy= 0.327180  
 Thermal correction to Gibbs Free Energy= 0.244915  
 Sum of electronic and zero-point Energies= -1313.668228  
 Sum of electronic and thermal Energies= -1313.644002  
 Sum of electronic and thermal Enthalpies= -1313.643058  
 Sum of electronic and thermal Free Energies= -1313.725323

### TS-OG\_PT1

C1 -1.943908 0.566900 -0.004358  
 C2 -3.387138 0.597035 -0.006034  
 H3 -0.175164 -0.868735 -0.003750  
 C4 -2.218072 -1.803365 0.013346  
 C5 -5.594142 1.073966 -0.013093  
 N6 -1.432558 -0.704894 0.004496  
 N7 -4.277127 1.597753 -0.015721  
 N8 -5.431670 -0.320987 -0.002623  
 N9 -3.576242 -1.820037 0.015348  
 C10 -4.113731 -0.632051 0.004038  
 N11 -1.613551 -2.985417 0.021423  
 H12 -2.178769 -3.819222 0.027916  
 H13 -0.606516 -3.056599 0.019849  
 O14 -1.237894 1.571980 -0.009991

C15 -6.542309 -1.263228 0.015941  
 H16 -6.407326 -1.997756 -0.777098  
 H17 -6.589011 -1.766188 0.981898  
 H18 -7.458086 -0.698930 -0.150296  
 O19 -6.608247 1.697131 -0.020718  
 H20 -4.080576 2.588919 -0.025021  
 C21 1.901967 -0.309204 -0.005862  
 C22 3.253022 -0.549556 -0.007133  
 H23 0.565880 1.274255 -0.000415  
 C24 2.486610 2.041515 0.011867  
 C25 5.370811 -1.359282 -0.012949  
 N26 1.564992 1.035666 0.002635  
 N27 5.392576 0.057926 -0.002042  
 N28 3.787102 1.828297 0.013533  
 C29 4.130405 0.541242 0.002904  
 N30 2.020801 3.302848 0.019990  
 H31 2.691589 4.052016 0.026770  
 H32 1.038822 3.516087 0.018798  
 O33 0.977652 -1.198510 -0.012327  
 C34 6.619796 0.833386 0.013803  
 H35 6.606506 1.565248 -0.793448  
 H36 6.733415 1.344748 0.970365  
 H37 7.443244 0.135234 -0.128336  
 O38 6.326771 -2.083959 -0.020356  
 N39 4.030955 -1.696425 -0.015138  
 H40 3.712922 -2.649466 -0.028221

Zero-point correction= 0.298354 (Hartree/Particle)  
 Thermal correction to Energy= 0.322142  
 Thermal correction to Enthalpy= 0.323086  
 Thermal correction to Gibbs Free Energy= 0.242609  
 Sum of electronic and zero-point Energies= -1313.670108  
 Sum of electronic and thermal Energies= -1313.646320  
 Sum of electronic and thermal Enthalpies= -1313.645376  
 Sum of electronic and thermal Free Energies= -1313.725852

$[9\text{MOG} - \text{H}_{\text{N1}}]_{\text{WC}}^{\bullet} \cdot [9\text{MOG} + \text{H}_{\text{O6}}]_{\text{WC}}^{+}$   
 C1 -1.912813 -0.424885 -0.011335  
 C2 -3.349596 -0.564858 0.003161  
 H3 0.143753 1.133239 -0.004852  
 C4 -2.336242 1.886619 -0.036714  
 C5 -5.518006 -1.198206 0.035144  
 N6 -1.466448 0.860446 -0.029743  
 N7 -4.167038 -1.626624 0.025747  
 N8 -5.456280 0.202747 0.018343  
 N9 -3.701020 1.823858 -0.024783  
 C10 -4.160995 0.607210 -0.003513  
 N11 -1.835784 3.121115 -0.057674  
 H12 -2.470835 3.902635 -0.062751  
 H13 -0.842216 3.282764 -0.069770  
 O14 -1.156679 -1.405510 -0.006628  
 C15 -6.630651 1.062878 0.010048  
 H16 -6.537493 1.810911 0.796530  
 H17 -6.727904 1.555046 -0.957821  
 H18 -7.501257 0.435732 0.193432  
 O19 -6.484852 -1.894115 0.055497

H20 -3.900525 -2.600662 0.036459  
 C21 1.976113 0.429191 0.001369  
 C22 3.330100 0.584446 0.010355  
 H23 0.495427 -1.039455 -0.018302  
 C24 2.359909 -1.940923 -0.029762  
 C25 5.505546 1.220264 0.033924  
 N26 1.521492 -0.867155 -0.018408  
 N27 5.415362 -0.196366 0.013785  
 N28 3.676920 -1.829323 -0.023180  
 C29 4.122587 -0.579179 -0.001908  
 N30 1.795128 -3.157359 -0.049460  
 H31 2.400221 -3.960626 -0.055874  
 H32 0.796935 -3.282591 -0.051952  
 O33 1.120838 1.418060 0.011107  
 C34 6.578680 -1.066099 -0.000477  
 H35 6.491107 -1.812167 0.788794  
 H36 6.668885 -1.562742 -0.967124  
 H37 7.452769 -0.440471 0.172703  
 O38 6.514073 1.865381 0.051441  
 N39 4.195012 1.664207 0.031103  
 H40 3.954903 2.640291 0.047325

Zero-point correction= 0.302528 (Hartree/Particle)  
 Thermal correction to Energy= 0.326391  
 Thermal correction to Enthalpy= 0.327335  
 Thermal correction to Gibbs Free Energy= 0.246450  
 Sum of electronic and zero-point Energies= -1313.668310  
 Sum of electronic and thermal Energies= -1313.644446  
 Sum of electronic and thermal Enthalpies= -1313.643502  
 Sum of electronic and thermal Free Energies= -1313.724387

### 9MOG<sup>++</sup>

C1 1.261357 1.483533 0.000736  
 C2 -0.057794 0.899485 0.001156  
 H3 3.199490 0.810088 -0.000111  
 C4 1.993296 -0.873416 -0.000485  
 C5 -2.262870 0.436519 -0.000792  
 N6 2.246226 0.466654 -0.000134  
 N7 -1.275271 1.452014 0.001061  
 N8 -1.538239 -0.775901 -0.002779  
 N9 0.759287 -1.396544 0.000514  
 C10 -0.217381 -0.519264 0.000353  
 N11 3.015074 -1.717509 -0.001510  
 H12 2.810123 -2.705534 -0.001119  
 H13 3.978410 -1.423233 -0.002503  
 O14 1.539890 2.651554 0.001102  
 C15 -2.171771 -2.090312 0.003496  
 H16 -1.996783 -2.581349 0.960530  
 H17 -3.239346 -1.940277 -0.145675  
 H18 -1.761963 -2.692477 -0.806228  
 O19 -3.441203 0.582572 -0.002657  
 H20 -1.497986 2.439504 0.000701

Zero-point correction= 0.151234 (Hartree/Particle)  
 Thermal correction to Energy= 0.162256  
 Thermal correction to Enthalpy= 0.163200  
 Thermal correction to Gibbs Free Energy= 0.113871

Sum of electronic and zero-point Energies= -656.675467  
 Sum of electronic and thermal Energies= -656.664444  
 Sum of electronic and thermal Enthalpies= -656.663500  
 Sum of electronic and thermal Free Energies= -656.712830

**9MOG**

C1 1.219433 1.490018 0.000523  
 C2 -0.059254 0.886209 -0.008206  
 H3 3.164339 0.835915 0.076800  
 C4 1.995041 -0.865435 0.001401  
 C5 -2.278101 0.420012 -0.004179  
 N6 2.221934 0.478784 0.005654  
 N7 -1.339337 1.426260 -0.008786  
 N8 -1.530399 -0.770525 -0.002368  
 N9 0.801019 -1.394796 -0.009319  
 C10 -0.193095 -0.479735 -0.001963  
 N11 3.093064 -1.680992 0.056987  
 H12 2.886848 -2.654341 -0.101646  
 H13 3.955112 -1.354450 -0.347772  
 O14 1.532059 2.665821 0.008864  
 C15 -2.128173 -2.086899 0.012906  
 H16 -1.923443 -2.593027 0.958243  
 H17 -3.202971 -1.953454 -0.104242  
 H18 -1.736689 -2.687707 -0.809001  
 O19 -3.485272 0.510213 -0.003988  
 H20 -1.576562 2.402667 -0.009469

Zero-point correction= 0.150795 (Hartree/Particle)  
 Thermal correction to Energy= 0.162073  
 Thermal correction to Enthalpy= 0.163017  
 Thermal correction to Gibbs Free Energy= 0.113745  
 Sum of electronic and zero-point Energies= -656.944069  
 Sum of electronic and thermal Energies= -656.932790  
 Sum of electronic and thermal Enthalpies= -656.931846  
 Sum of electronic and thermal Free Energies= -656.981119

**[9MOG + H<sub>06</sub>]<sup>+</sup>**

C1 1.214187 1.344573 0.005670  
 C2 -0.053459 0.883740 -0.005595  
 H3 3.171371 0.712049 -0.132227  
 C4 1.959541 -0.953310 0.000929  
 C5 -2.278292 0.464794 -0.001759  
 N6 2.221142 0.390415 -0.006314  
 N7 -1.305687 1.454217 0.008042  
 N8 -1.553697 -0.768087 -0.004886  
 N9 0.726958 -1.432580 0.007908  
 C10 -0.238593 -0.528578 -0.007290  
 N11 2.989119 -1.804704 -0.006327  
 H12 2.778583 -2.790183 -0.008265  
 H13 3.952078 -1.518604 0.036624  
 O14 1.532903 2.632878 -0.052660  
 C15 -2.206200 -2.069515 0.014188  
 H16 -2.035330 -2.560059 0.972564  
 H17 -3.271846 -1.897893 -0.127105  
 H18 -1.816646 -2.686866 -0.794304  
 O19 -3.463303 0.580110 -0.005738

H20 -1.531234 2.435238 -0.024814  
 H21 2.268267 2.877352 0.518892

Zero-point correction= 0.162411 (Hartree/Particle)  
 Thermal correction to Energy= 0.174411  
 Thermal correction to Enthalpy= 0.175355  
 Thermal correction to Gibbs Free Energy= 0.124915  
 Sum of electronic and zero-point Energies= -657.287535  
 Sum of electronic and thermal Energies= -657.275534  
 Sum of electronic and thermal Enthalpies= -657.274590  
 Sum of electronic and thermal Free Energies= -657.325031

**[9MOG - H<sub>N1</sub>]<sup>\*</sup>**

C1 1.338047 1.439829 0.001018  
 C2 -0.004850 0.870869 0.000984  
 C3 2.039509 -0.779548 -0.000425  
 C4 -2.224101 0.433668 -0.001156  
 N5 2.337289 0.500571 0.000062  
 N6 -1.232684 1.429075 0.000110  
 N7 -1.527833 -0.776258 -0.002859  
 N8 0.790742 -1.397710 0.000821  
 C9 -0.177332 -0.535734 0.000542  
 N10 3.055884 -1.662560 -0.002201  
 H11 2.860867 -2.647331 -0.001796  
 H12 3.999215 -1.316372 -0.002972  
 O13 1.506547 2.649790 0.001763  
 C14 -2.163241 -2.077726 0.003834  
 H15 -1.974017 -2.587647 0.949755  
 H16 -3.233767 -1.924432 -0.123408  
 H17 -1.773406 -2.681765 -0.815984  
 O18 -3.413637 0.597730 -0.002501  
 H19 -1.434151 2.417411 -0.000014

Zero-point correction= 0.137707 (Hartree/Particle)  
 Thermal correction to Energy= 0.148816  
 Thermal correction to Enthalpy= 0.149760  
 Thermal correction to Gibbs Free Energy= 0.100002  
 Sum of electronic and zero-point Energies= -656.308079  
 Sum of electronic and thermal Energies= -656.296971  
 Sum of electronic and thermal Enthalpies= -656.296027  
 Sum of electronic and thermal Free Energies= -656.345784

**[9MOG - H<sub>N7</sub>]<sup>\*</sup>**

C1 1.221512 1.494995 0.001606  
 C2 -0.110970 0.931471 0.003611  
 H3 3.151880 0.793544 -0.033984  
 C4 1.949111 -0.883877 -0.001286  
 C5 -2.231953 0.527962 0.000547  
 N6 2.200611 0.453968 -0.000321  
 N7 -1.285008 1.542898 0.004369  
 N8 -1.552845 -0.740167 -0.004202  
 N9 0.738725 -1.403617 0.003188  
 C10 -0.238809 -0.491098 -0.000453  
 N11 3.009595 -1.721431 -0.034064  
 H12 2.809965 -2.702185 0.067503  
 H13 3.941313 -1.402653 0.164439  
 O14 1.581622 2.644798 -0.001004  
 C15 -2.207127 -2.028934 0.001010



|     |           |           |           |
|-----|-----------|-----------|-----------|
| H16 | -3.274367 | -1.848673 | -0.121711 |
| H17 | -1.836668 | -2.643015 | -0.820990 |
| H18 | -2.030290 | -2.545749 | 0.946239  |
| O19 | -3.435368 | 0.620710  | -0.000808 |

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.137264 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.148400                    |
| Thermal correction to Enthalpy=              | 0.149344                    |
| Thermal correction to Gibbs Free Energy=     | 0.099626                    |
| Sum of electronic and zero-point Energies=   | -656.305795                 |
| Sum of electronic and thermal Energies=      | -656.294659                 |
| Sum of electronic and thermal Enthalpies=    | -656.293715                 |
| Sum of electronic and thermal Free Energies= | -656.343433                 |