

Supplementary Information

1 BSSE correction energies

Table S1 BSSE correction energies (kcal mol⁻¹) for 1-X⁻ complexes

| X | Binding mode | B3LYP/6-31(1)++G(d,p) | B3LYP/6-311++G(d,p) ^a |
|-----------------|--------------|-----------------------|----------------------------------|
| F | I | 3.69 | 3.63 |
| Cl | I | 1.64 | 1.75 |
| Br | I | 0.54 | 0.53 |
| I | I | 0.40 | 0.41 |
| NO ₃ | I | 2.70 | 2.70 |
| F | II | 3.48 | 3.43 |
| Cl | II | 1.51 | 1.52 |
| Br | II | 0.44 | 0.42 |
| I | II | 0.30 | 0.29 |
| NO ₃ | II | 2.42 | 2.38 |
| F | III | 3.61 | 3.58 |
| Cl | III | 1.61 | 1.62 |
| Br | III | 0.51 | 0.50 |
| I | III | 0.39 | 0.36 |
| NO ₃ | III | 2.72 | 2.72 |

^a Correction energies were calculated based on the geometries optimized at the B3LYP/6-31(1)++G(d,p) level.

2 Gibbs free energy changes for 1-X⁻ complexes with different alpha values

Table S2 The calculated Gibbs free energy changes (kcal mol⁻¹) for 1-X⁻ complex with different alpha values in solution

| alpha | experiment | 1.20 | 1.25 | 1.30 | 1.35 | 1.40 |
|-----------------|----------------------|---------|---------|---------|---------|---------|
| Cl | -4.52 | -1.31 | -3.84 | -4.41 | -6.93 | -8.42 |
| | (-1.38) ^a | (-1.56) | (-2.71) | (-1.89) | (-3.03) | (-3.17) |
| Br | -3.14 | 0.25 | -1.13 | -2.52 | -3.90 | -5.25 |
| | (0.00) | (0.00) | (0.00) | (0.00) | (0.00) | (0.00) |
| NO ₃ | -3.70 | -0.46 | -1.76 | -3.03 | -4.23 | -5.37 |
| | (-0.56) | (-0.71) | (-0.63) | (-0.51) | (-0.33) | (-0.12) |
| I | > 0 | 4.02 | 2.45 | 1.66 | 0.44 | -0.76 |
| | | (3.77) | (3.58) | (4.18) | (4.34) | (4.49) |

^a The values in parentheses are the relative energies to Br⁻ complex.

As shown in Table S2, although the calculated Gibbs free energy changes with different alpha values exhibit obvious differences, the relative values (in parentheses) of Gibbs free energy changes with different alpha are all consistent with the experiment.

3 Cartesian coordinates of the optimized geometries listed in Tables 4 and 6

C1 B3LYP/6-31++G(d,p)

| | | | |
|---|-------------|-------------|-------------|
| C | 3.94188000 | 1.48449900 | 0.57175700 |
| C | 4.36952500 | -3.40309300 | 0.79036200 |
| N | 3.58473900 | -2.17663100 | 0.92557900 |
| C | 4.17436600 | -0.97084300 | 0.58002300 |
| N | 3.45686200 | 0.15546400 | 0.92899100 |
| O | 5.26154100 | -0.91064700 | 0.00809600 |
| C | 3.70775300 | 1.84353000 | -0.90107900 |
| C | 4.35414200 | -4.00213000 | -0.61773000 |
| C | -5.25190700 | -2.72803700 | 0.17683000 |
| N | -3.90438300 | -3.06072000 | 0.62076100 |
| C | -2.90434200 | -3.29414500 | -0.30230900 |
| N | -1.65874400 | -3.56986100 | 0.24267100 |
| C | -0.59153200 | -4.08189600 | -0.62045700 |
| O | -3.10538600 | -3.27219900 | -1.51542100 |
| C | -5.46685500 | -1.26954200 | -0.24596600 |
| C | 0.39219000 | -2.98630300 | -1.04643100 |
| C | -3.21963600 | 2.76601100 | 1.13577900 |
| N | -1.82700800 | 3.07053600 | 0.82218900 |
| C | -1.50273000 | 4.18056300 | 0.06083100 |
| N | -0.16105400 | 4.26450000 | -0.26770000 |
| C | 0.35093800 | 5.44890700 | -0.94541500 |
| O | -2.33734800 | 5.00969900 | -0.29616000 |
| C | -4.02845600 | 2.28824500 | -0.07702200 |
| C | 1.68450300 | 5.15091000 | -1.62865700 |
| S | 2.82754400 | -4.92568000 | -1.10247400 |
| S | 1.67041800 | -3.59409100 | -2.22260300 |
| S | -5.39448200 | -0.14663500 | 1.22431200 |
| S | -5.72394500 | 1.72879300 | 0.37169900 |
| S | 2.99857500 | 4.80387700 | -0.35791700 |
| S | 4.32497900 | 3.52363200 | -1.33594900 |
| H | 3.44084700 | 2.20823000 | 1.22110700 |
| H | 5.01174800 | 1.52361300 | 0.78703400 |
| H | 5.41355500 | -3.18849500 | 1.04944300 |
| H | 3.98209900 | -4.12879700 | 1.51114900 |
| H | 2.90068900 | -2.15804100 | 1.66819700 |
| H | 2.47963800 | 0.05304900 | 1.16203700 |
| H | 2.65063400 | 1.76392200 | -1.17442500 |
| H | 4.28153700 | 1.16830500 | -1.54422500 |
| H | 5.14545800 | -4.75708700 | -0.68938800 |
| H | 4.55812300 | -3.23633100 | -1.36874200 |
| H | -5.47240100 | -3.35889700 | -0.68826700 |
| H | -5.94798700 | -3.00372600 | 0.97610700 |
| H | -3.64481200 | -2.81389100 | 1.56511100 |
| H | -1.64143600 | -3.86929700 | 1.20753000 |
| H | -0.05495900 | -4.86595800 | -0.07826800 |
| H | -1.04327600 | -4.52681200 | -1.51021700 |
| H | -6.45491500 | -1.16291800 | -0.70229800 |
| H | -4.70647100 | -0.97654100 | -0.97278800 |
| H | 0.88105700 | -2.52289300 | -0.18455700 |
| H | -0.13726500 | -2.20985200 | -1.61006400 |
| H | -3.21781200 | 1.99537200 | 1.91190000 |
| H | -3.68322900 | 3.66300700 | 1.55264000 |
| H | -1.19141800 | 2.28577700 | 0.78159200 |
| H | 0.49575400 | 3.81477400 | 0.35827600 |
| H | 0.45133800 | 6.29902000 | -0.25444200 |
| H | -0.38373000 | 5.74359700 | -1.69909700 |
| H | -3.51752200 | 1.47720100 | -0.60530400 |
| H | -4.17629300 | 3.11501500 | -0.77852100 |
| H | 2.00311800 | 6.01092400 | -2.22261600 |
| H | 1.59840400 | 4.27743600 | -2.27910000 |

C1a B3LYP/6-31++G(d,p)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.00000000 | 4.25265800 | 0.16977200 |
| O | -0.38842600 | 5.20479000 | 0.84728300 |
| N | -0.64361000 | 3.86113800 | -0.99131700 |
| N | 1.10729600 | 3.50239200 | 0.50960500 |
| C | -1.86490200 | 4.53721200 | -1.40006700 |
| C | 1.97104100 | 3.99500500 | 1.58117700 |
| C | -3.12496400 | 4.14128700 | -0.61833200 |
| C | 3.28427100 | 3.22414000 | 1.65583500 |
| C | 3.68291000 | -2.12632900 | 0.16977200 |
| O | 4.70169300 | -2.26600800 | 0.84728300 |
| N | 3.66564900 | -1.37318600 | -0.99131700 |
| N | 2.47951300 | -2.71014200 | 0.50960500 |
| C | 4.86179200 | -0.65355400 | -1.40006700 |
| C | 2.47425500 | -3.70447400 | 1.58117700 |
| C | 5.14894200 | 0.63565500 | -0.61833200 |
| C | 1.15005200 | -4.45633200 | 1.65583500 |
| C | -3.68291000 | -2.12632900 | 0.16977200 |
| O | -4.31326700 | -2.93878200 | 0.84728300 |
| N | -3.02203900 | -2.48795200 | -0.99131700 |
| N | -3.58680900 | -0.79225000 | 0.50960500 |
| C | -2.99689000 | -3.88365900 | -1.40006700 |
| C | -4.44529600 | -0.29053100 | 1.58117700 |
| C | -2.02397800 | -4.77694200 | -0.61833200 |
| C | -4.43432300 | 1.23219200 | 1.65583500 |
| S | -0.27459900 | -4.43832300 | -1.12180600 |
| S | 0.82591700 | -5.59031400 | 0.22543800 |
| S | 3.98100000 | 1.98135200 | -1.12180600 |
| S | 4.42839500 | 3.51042200 | 0.22543800 |
| S | -3.70640100 | 2.45697100 | -1.12180600 |
| S | -5.25431200 | 2.07989200 | 0.22543800 |
| H | -0.47520200 | 2.92973700 | -1.34355600 |
| H | 1.56618400 | 2.98838600 | -0.23223400 |
| H | -2.00338700 | 4.37388800 | -2.47421400 |
| H | -1.71049800 | 5.60861600 | -1.24698600 |
| H | 1.44645700 | 3.88730300 | 2.53820900 |
| H | 2.16961100 | 5.06531400 | 1.44801000 |
| H | -3.93320800 | 4.84625500 | -0.83145700 |
| H | -2.91618100 | 4.15139000 | 0.45277600 |
| H | 3.84694600 | 3.56814100 | 2.52973300 |
| H | 3.12569200 | 2.14721900 | 1.76501300 |
| H | 2.77482800 | -1.05333200 | -1.34355600 |
| H | 1.80492600 | -2.85054800 | -0.23223400 |
| H | 4.78959200 | -0.45196000 | -2.47421400 |
| H | 5.71245300 | -1.32297300 | -1.24698600 |
| H | 2.64327500 | -3.19632000 | 2.53820900 |
| H | 3.30188500 | -4.41159500 | 1.44801000 |
| H | 6.16358400 | 0.98313100 | -0.83145700 |
| H | 5.05330000 | 0.44979200 | 0.45277600 |
| H | 1.16662800 | -5.11562400 | 2.52973300 |
| H | 0.29670000 | -3.78053800 | 1.76501300 |
| H | -2.29962600 | -1.87640600 | -1.34355600 |
| H | -3.37111000 | -0.13783800 | -0.23223400 |
| H | -2.78620500 | -3.92192800 | -2.47421400 |
| H | -4.00195500 | -4.28564300 | -1.24698600 |
| H | -4.08973200 | -0.69098300 | 2.53820900 |
| H | -5.47149600 | -0.65371900 | 1.44801000 |
| H | -2.23037600 | -5.82938600 | -0.83145700 |
| H | -2.13711900 | -4.60118200 | 0.45277600 |
| H | -5.01357400 | 1.54748200 | 2.52973300 |
| H | -3.42239200 | 1.63331900 | 1.76501300 |

C2 B3LYP/6-31++G(d,p)

| | | | |
|---|-------------|-------------|-------------|
| C | -1.82716605 | -2.56561112 | -1.83926787 |
| C | -3.70357440 | 1.10105217 | 0.71858613 |
| N | -2.53534697 | 0.27069087 | 0.40607013 |
| C | -2.64464903 | -0.51775077 | -0.76322187 |
| N | -1.67779075 | -1.46782178 | -0.89569887 |
| O | -3.52694063 | -0.31851843 | -1.59833588 |
| C | -2.84146690 | -3.62014735 | -1.37964188 |
| C | -3.47634064 | 2.06458942 | 1.87508513 |
| C | 2.80532635 | 2.65686343 | 0.71858613 |
| N | 1.50209865 | 2.06032945 | 0.40607013 |
| C | 0.87393920 | 2.54920863 | -0.76322187 |
| N | -0.43227557 | 2.18692030 | -0.89569887 |
| C | -1.30830138 | 2.86517777 | -1.83926787 |
| O | 1.48762526 | 3.21367940 | -1.59833588 |
| C | 3.52615720 | 1.97830460 | 1.87508513 |
| C | -1.71440612 | 4.27085619 | -1.37964188 |
| C | 3.13546743 | -0.29956666 | -1.83926787 |
| N | 2.11006632 | -0.71909852 | -0.89569887 |
| C | 1.77070983 | -2.03145786 | -0.76322187 |
| N | 1.03324832 | -2.33102032 | 0.40607013 |
| C | 0.89824805 | -3.75791560 | 0.71858613 |
| O | 2.03931537 | -2.89516097 | -1.59833588 |
| C | 4.55587302 | -0.65070884 | -1.37964188 |
| C | -0.04981656 | -4.04289402 | 1.87508513 |
| S | -2.25519070 | 3.44167733 | 1.65670314 |
| S | -2.97357027 | 4.46176032 | -0.03592686 |
| S | 4.10817534 | 0.23221377 | 1.65670314 |
| S | 5.35078292 | 0.34430723 | -0.03592686 |
| S | -1.85298465 | -3.67389110 | 1.65670314 |
| S | -2.37721265 | -4.80606755 | -0.03592686 |
| H | -2.18155133 | -2.15408299 | -2.78959687 |
| H | -0.84171927 | -3.00668554 | -2.00809987 |
| H | -4.57384390 | 0.47660427 | 0.97083712 |
| H | -3.97372783 | 1.65046514 | -0.18447387 |
| H | -2.20020226 | -0.26653674 | 1.20140513 |
| H | -0.97539621 | -1.58894282 | -0.17394186 |
| H | -3.04830673 | -4.31589494 | -2.20281389 |
| H | -3.78542099 | -3.13902877 | -1.11328289 |
| H | -4.43592731 | 2.51509803 | 2.14237912 |
| H | -3.10438074 | 1.54850385 | 2.77001613 |
| H | 2.69967335 | 3.72276287 | 0.97083712 |
| H | 3.41620865 | 2.61611668 | -0.18447387 |
| H | 0.86927354 | 2.03869942 | 1.20140513 |
| H | -0.88836674 | 1.63918930 | -0.17394186 |
| H | -2.18300643 | 2.23229305 | -2.00809987 |
| H | -0.77471493 | 2.96632037 | -2.78959687 |
| H | 4.39610245 | 2.58407673 | 2.14237912 |
| H | 2.89323404 | 1.91422066 | 2.77001613 |
| H | -0.82576816 | 4.84778513 | -1.11328289 |
| H | -2.21352130 | 4.79785854 | -2.20281389 |
| H | 3.02472570 | 0.77439250 | -2.00809987 |
| H | 2.95626626 | -0.81223738 | -2.78959687 |
| H | 1.86376295 | -0.05024648 | -0.17394186 |
| H | 1.33092872 | -1.77216268 | 1.20140513 |
| H | 0.55751918 | -4.26658182 | -0.18447387 |
| H | 1.87417054 | -4.19936714 | 0.97083712 |
| H | 5.26182802 | -0.48196359 | -2.20281389 |
| H | 4.61118915 | -1.70875636 | -1.11328289 |
| H | 0.03982487 | -5.09917476 | 2.14237912 |
| H | 0.21114670 | -3.46272451 | 2.77001613 |

C3 B3LYP/6-31++G(d,p)

| | | | |
|---|-------------|-------------|-------------|
| C | 1.54465861 | 4.64290701 | 0.36253897 |
| O | 1.28404787 | 5.17591726 | 1.44187597 |
| N | 0.91903462 | 5.00975661 | -0.81698503 |
| N | 2.47410179 | 3.63371632 | 0.22394598 |
| C | -0.20129136 | 5.94172114 | -0.78896103 |
| C | 3.31316265 | 3.24265589 | 1.34657898 |
| C | -1.49763978 | 5.39608830 | -0.17298203 |
| C | 3.80170674 | 1.80314769 | 1.19556799 |
| C | 3.24854611 | -3.65916710 | 0.36253897 |
| O | 3.84045189 | -3.69997671 | 1.44187597 |
| N | 3.87905918 | -3.30078563 | -0.81698503 |
| N | 1.90983975 | -3.95949316 | 0.22394598 |
| C | 5.24632713 | -2.79653714 | -0.78896103 |
| C | 1.15164105 | -4.49061097 | 1.34657898 |
| C | 5.42196944 | -1.40105005 | -0.17298203 |
| C | -0.33928167 | -4.19394846 | 1.19556799 |
| C | -4.79320473 | -0.98373991 | 0.36253897 |
| O | -5.12449977 | -1.47594055 | 1.44187597 |
| N | -4.79809380 | -1.70897097 | -0.81698503 |
| N | -4.38394153 | 0.32577684 | 0.22394598 |
| C | -5.04503577 | -3.14518401 | -0.78896103 |
| C | -4.46480370 | 1.24795508 | 1.34657898 |
| C | -3.92432966 | -3.99503825 | -0.17298203 |
| C | -3.46242508 | 2.39080077 | 1.19556799 |
| S | -2.36446214 | -3.80159387 | -1.15041800 |
| S | -1.05607291 | -5.13707045 | -0.24066699 |
| S | 4.47450794 | -0.14688734 | -1.15041800 |
| S | 4.97686996 | 1.65394925 | -0.24066699 |
| S | -2.11004580 | 3.94848122 | -1.15041800 |
| S | -3.92079705 | 3.48312119 | -0.24066699 |
| H | 0.93678297 | 4.34220972 | -1.57576602 |
| H | 2.86356690 | 3.46430758 | -0.69509402 |
| H | -0.37581623 | 6.27725996 | -1.81617903 |
| H | 0.10050749 | 6.81259322 | -0.19994503 |
| H | 2.70934300 | 3.32749384 | 2.25379398 |
| H | 4.16564328 | 3.92741751 | 1.47075298 |
| H | -2.26792437 | 6.17241863 | -0.18946003 |
| H | -1.31497349 | 5.08652280 | 0.85735597 |
| H | 4.32473610 | 1.48985465 | 2.10288299 |
| H | 2.96421578 | 1.12646402 | 1.00882599 |
| H | 3.29207244 | -2.98238271 | -1.57576602 |
| H | 1.56839492 | -4.21207547 | -0.69509402 |
| H | 5.62417471 | -2.81316358 | -1.81617903 |
| H | 5.84962505 | -3.49333865 | -0.19994503 |
| H | 1.52702270 | -4.01010679 | 2.25379398 |
| H | 1.31842170 | -5.57126166 | 1.47075298 |
| H | 6.47943352 | -1.12212920 | -0.18946003 |
| H | 5.06254471 | -1.40446095 | 0.85735597 |
| H | -0.87211608 | -4.49025865 | 2.10288299 |
| H | -0.50656143 | -3.13031818 | 1.00882599 |
| H | -4.22885541 | -1.35982701 | -1.57576602 |
| H | -4.43196182 | 0.74776789 | -0.69509402 |
| H | -5.24835848 | -3.46409638 | -1.81617903 |
| H | -5.95013254 | -3.31925457 | -0.19994503 |
| H | -4.23636570 | 0.68261295 | 2.25379398 |
| H | -5.48406498 | 1.64384415 | 1.47075298 |
| H | -4.21150915 | -5.05028943 | -0.18946003 |
| H | -3.74757121 | -3.68206185 | 0.85735597 |
| H | -3.45262002 | 3.00040401 | 2.10288299 |
| H | -2.45765435 | 2.00385416 | 1.00882599 |

C4 B3LYP/6-31++G(d,p)

| | | | |
|---|-------------|-------------|-------------|
| C | -4.60805824 | -1.02829612 | -0.50281608 |
| O | -3.63611832 | -0.57390637 | -1.10073008 |
| N | -5.62533495 | -0.22800961 | -0.01380909 |
| N | -4.78109588 | -2.38121402 | -0.27570307 |
| C | -5.52900150 | 1.22570652 | -0.07140310 |
| C | -3.86644761 | -3.36794189 | -0.83647506 |
| C | -4.71120130 | 1.81956115 | 1.08304990 |
| C | -2.85890332 | -3.86389187 | 0.21149595 |
| C | 3.19455968 | -3.47654743 | -0.50281608 |
| O | 2.31507666 | -2.86201765 | -1.10073008 |
| N | 3.01012959 | -4.75767817 | -0.01380909 |
| N | 4.45273977 | -2.94994348 | -0.27570307 |
| C | 1.70300777 | -5.40110902 | -0.07140310 |
| C | 4.84994704 | -1.66447091 | -0.83647506 |
| C | 0.77981447 | -4.98980058 | 1.08304990 |
| C | 4.77568018 | -0.54393697 | 0.21149595 |
| C | 1.41349855 | 4.50484356 | -0.50281608 |
| O | 1.32104166 | 3.43592402 | -1.10073008 |
| N | 2.61520537 | 4.98568777 | -0.01380909 |
| N | 0.32835611 | 5.33115750 | -0.27570307 |
| C | 3.82599374 | 4.17540250 | -0.07140310 |
| C | -0.98349943 | 5.03241280 | -0.83647506 |
| C | 3.93138682 | 3.17023943 | 1.08304990 |
| C | -1.91677685 | 4.40782884 | 0.21149595 |
| S | -4.75224485 | 3.66245088 | 1.13704589 |
| S | -1.87867732 | -5.25995772 | -0.50547103 |
| S | -0.79565308 | -5.94679020 | 1.13704589 |
| S | 5.49459567 | 1.00299657 | -0.50547103 |
| S | 5.54789793 | 2.28433932 | 1.13704589 |
| S | -3.61591835 | 4.25696114 | -0.50547103 |
| H | -6.26005439 | -0.62155422 | 0.66682391 |
| H | -5.68072408 | -2.70771026 | 0.04509893 |
| H | -6.54319939 | 1.63672036 | -0.06138811 |
| H | -5.06363095 | 1.49021074 | -1.02275210 |
| H | -3.34139146 | -2.90214129 | -1.67390806 |
| H | -4.45345040 | -4.20854280 | -1.22272205 |
| H | -5.13618722 | 1.52798227 | 2.05196890 |
| H | -3.67646441 | 1.47044591 | 1.04367291 |
| H | -2.18792541 | -3.05048233 | 0.49787095 |
| H | -3.37764524 | -4.23537136 | 1.09945296 |
| H | 3.66830894 | -5.11058902 | 0.66682391 |
| H | 5.18530791 | -3.56579623 | 0.04509893 |
| H | 1.85415829 | -6.48493707 | -0.06138811 |
| H | 1.24125512 | -5.13033841 | -1.02275210 |
| H | 4.18402382 | -1.44265924 | -1.67390806 |
| H | 5.87143017 | -1.75252978 | -1.22272205 |
| H | 1.24482215 | -5.21205974 | 2.05196890 |
| H | 0.56478869 | -3.91913453 | 1.04367291 |
| H | 5.35676181 | -0.80744090 | 1.09945296 |
| H | 3.73575790 | -0.36955782 | 0.49787095 |
| H | 2.59174545 | 5.73214324 | 0.66682391 |
| H | 0.49541616 | 6.27350650 | 0.04509893 |
| H | 4.68904110 | 4.84821672 | -0.06138811 |
| H | 3.82237583 | 3.64012767 | -1.02275210 |
| H | -0.84263235 | 4.34480054 | -1.67390806 |
| H | -1.41797978 | 5.96107258 | -1.22272205 |
| H | 3.89136507 | 3.68407747 | 2.05196890 |
| H | 3.11167572 | 2.44868862 | 1.04367291 |
| H | -1.54783249 | 3.42004015 | 0.49787095 |
| H | -1.97911657 | 5.04281226 | 1.09945296 |

C5 B3LYP/6-31++G(d,p)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.42215300 | -1.48533000 | 3.42175400 |
| C | -0.24963500 | -2.68756400 | 2.74385100 |
| S | -1.42333800 | -2.21827500 | 1.39529100 |
| S | -0.28711700 | -2.28495100 | -0.36140800 |
| C | -0.77738400 | -3.88285800 | -1.14836500 |
| C | -2.00134500 | -3.80001200 | -2.07255900 |
| N | -3.20395100 | -3.32561600 | -1.41139500 |
| C | -3.69200200 | -2.05495200 | -1.65452300 |
| N | -4.63080000 | -1.60894300 | -0.73664100 |
| C | -4.99506500 | -0.19449500 | -0.72663300 |
| C | -3.83995000 | 0.67800900 | -0.20897700 |
| S | -4.35914500 | 2.44623900 | -0.05154700 |
| S | -2.63398200 | 3.52067400 | -0.52535400 |
| C | -1.78249800 | 3.77906900 | 1.08820700 |
| C | -1.03297100 | 2.56825000 | 1.65894700 |
| N | -0.00904300 | 1.99358000 | 0.78145500 |
| C | 1.10654900 | 2.77514000 | 0.47519600 |
| N | 1.90807000 | 2.25979100 | -0.52319800 |
| C | 2.95748900 | 3.06969400 | -1.13563100 |
| C | 4.35304300 | 2.44671700 | -1.05496700 |
| S | 4.75905300 | 1.10944400 | -2.26691600 |
| S | 3.43706800 | -0.47000200 | -1.90205700 |
| C | 4.27903300 | -1.50081900 | -0.62265800 |
| C | 4.47605400 | -0.83438200 | 0.74356400 |
| N | 3.25307900 | -0.36304000 | 1.36460400 |
| C | 2.52078800 | -1.18535500 | 2.19363200 |
| N | 1.28390100 | -0.70176400 | 2.55697300 |
| O | -3.35640600 | -1.38340500 | -2.62774900 |
| O | 1.38419000 | 3.79659600 | 1.09990800 |
| O | 2.95091600 | -2.26455700 | 2.61265600 |
| H | 1.02159700 | -1.86681100 | 4.25553800 |
| H | -0.33762800 | -0.81381300 | 3.83286700 |
| H | -0.85599700 | -3.23438900 | 3.47573000 |
| H | 0.50018000 | -3.36902600 | 2.33723800 |
| H | -0.91813500 | -4.61743000 | -0.34945300 |
| H | 0.09702300 | -4.19517800 | -1.73143200 |
| H | -2.17559200 | -4.79832000 | -2.49735400 |
| H | -1.81404700 | -3.11487800 | -2.90186900 |
| H | -3.45719300 | -3.77231200 | -0.54094300 |
| H | -4.65343000 | -2.07477700 | 0.16108900 |
| H | -5.25593000 | 0.10212400 | -1.74411000 |
| H | -5.88698800 | -0.08667300 | -0.10155200 |
| H | -3.01580500 | 0.63252000 | -0.92299900 |
| H | -3.49691100 | 0.31233200 | 0.76350000 |
| H | -1.07412100 | 4.58934800 | 0.88820100 |
| H | -2.51664500 | 4.14019800 | 1.81439800 |
| H | -1.73350000 | 1.76596300 | 1.90744900 |
| H | -0.54150600 | 2.88201600 | 2.58474900 |
| H | -0.38510400 | 1.45427500 | 0.00899000 |
| H | 1.58624200 | 1.45286400 | -1.04230100 |
| H | 2.96822900 | 4.01548600 | -0.58690900 |
| H | 2.70460400 | 3.28264100 | -2.18134100 |
| H | 4.56906600 | 2.11536700 | -0.03650500 |
| H | 5.09705300 | 3.20891200 | -1.31866800 |
| H | 5.23982900 | -1.83316800 | -1.02725000 |
| H | 3.62190000 | -2.37243000 | -0.52689100 |
| H | 4.92347600 | -1.56621300 | 1.42157600 |
| H | 5.17655900 | 0.00153400 | 0.65110300 |
| H | 2.80584500 | 0.44875000 | 0.95741400 |
| H | 0.89603500 | 0.10874600 | 2.08785800 |

C6 B3LYP/6-31++G(d,p)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.65237500 | -1.68697800 | -1.18306000 |
| C | 3.59355300 | -2.56316800 | 1.14148400 |
| N | 2.55132200 | -1.70645400 | 0.61709800 |
| C | 1.45730300 | -2.23011100 | -0.02406200 |
| N | 0.55617600 | -1.29352700 | -0.48333800 |
| O | 1.28954800 | -3.44501700 | -0.18138600 |
| C | -1.77249400 | -2.12312800 | -0.22103200 |
| C | 4.49173400 | -3.23378000 | 0.09645100 |
| C | 1.08200500 | 3.72391800 | 0.45389700 |
| N | 2.48029300 | 3.56348900 | 0.84067400 |
| C | 3.06250400 | 2.32481600 | 0.94600500 |
| N | 4.36664100 | 2.30846900 | 1.37989100 |
| C | 5.14636300 | 1.07264500 | 1.40002100 |
| O | 2.43728100 | 1.28754400 | 0.68296300 |
| C | 0.89661600 | 3.75504600 | -1.06678000 |
| C | 5.71653200 | 0.71326800 | 0.02137900 |
| C | -4.08571700 | 2.88036000 | 0.33944500 |
| N | -4.85807200 | 1.77305500 | -0.19642300 |
| C | -5.41315500 | 0.83128400 | 0.64868600 |
| N | -5.95276800 | -0.27253600 | 0.01922000 |
| C | -6.40990000 | -1.40203500 | 0.81827100 |
| O | -5.46351200 | 0.99438700 | 1.87036800 |
| C | -2.60624000 | 2.54277900 | 0.55648100 |
| C | -5.29808400 | -2.33538100 | 1.31475500 |
| S | -3.35040800 | -2.30437600 | -1.17069700 |
| S | -4.55535200 | -3.47781700 | 0.06776000 |
| S | -1.71783200 | 2.12643400 | -1.01676400 |
| S | -0.85353900 | 3.93529500 | -1.61452900 |
| S | 5.35457800 | -2.15190000 | -1.11860300 |
| S | 6.61919400 | -0.90350300 | -0.01405800 |
| H | -0.41665200 | -2.51275600 | -1.85917900 |
| H | -0.97658800 | -0.83286700 | -1.78565500 |
| H | 3.13827000 | -3.36902600 | 1.73030100 |
| H | 4.20528400 | -1.96673000 | 1.82497200 |
| H | 2.66820000 | -0.69909800 | 0.64845400 |
| H | 0.70119200 | -0.31666600 | -0.26424400 |
| H | -1.91050100 | -1.37590000 | 0.56586400 |
| H | -1.52749400 | -3.08610400 | 0.23112400 |
| H | 5.23291800 | -3.86449400 | 0.59694100 |
| H | 3.88158800 | -3.87105000 | -0.55323100 |
| H | 0.70774100 | 4.64859000 | 0.90301900 |
| H | 0.51817100 | 2.88671400 | 0.87193600 |
| H | 3.00683000 | 4.38610200 | 1.09349200 |
| H | 4.86972900 | 3.18179300 | 1.44369400 |
| H | 4.49939000 | 0.27554800 | 1.76731500 |
| H | 5.95175700 | 1.19724200 | 2.12962200 |
| H | 1.31796300 | 2.85383800 | -1.51849800 |
| H | 1.39792100 | 4.62526100 | -1.50706100 |
| H | 6.43582700 | 1.47334300 | -0.30275600 |
| H | 4.91849300 | 0.65673200 | -0.72197600 |
| H | -4.18411800 | 3.73847400 | -0.33303300 |
| H | -4.52940200 | 3.14691100 | 1.30260000 |
| H | -4.72918900 | 1.54339200 | -1.17203400 |
| H | -5.60130800 | -0.49577200 | -0.90238000 |
| H | -6.92504700 | -0.98890400 | 1.68986000 |
| H | -7.13737500 | -1.96569900 | 0.22613800 |
| H | -2.07973100 | 3.37129600 | 1.03728300 |
| H | -2.51627600 | 1.65810000 | 1.19517600 |
| H | -5.71662800 | -3.03617500 | 2.04832900 |
| H | -4.51077300 | -1.76822200 | 1.81712300 |

C6 B3LYP/6-31(1)++G(d,p)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.65051275 | -1.67535479 | -1.16640847 |
| C | 3.60003350 | -2.56461827 | 1.14389661 |
| N | 2.55823213 | -1.70855024 | 0.61997639 |
| C | 1.45798811 | -2.22880454 | -0.01041608 |
| N | 0.55557302 | -1.29054908 | -0.45907985 |
| O | 1.28541704 | -3.44378000 | -0.16663050 |
| C | -1.77331929 | -2.12199794 | -0.21158620 |
| C | 4.49438347 | -3.23938796 | 0.09744237 |
| C | 1.08325215 | 3.72599060 | 0.45601077 |
| N | 2.48029466 | 3.55932229 | 0.84167237 |
| C | 3.06160060 | 2.32118004 | 0.94100348 |
| N | 4.36585027 | 2.30328661 | 1.36936199 |
| C | 5.14672589 | 1.06920562 | 1.39068327 |
| O | 2.43564058 | 1.28430658 | 0.67525928 |
| C | 0.89738019 | 3.76511609 | -1.06504684 |
| C | 5.71462697 | 0.70688521 | 0.01111897 |
| C | -4.09143929 | 2.87938248 | 0.33848146 |
| N | -4.85582688 | 1.76632387 | -0.19437886 |
| C | -5.41372006 | 0.82607880 | 0.64805058 |
| N | -5.94989634 | -0.27680058 | 0.01703157 |
| C | -6.41133543 | -1.40763797 | 0.81016648 |
| O | -5.46658159 | 0.98821101 | 1.87039114 |
| C | -2.60769422 | 2.55392068 | 0.54857102 |
| C | -5.30168741 | -2.34298970 | 1.30957080 |
| S | -3.34684168 | -2.29947847 | -1.16788294 |
| S | -4.55388589 | -3.48009845 | 0.06184259 |
| S | -1.72407747 | 2.14851369 | -1.02988322 |
| S | -0.85117173 | 3.95858815 | -1.61098054 |
| S | 5.35464166 | -2.16094613 | -1.12162452 |
| S | 6.61865928 | -0.90842808 | -0.02097724 |
| H | -0.41471869 | -2.49334801 | -1.85246830 |
| H | -0.97272136 | -0.81349422 | -1.75905221 |
| H | 3.14542428 | -3.36806667 | 1.73684704 |
| H | 4.21481805 | -1.96670837 | 1.82342778 |
| H | 2.67304096 | -0.70257950 | 0.65416701 |
| H | 0.71578139 | -0.31434307 | -0.25578063 |
| H | -1.91524280 | -1.38135116 | 0.58091770 |
| H | -1.52753211 | -3.08815636 | 0.23354867 |
| H | 5.23611800 | -3.87008166 | 0.59735575 |
| H | 3.88140121 | -3.87753171 | -0.54894423 |
| H | 0.71255511 | 4.64994919 | 0.90976121 |
| H | 0.51626409 | 2.88892152 | 0.87057471 |
| H | 3.00873119 | 4.37842130 | 1.09531674 |
| H | 4.86480171 | 3.17603852 | 1.44527055 |
| H | 4.50224443 | 0.27138607 | 1.76147471 |
| H | 5.95360917 | 1.19692798 | 2.11820844 |
| H | 1.31324796 | 2.86350357 | -1.52137005 |
| H | 1.40411167 | 4.63439817 | -1.50121126 |
| H | 6.43210085 | 1.46732688 | -0.31636582 |
| H | 4.91495759 | 0.64755111 | -0.73042800 |
| H | -4.19997118 | 3.73735719 | -0.33278027 |
| H | -4.53334215 | 3.14142711 | 1.30395780 |
| H | -4.73704013 | 1.54238536 | -1.17077736 |
| H | -5.59753167 | -0.49632490 | -0.90324695 |
| H | -6.93144312 | -0.99707106 | 1.68026500 |
| H | -7.13578692 | -1.96948650 | 0.21246877 |
| H | -2.08615776 | 3.38683770 | 1.02732726 |
| H | -2.50716716 | 1.66975816 | 1.18657933 |
| H | -5.72389767 | -3.04601295 | 2.03902953 |
| H | -4.51657743 | -1.77757220 | 1.81760415 |

1-F^r (model) B3LYP/6-31(1)++G(d,p)

| | | | |
|---|-------------|-------------|-------------|
| F | 0.00000000 | 0.00000000 | 0.33953000 |
| C | 0.00000000 | 3.33289100 | -0.09094900 |
| O | 0.06270800 | 4.55349800 | -0.31162100 |
| N | 0.64993900 | 2.72969900 | 0.95948800 |
| N | -0.71536800 | 2.45262500 | -0.86169500 |
| C | 1.54004400 | 3.47387600 | 1.81594400 |
| C | -1.54670200 | 2.87133100 | -1.96255700 |
| C | 2.97019500 | 3.63692900 | 1.26911600 |
| C | -2.98188400 | 2.33336900 | -1.89029100 |
| C | -2.88636800 | -1.66644600 | -0.09094900 |
| O | -3.97479900 | -2.22244200 | -0.31162100 |
| N | -2.68895900 | -0.80198600 | 0.95948800 |
| N | -1.76635200 | -1.84584000 | -0.86169500 |
| C | -3.77848700 | -0.40322100 | 1.81594400 |
| C | -1.71329500 | -2.77514800 | -1.96255700 |
| C | -4.63477000 | 0.75380000 | 1.26911600 |
| C | -0.52981400 | -3.74907200 | -1.89029100 |
| C | 2.88636800 | -1.66644600 | -0.09094900 |
| O | 3.91209100 | -2.33105600 | -0.31162100 |
| N | 2.03901900 | -1.92771400 | 0.95948800 |
| N | 2.48172000 | -0.60678600 | -0.86169500 |
| C | 2.23844300 | -3.07065500 | 1.81594400 |
| C | 3.25999600 | -0.09618300 | -1.96255700 |
| C | 1.66457500 | -4.39072900 | 1.26911600 |
| C | 3.51169900 | 1.41570300 | -1.89029100 |
| S | -0.18634400 | -4.33212600 | 1.18290500 |
| S | -0.65743200 | -5.13762400 | -0.67949900 |
| S | -3.65855900 | 2.32744200 | 1.18290500 |
| S | -4.12059700 | 3.13816500 | -0.67949900 |
| S | 3.84490300 | 2.00468500 | 1.18290500 |
| S | 4.77802900 | 1.99945900 | -0.67949900 |
| H | 0.59674100 | 1.71345600 | 1.02005000 |
| H | -0.66658600 | 1.46788200 | -0.59266700 |
| H | 1.56460400 | 2.98480400 | 2.79689000 |
| H | 1.12523200 | 4.47856700 | 1.95506500 |
| H | -1.12259800 | 2.52353200 | -2.92114600 |
| H | -1.54189100 | 3.96440000 | -1.98092900 |
| H | 3.54879200 | 4.30760800 | 1.91468600 |
| H | 2.93644700 | 4.06300700 | 0.26440600 |
| H | -3.48255000 | 2.51645700 | -2.85023800 |
| H | -2.99557000 | 1.25247500 | -1.71836600 |
| H | -1.78226700 | -0.33993500 | 1.02005000 |
| H | -0.93793000 | -1.31122200 | -0.59266700 |
| H | -3.36721900 | -0.13741500 | 2.79689000 |
| H | -4.44116900 | -1.26480400 | 1.95506500 |
| H | -1.62414400 | -2.23396400 | -2.92114600 |
| H | -2.66232600 | -3.31751700 | -1.98092900 |
| H | -5.50489400 | 0.91954000 | 1.91468600 |
| H | -4.98689000 | 0.51153400 | 0.26440600 |
| H | -0.43804100 | -4.27420500 | -2.85023800 |
| H | 0.41311000 | -3.22047700 | -1.71836600 |
| H | 1.18552600 | -1.37352100 | 1.02005000 |
| H | 1.60451600 | -0.15666000 | -0.59266700 |
| H | 1.80261400 | -2.84738900 | 2.79689000 |
| H | 3.31593700 | -3.21376400 | 1.95506500 |
| H | 2.74674200 | -0.28956800 | -2.92114600 |
| H | 4.20421700 | -0.64688300 | -1.98092900 |
| H | 1.95610100 | -5.22714800 | 1.91468600 |
| H | 2.05044400 | -4.57454100 | 0.26440600 |
| H | 3.92059000 | 1.75774800 | -2.85023800 |
| H | 2.58246000 | 1.96800200 | -1.71836600 |

1-Cl (model) B3LYP/6-31(1)++G(d,p)

| | | | |
|----|-------------|-------------|-------------|
| Cl | 0.00000000 | 0.00000000 | 0.42940900 |
| C | 0.00000000 | 3.90398900 | -0.07318600 |
| O | 0.12639900 | 5.09357800 | -0.40261900 |
| N | 0.74827200 | 3.32755200 | 0.92840800 |
| N | -0.91120800 | 3.05433500 | -0.64804100 |
| C | 1.80268100 | 4.06384600 | 1.58662700 |
| C | -1.68606100 | 3.44032600 | -1.80380600 |
| C | 3.17702800 | 3.96580300 | 0.89974100 |
| C | -3.07781900 | 2.80312300 | -1.82632700 |
| C | -3.38095400 | -1.95199500 | -0.07318600 |
| O | -4.47436800 | -2.43732400 | -0.40261900 |
| N | -3.25588100 | -1.01575300 | 0.92840800 |
| N | -2.18952700 | -2.31629700 | -0.64804100 |
| C | -4.42073400 | -0.47075500 | 1.58662700 |
| C | -2.13637900 | -3.18033500 | -1.80380600 |
| C | -5.02300000 | 0.76848500 | 0.89974100 |
| C | -0.88866600 | -4.06703100 | -1.82632700 |
| C | 3.38095400 | -1.95199500 | -0.07318600 |
| O | 4.34796800 | -2.65625400 | -0.40261900 |
| N | 2.50760900 | -2.31179900 | 0.92840800 |
| N | 3.10073600 | -0.73803800 | -0.64804100 |
| C | 2.61805300 | -3.59309100 | 1.58662700 |
| C | 3.82244000 | -0.25999200 | -1.80380600 |
| C | 1.84597200 | -4.73428800 | 0.89974100 |
| C | 3.96648500 | 1.26390800 | -1.82632700 |
| S | 0.02260400 | -4.49470200 | 1.12340100 |
| S | -0.82213600 | -5.40209500 | -0.55022600 |
| S | -3.90382800 | 2.22777600 | 1.12340100 |
| S | -4.26728400 | 3.41303800 | -0.55022600 |
| S | 3.88122400 | 2.26692600 | 1.12340100 |
| S | 5.08942000 | 1.98905700 | -0.55022600 |
| H | 0.68517800 | 2.32163600 | 1.05695000 |
| H | -0.84346200 | 2.06554000 | -0.41311900 |
| H | 1.87248000 | 3.72515200 | 2.62770300 |
| H | 1.51211800 | 5.11884200 | 1.59914400 |
| H | -1.17902500 | 3.14705200 | -2.74123100 |
| H | -1.75727100 | 4.53074900 | -1.80507300 |
| H | 3.87003300 | 4.69762600 | 1.32867400 |
| H | 3.06986400 | 4.16516000 | -0.16863000 |
| H | -3.56317200 | 3.03869100 | -2.78152100 |
| H | -3.02202400 | 1.71296100 | -1.74693400 |
| H | -2.35318500 | -0.56743600 | 1.05695000 |
| H | -1.36708000 | -1.76323000 | -0.41311900 |
| H | -4.16231600 | -0.24096100 | 2.62770300 |
| H | -5.18910600 | -1.24988900 | 1.59914400 |
| H | -2.13591400 | -2.59459200 | -2.74123100 |
| H | -3.04510800 | -3.78721600 | -1.80507300 |
| H | -6.00328000 | 1.00273400 | 1.32867400 |
| H | -5.14206600 | 0.57600000 | -0.16863000 |
| H | -0.84999800 | -4.60514200 | -2.78152100 |
| H | 0.02754400 | -3.47363000 | -1.74693400 |
| H | 1.66800700 | -1.75420000 | 1.05695000 |
| H | 2.21054100 | -0.30231100 | -0.41311900 |
| H | 2.28983600 | -3.48419100 | 2.62770300 |
| H | 3.67698800 | -3.86895400 | 1.59914400 |
| H | 3.31494000 | -0.55246000 | -2.74123100 |
| H | 4.80237900 | -0.74353300 | -1.80507300 |
| H | 2.13324700 | -5.70036000 | 1.32867400 |
| H | 2.07220300 | -4.74116000 | -0.16863000 |
| H | 4.41316900 | 1.56645200 | -2.78152100 |
| H | 2.99448000 | 1.76066900 | -1.74693400 |

1-Br⁻ (model) B3LYP/6-31(1)++G(d,p)

| | | | |
|----|-------------|-------------|-------------|
| Br | 0.00000000 | 0.00000000 | 0.39474900 |
| C | 0.00000000 | 4.07908300 | -0.07783600 |
| O | 0.14211200 | 5.26241500 | -0.42126400 |
| N | 0.77243700 | 3.49189400 | 0.89943600 |
| N | -0.95844600 | 3.25234800 | -0.61039500 |
| C | 1.87995200 | 4.20423200 | 1.49619100 |
| C | -1.73233100 | 3.65169600 | -1.76438800 |
| C | 3.22422400 | 4.02557900 | 0.76703200 |
| C | -3.10135200 | 2.97113000 | -1.82386600 |
| C | -3.53259000 | -2.03954200 | -0.07783600 |
| O | -4.62844100 | -2.50813500 | -0.42126400 |
| N | -3.41028800 | -1.07699700 | 0.89943600 |
| N | -2.33739300 | -2.45621300 | -0.61039500 |
| C | -4.58094800 | -0.47402900 | 1.49619100 |
| C | -2.29629600 | -3.32609100 | -1.76438800 |
| C | -5.09836600 | 0.77947100 | 0.76703200 |
| C | -1.02239800 | -4.17141500 | -1.82386600 |
| C | 3.53259000 | -2.03954200 | -0.07783600 |
| O | 4.48632900 | -2.75428000 | -0.42126400 |
| N | 2.63785100 | -2.41489700 | 0.89943600 |
| N | 3.29583900 | -0.79613500 | -0.61039500 |
| C | 2.70099600 | -3.73020300 | 1.49619100 |
| C | 4.02862700 | -0.32560500 | -1.76438800 |
| C | 1.87414100 | -4.80504900 | 0.76703200 |
| C | 4.12375000 | 1.20028500 | -1.82386600 |
| S | 0.06842800 | -4.52612200 | 1.07062400 |
| S | -0.86478000 | -5.48038300 | -0.52836200 |
| S | -3.95395100 | 2.20380000 | 1.07062400 |
| S | -4.31376100 | 3.48911300 | -0.52836200 |
| S | 3.88552200 | 2.32232200 | 1.07062400 |
| S | 5.17854100 | 1.99127100 | -0.52836200 |
| H | 0.70219900 | 2.48692600 | 1.02951400 |
| H | -0.89196800 | 2.25932900 | -0.39582200 |
| H | 1.97318900 | 3.90003800 | 2.54620400 |
| H | 1.63065300 | 5.26926200 | 1.47954600 |
| H | -1.20533600 | 3.40729600 | -2.70464000 |
| H | -1.84000300 | 4.73861500 | -1.73223500 |
| H | 3.95310800 | 4.75858500 | 1.12860500 |
| H | 3.08270700 | 4.16668700 | -0.30676000 |
| H | -3.58650100 | 3.23155600 | -2.77242500 |
| H | -3.01099400 | 1.88106700 | -1.78955200 |
| H | -2.50484000 | -0.63534100 | 1.02951400 |
| H | -1.51065200 | -1.90213100 | -0.39582200 |
| H | -4.36412700 | -0.24118700 | 2.54620400 |
| H | -5.37864200 | -1.22244400 | 1.47954600 |
| H | -2.34813600 | -2.74750000 | -2.70464000 |
| H | -3.18375900 | -3.96279700 | -1.73223500 |
| H | -6.09760900 | 1.04420000 | 1.12860500 |
| H | -5.14981000 | 0.58635900 | -0.30676000 |
| H | -1.00535900 | -4.72177900 | -2.77242500 |
| H | -0.12355500 | -3.54813000 | -1.78955200 |
| H | 1.80264200 | -1.85158500 | 1.02951400 |
| H | 2.40262000 | -0.35719800 | -0.39582200 |
| H | 2.39093700 | -3.65885100 | 2.54620400 |
| H | 3.74798800 | -4.04681800 | 1.47954600 |
| H | 3.55347300 | -0.65979600 | -2.70464000 |
| H | 5.02376300 | -0.77581800 | -1.73223500 |
| H | 2.14450100 | -5.80278500 | 1.12860500 |
| H | 2.06710300 | -4.75304600 | -0.30676000 |
| H | 4.59186000 | 1.49022300 | -2.77242500 |
| H | 3.13454800 | 1.66706400 | -1.78955200 |

1-Γ (model) B3LYP/6-31(1)++G(d,p)

| | | | |
|---|-------------|-------------|-------------|
| I | 0.00000000 | 0.00000000 | 1.43711900 |
| C | 1.61369900 | 3.66761900 | -0.26363900 |
| O | 2.22663200 | 4.55896600 | -0.87066600 |
| N | 2.12161800 | 3.05507600 | 0.85658400 |
| N | 0.36322900 | 3.23486600 | -0.63986400 |
| C | 3.46216100 | 3.34634900 | 1.31562100 |
| C | -0.19273200 | 3.63325500 | -1.91639700 |
| C | 4.58350600 | 2.65327000 | 0.51972200 |
| C | -1.71158600 | 3.47523300 | -1.98436800 |
| C | -3.98310000 | -0.43630500 | -0.26363900 |
| O | -5.06149600 | -0.35116300 | -0.87066600 |
| N | -3.70658200 | 0.30983700 | 0.85658400 |
| N | -2.98309000 | -1.30286700 | -0.63986400 |
| C | -4.62910400 | 1.32514500 | 1.31562100 |
| C | -3.05012500 | -1.98353800 | -1.91639700 |
| C | -4.58955200 | 2.64279800 | 0.51972200 |
| C | -2.15384700 | -3.21989300 | -1.98436800 |
| C | 2.36940100 | -3.23131400 | -0.26363900 |
| O | 2.83486400 | -4.20780300 | -0.87066600 |
| N | 1.58496400 | -3.36491300 | 0.85658400 |
| N | 2.61986100 | -1.93199800 | -0.63986400 |
| C | 1.16694200 | -4.67149400 | 1.31562100 |
| C | 3.24285700 | -1.64971700 | -1.91639700 |
| C | 0.00604600 | -5.29606800 | 0.51972200 |
| C | 3.86543300 | -0.25534000 | -1.98436800 |
| S | -1.57600000 | -4.38589600 | 0.83964600 |
| S | -2.66335900 | -4.64239900 | -0.91856000 |
| S | -3.01029700 | 3.55780400 | 0.83964600 |
| S | -2.68875600 | 4.62773600 | -0.91856000 |
| S | 4.58629700 | 0.82809200 | 0.83964600 |
| S | 5.35211500 | 0.01466300 | -0.91856000 |
| H | 1.65078800 | 2.22866800 | 1.21449000 |
| H | 0.00000000 | 2.39605100 | -0.19503900 |
| H | 3.52224400 | 3.08034100 | 2.37700000 |
| H | 3.62517000 | 4.42616400 | 1.23439600 |
| H | 0.23562400 | 3.03760300 | -2.74266500 |
| H | 0.09547100 | 4.67211100 | -2.09567200 |
| H | 5.55693000 | 3.06415300 | 0.80825600 |
| H | 4.43254400 | 2.82463500 | -0.54773700 |
| H | -2.04042400 | 3.69101200 | -3.00771600 |
| H | -2.02504000 | 2.45352200 | -1.74914100 |
| H | -2.75547700 | 0.31529100 | 1.21449000 |
| H | -2.07504100 | -1.19802600 | -0.19503900 |
| H | -4.42877600 | 1.51018200 | 2.37700000 |
| H | -5.64575500 | 0.92640700 | 1.23439600 |
| H | -2.74845300 | -1.31474500 | -2.74266500 |
| H | -4.09390200 | -2.25337500 | -2.09567200 |
| H | -5.43209900 | 3.28036700 | 0.80825600 |
| H | -4.66247700 | 2.42637800 | -0.54773700 |
| H | -2.17629800 | -3.61256500 | -3.00771600 |
| H | -1.11229200 | -2.98049700 | -1.74914100 |
| H | 1.10468900 | -2.54395900 | 1.21449000 |
| H | 2.07504100 | -1.19802600 | -0.19503900 |
| H | 0.90653200 | -4.59052300 | 2.37700000 |
| H | 2.02058500 | -5.35257100 | 1.23439600 |
| H | 2.51282900 | -1.72285800 | -2.74266500 |
| H | 3.99843100 | -2.41873500 | -2.09567200 |
| H | -0.12483100 | -6.34451900 | 0.80825600 |
| H | 0.22993400 | -5.25101300 | -0.54773700 |
| H | 4.21672200 | -0.07844700 | -3.00771600 |
| H | 3.13733300 | 0.52697500 | -1.74914100 |

1- NO₃⁻ (model) B3LYP/6-31(1)++G(d,p)

| | | | |
|---|-------------|-------------|-------------|
| N | 0.00000000 | 0.00000000 | 0.35640000 |
| O | 1.12202100 | 0.56393800 | 0.35467100 |
| O | -0.07262600 | -1.25366800 | 0.35467100 |
| O | -1.04939500 | 0.68973000 | 0.35467100 |
| C | 0.00000000 | 4.33044300 | 0.08820900 |
| O | -0.05667800 | 5.56485900 | 0.20021100 |
| N | -0.91774700 | 3.60419400 | -0.64081500 |
| N | 0.99511700 | 3.57675300 | 0.65643600 |
| C | -2.00658200 | 4.26104800 | -1.33159000 |
| C | 1.90847700 | 4.14740100 | 1.62087500 |
| C | -3.39447000 | 3.97531200 | -0.73661900 |
| C | 3.28178400 | 3.47273700 | 1.61703600 |
| C | 3.75027400 | -2.16522200 | 0.08820900 |
| O | 4.84764800 | -2.73334500 | 0.20021100 |
| N | 3.58019700 | -1.00730500 | -0.64081500 |
| N | 2.60000000 | -2.65017400 | 0.65643600 |
| C | 4.69346700 | -0.39277300 | -1.33159000 |
| C | 2.63751600 | -3.72649000 | 1.62087500 |
| C | 5.13995600 | 0.95204100 | -0.73661900 |
| C | 1.36658600 | -4.57847700 | 1.61703600 |
| C | -3.75027400 | -2.16522200 | 0.08820900 |
| O | -4.79097000 | -2.83151400 | 0.20021100 |
| N | -2.66245000 | -2.59688900 | -0.64081500 |
| N | -3.59511800 | -0.92657900 | 0.65643600 |
| C | -2.68688500 | -3.86827500 | -1.33159000 |
| C | -4.54599300 | -0.42091100 | 1.62087500 |
| C | -1.74548600 | -4.92735300 | -0.73661900 |
| C | -4.64837100 | 1.10574000 | 1.61703600 |
| S | 0.00767200 | -4.53194600 | -1.19027000 |
| S | 1.13327100 | -5.66898200 | 0.14145600 |
| S | 3.92094400 | 2.27261800 | -1.19027000 |
| S | 4.34284700 | 3.81593200 | 0.14145600 |
| S | -3.92861700 | 2.25932900 | -1.19027000 |
| S | -5.47611800 | 1.85305000 | 0.14145600 |
| H | -0.95040600 | 2.59736200 | -0.51224200 |
| H | 0.97338400 | 2.56440300 | 0.55385800 |
| H | -1.99702300 | 3.99274800 | -2.39822500 |
| H | -1.81466800 | 5.33533000 | -1.26140400 |
| H | 1.50800300 | 4.05996500 | 2.64744800 |
| H | 1.99921600 | 5.21459700 | 1.40352200 |
| H | -4.13005600 | 4.68478700 | -1.12891900 |
| H | -3.36041000 | 4.06056900 | 0.35223900 |
| H | 3.86353000 | 3.84996600 | 2.46667500 |
| H | 3.19805200 | 2.38756500 | 1.73061200 |
| H | 2.72458500 | -0.47560500 | -0.51224200 |
| H | 1.73414600 | -2.12517700 | 0.55385800 |
| H | 4.45633300 | -0.26690100 | -2.39822500 |
| H | 5.52786500 | -1.09611700 | -1.26140400 |
| H | 2.76203200 | -3.33595100 | 2.64744800 |
| H | 3.51636600 | -4.33867000 | 1.40352200 |
| H | 6.12217200 | 1.23434000 | -1.12891900 |
| H | 5.19676100 | 0.87991600 | 0.35223900 |
| H | 1.40240400 | -5.27089800 | 2.46667500 |
| H | 0.46866600 | -3.96337700 | 1.73061200 |
| H | -1.77417900 | -2.12175700 | -0.51224200 |
| H | -2.70753100 | -0.43922600 | 0.55385800 |
| H | -2.45931000 | -3.72584700 | -2.39822500 |
| H | -3.71319800 | -4.23921300 | -1.26140400 |
| H | -4.27003500 | -0.72401400 | 2.64744800 |
| H | -5.51558100 | -0.87592700 | 1.40352200 |
| H | -1.99211600 | -5.91912700 | -1.12891900 |

| | | | |
|---|-------------|-------------|-------------|
| H | -1.83635100 | -4.94048500 | 0.35223900 |
| H | -5.26593300 | 1.42093200 | 2.46667500 |
| H | -3.66671800 | 1.57581200 | 1.73061200 |
| 1-F⁻ (model) B3LYP/6-31(1)++G(d,p) | | | |
| C | -0.80679000 | 3.52535400 | -0.65430000 |
| C | 3.29566100 | 2.66524200 | 1.81572800 |
| N | 2.14098200 | 2.21819500 | 1.06082000 |
| C | 1.36250500 | 3.15083400 | 0.39620500 |
| N | 0.24725300 | 2.62774900 | -0.19802300 |
| O | 1.68594700 | 4.34572800 | 0.32952100 |
| C | -1.84879000 | 2.73966400 | -1.45070400 |
| C | 4.52145900 | 3.00998200 | 0.95442800 |
| C | 0.66033600 | -4.18674700 | 1.81572800 |
| N | 0.85052200 | -2.96324200 | 1.06082000 |
| C | 2.04745000 | -2.75538100 | 0.39620500 |
| N | 2.15207100 | -1.52800200 | -0.19802300 |
| C | 3.45644100 | -1.06397600 | -0.65430000 |
| O | 2.92053700 | -3.63293700 | 0.32952100 |
| C | 0.34599200 | -5.42068900 | 0.95442800 |
| C | 3.29701400 | 0.23126700 | -1.45070400 |
| C | -2.64965100 | -2.46137800 | -0.65430000 |
| N | -2.39932400 | -1.09974700 | -0.19802300 |
| C | -3.40995500 | -0.39545300 | 0.39620500 |
| N | -2.99150400 | 0.74504700 | 1.06082000 |
| C | -3.95599700 | 1.52150500 | 1.81572800 |
| O | -4.60648400 | -0.71279100 | 0.32952100 |
| C | -1.44822300 | -2.97093100 | -1.45070400 |
| C | -4.86745000 | 2.41070700 | 0.95442800 |
| S | 5.48886100 | 1.56528300 | 0.32436700 |
| S | 4.85535900 | 1.20021200 | -1.63029500 |
| S | -1.38885600 | -5.53613500 | 0.32436700 |
| S | -1.38826500 | -4.80497100 | -1.63029500 |
| S | -4.10000500 | 3.97085200 | 0.32436700 |
| S | -3.46709400 | 3.60475800 | -1.63029500 |
| H | -1.29330300 | 4.01303200 | 0.20095100 |
| H | -0.36366900 | 4.31771300 | -1.26332900 |
| H | 3.03798700 | 3.57223700 | 2.38096500 |
| H | 3.55348500 | 1.87931800 | 2.53228300 |
| H | 1.69044800 | 1.34026800 | 1.29906700 |
| H | 0.00000000 | 1.66799300 | 0.07275600 |
| H | -2.04581800 | 1.76810100 | -0.99501100 |
| H | -1.52622200 | 2.57139700 | -2.48492000 |
| H | 5.24431200 | 3.56453200 | 1.56607100 |
| H | 4.23335300 | 3.64618200 | 0.11494800 |
| H | 1.57465400 | -4.41709200 | 2.38096500 |
| H | -0.14920600 | -4.01706700 | 2.53228300 |
| H | 0.31548200 | -2.13410500 | 1.29906700 |
| H | 1.44452500 | -0.83399700 | 0.07275600 |
| H | 4.12203900 | -0.88648300 | 0.20095100 |
| H | 3.92108400 | -1.84391000 | -1.26332900 |
| H | 0.46481900 | -6.32397300 | 1.56607100 |
| H | 1.04101000 | -5.48928200 | 0.11494800 |
| H | 2.55413000 | 0.88768000 | -0.99501100 |
| H | 2.99000600 | 0.03604800 | -2.48492000 |
| H | -2.82873600 | -3.12654900 | 0.20095100 |
| H | -3.55741500 | -2.47380300 | -1.26332900 |
| H | -1.44452500 | -0.83399700 | 0.07275600 |
| H | -2.00593000 | 0.79383700 | 1.29906700 |
| H | -3.40427900 | 2.13775000 | 2.53228300 |
| H | -4.61264100 | 0.84485500 | 2.38096500 |
| H | -0.50831100 | -2.65578100 | -0.99501100 |
| H | -1.46378400 | -2.60744600 | -2.48492000 |
| H | -5.70913100 | 2.75944100 | 1.56607100 |
| H | -5.27436300 | 1.84310000 | 0.11494800 |
| F | 0.00000000 | 0.00000000 | 0.80906100 |

1-Cl (model) B3LYP/6-31(1)++G(d,p)

| | | | |
|----|-------------|-------------|-------------|
| C | -2.11567100 | 3.14091000 | -0.43994800 |
| C | 2.18821900 | 4.28832600 | 1.56113900 |
| N | 1.24019700 | 3.32410600 | 1.03304500 |
| C | 0.12543000 | 3.77755400 | 0.34764700 |
| N | -0.78335700 | 2.80049100 | 0.03699500 |
| O | 0.00000000 | 4.96516500 | 0.02072600 |
| C | -2.68143200 | 1.98787300 | -1.27059400 |
| C | 3.20666500 | 4.80823700 | 0.53565500 |
| C | 2.61969000 | -4.03921600 | 1.56113900 |
| N | 2.25866100 | -2.73609500 | 1.03304500 |
| C | 3.20874300 | -1.99740300 | 0.34764700 |
| N | 2.81697500 | -0.72183800 | 0.03699500 |
| C | 3.77794300 | 0.26177000 | -0.43994800 |
| O | 4.29995900 | -2.48258200 | 0.02072600 |
| C | 2.56072300 | -5.18117200 | 0.53565500 |
| C | 3.06226500 | 1.32825100 | -1.27059400 |
| C | -1.66227200 | -3.40268000 | -0.43994800 |
| N | -2.03361800 | -2.07865300 | 0.03699500 |
| C | -3.33417300 | -1.78015100 | 0.34764700 |
| N | -3.49885900 | -0.58801100 | 1.03304500 |
| C | -4.80790800 | -0.24911000 | 1.56113900 |
| O | -4.29995900 | -2.48258200 | 0.02072600 |
| C | -0.38083300 | -3.31612500 | -1.27059400 |
| C | -5.76738800 | 0.37293500 | 0.53565500 |
| S | 4.59162900 | 3.64958700 | 0.13191500 |
| S | 4.12302800 | 2.77014900 | -1.70122200 |
| S | 0.86482100 | -5.80126100 | 0.13191500 |
| S | 0.33750500 | -4.95572100 | -1.70122200 |
| S | -5.45645000 | 2.15167400 | 0.13191500 |
| S | -4.46053300 | 2.18557200 | -1.70122200 |
| H | -2.79097700 | 3.34714400 | 0.40203000 |
| H | -2.04259200 | 4.05447000 | -1.03339700 |
| H | 1.64266400 | 5.16187800 | 1.94325800 |
| H | 2.71088200 | 3.81982800 | 2.40086400 |
| H | 1.17181000 | 2.41666700 | 1.48016300 |
| H | -0.66828100 | 1.89806400 | 0.49817400 |
| H | -2.56348000 | 1.03015500 | -0.75824700 |
| H | -2.17767300 | 1.91806500 | -2.24185500 |
| H | 3.70663700 | 5.69462800 | 0.94536900 |
| H | 2.70631500 | 5.10098600 | -0.38986400 |
| H | 3.64898600 | -4.00352800 | 1.94325800 |
| H | 1.95262700 | -4.25760600 | 2.40086400 |
| H | 1.50699000 | -2.22315100 | 1.48016300 |
| H | 1.97791200 | -0.37028400 | 0.49817400 |
| H | 4.29420000 | 0.74348500 | 0.40203000 |
| H | 4.53257000 | -0.25829900 | -1.03339700 |
| H | 3.07837400 | -6.05735600 | 0.94536900 |
| H | 3.06442600 | -4.89423100 | -0.38986400 |
| H | 2.17388000 | 1.70496200 | -0.75824700 |
| H | 2.74993000 | 0.92688800 | -2.24185500 |
| H | -1.50322300 | -4.09062900 | 0.40203000 |
| H | -2.48997800 | -3.79617100 | -1.03339700 |
| H | -1.30963100 | -1.52778000 | 0.49817400 |
| H | -2.67880000 | -0.19351600 | 1.48016300 |
| H | -4.66350900 | 0.43777800 | 2.40086400 |
| H | -5.29165000 | -1.15835100 | 1.94325800 |
| H | 0.38960000 | -2.73511700 | -0.75824700 |
| H | -0.57225700 | -2.84495300 | -2.24185500 |
| H | -6.78501100 | 0.36272800 | 0.94536900 |
| H | -5.77074100 | -0.20675500 | -0.38986400 |
| Cl | 0.00000000 | 0.00000000 | 1.72993100 |

1-Br⁻ (model) B3LYP/6-31(1)++G(d,p)

| | | | |
|----|-------------|-------------|-------------|
| C | -1.20025400 | 3.60460400 | -0.49697700 |
| C | 3.31126100 | 3.63759300 | 1.37610800 |
| N | 2.12730900 | 2.93837800 | 0.90847600 |
| C | 1.15560600 | 3.64368200 | 0.21890200 |
| N | 0.00000000 | 2.94223800 | -0.00883600 |
| O | 1.35089400 | 4.79851800 | -0.18150500 |
| C | -2.02194000 | 2.64257500 | -1.35673100 |
| C | 4.40902900 | 3.81370200 | 0.31678600 |
| C | 1.49461700 | -4.68643200 | 1.37610800 |
| N | 1.48105600 | -3.31149300 | 0.90847600 |
| C | 2.57771800 | -2.82262500 | 0.21890200 |
| N | 2.54805300 | -1.47111900 | -0.00883600 |
| C | 3.72180500 | -0.76285100 | -0.49697700 |
| O | 3.48019200 | -3.56916800 | -0.18150500 |
| C | 1.09824800 | -5.72518200 | 0.31678600 |
| C | 3.29950700 | 0.42976400 | -1.35673100 |
| C | -2.52155100 | -2.84175300 | -0.49697700 |
| N | -2.54805300 | -1.47111900 | -0.00883600 |
| C | -3.73332400 | -0.82105700 | 0.21890200 |
| N | -3.60836500 | 0.37311500 | 0.90847600 |
| C | -4.80587800 | 1.04883900 | 1.37610800 |
| O | -4.83108600 | -1.22935100 | -0.18150500 |
| C | -1.27756700 | -3.07233900 | -1.35673100 |
| C | -5.50727700 | 1.91148000 | 0.31678600 |
| S | 5.41357000 | 2.30226300 | -0.04289800 |
| S | 4.69895800 | 1.52378400 | -1.84192200 |
| S | -0.71296700 | -5.83942100 | -0.04289800 |
| S | -1.02984300 | -4.83130900 | -1.84192200 |
| S | -4.70060300 | 3.53715800 | -0.04289800 |
| S | -3.66911500 | 3.30752500 | -1.84192200 |
| H | -1.81755000 | 3.95824100 | 0.34029500 |
| H | -0.89121400 | 4.47901600 | -1.07275300 |
| H | 3.02840000 | 4.64295100 | 1.71647400 |
| H | 3.70729000 | 3.08708000 | 2.23510700 |
| H | 1.83065300 | 2.10862000 | 1.41001100 |
| H | -0.12547800 | 2.07210900 | 0.50651100 |
| H | -2.17775900 | 1.68623200 | -0.85174900 |
| H | -1.52147500 | 2.44591000 | -2.31219500 |
| H | 5.14060200 | 4.54663000 | 0.67873600 |
| H | 3.98725500 | 4.19134800 | -0.61702000 |
| H | 2.50671400 | -4.94414700 | 1.71647400 |
| H | 0.81984500 | -4.75414700 | 2.23510700 |
| H | 0.91079200 | -2.63970200 | 1.41001100 |
| H | 1.85723800 | -0.92738700 | 0.50651100 |
| H | 4.33671300 | -0.40507600 | 0.34029500 |
| H | 4.32454800 | -1.46769400 | -1.07275300 |
| H | 1.36719700 | -6.72520700 | 0.67873600 |
| H | 1.63618600 | -5.54873800 | -0.61702000 |
| H | 2.54919900 | 1.04287800 | -0.85174900 |
| H | 2.87895800 | 0.09468000 | -2.31219500 |
| H | -2.51916200 | -3.55316500 | 0.34029500 |
| H | -3.43333400 | -3.01132200 | -1.07275300 |
| H | -1.73176000 | -1.14472200 | 0.50651100 |
| H | -2.74144500 | 0.53108200 | 1.41001100 |
| H | -4.52713400 | 1.66706700 | 2.23510700 |
| H | -5.53511400 | 0.30119600 | 1.71647400 |
| H | -0.37144000 | -2.72911000 | -0.85174900 |
| H | -1.35748300 | -2.54059100 | -2.31219500 |
| H | -6.50779800 | 2.17857600 | 0.67873600 |
| H | -5.62344200 | 1.35739000 | -0.61702000 |
| Br | 0.00000000 | 0.00000000 | 1.96540500 |

1-I (model) B3LYP/6-31(1)++G(d,p)

| | | | |
|---|-------------|-------------|-------------|
| C | -2.24628100 | 3.10546200 | -0.60185900 |
| C | 2.06977400 | 4.59725000 | 1.14572200 |
| N | 1.14567300 | 3.54868200 | 0.74908700 |
| C | 0.00000000 | 3.88759500 | 0.05012300 |
| N | -0.90691600 | 2.86740300 | -0.08563000 |
| O | -0.15505800 | 5.01507500 | -0.43556100 |
| C | -2.70926900 | 1.92131300 | -1.45394400 |
| C | 3.05450400 | 5.02951700 | 0.05014500 |
| C | 2.94644800 | -4.09110100 | 1.14572200 |
| N | 2.50041200 | -2.76652300 | 0.74908700 |
| C | 3.36675600 | -1.94379800 | 0.05012300 |
| N | 2.93670200 | -0.64828900 | -0.08563000 |
| C | 3.81254900 | 0.39260600 | -0.60185900 |
| O | 4.42071100 | -2.37325300 | -0.43556100 |
| C | 2.82843800 | -5.16003700 | 0.05014500 |
| C | 3.01854000 | 1.38563900 | -1.45394400 |
| C | -1.56626800 | -3.49806700 | -0.60185900 |
| N | -2.02978600 | -2.21911300 | -0.08563000 |
| C | -3.36675600 | -1.94379800 | 0.05012300 |
| N | -3.64608500 | -0.78215900 | 0.74908700 |
| C | -5.01622200 | -0.50614800 | 1.14572200 |
| O | -4.26565300 | -2.64182200 | -0.43556100 |
| C | -0.30927100 | -3.30695200 | -1.45394400 |
| C | -5.88294200 | 0.13052000 | 0.05014500 |
| S | 4.46277300 | 3.86811100 | -0.25386100 |
| S | 4.00873800 | 2.83504600 | -2.00898600 |
| S | 1.11849600 | -5.79893100 | -0.25386100 |
| S | 0.45085300 | -4.88919200 | -2.00898600 |
| S | -5.58126900 | 1.93081900 | -0.25386100 |
| S | -4.45959100 | 2.05414600 | -2.00898600 |
| H | -2.95699600 | 3.25980300 | 0.22135300 |
| H | -2.21638600 | 4.02318000 | -1.19198000 |
| H | 1.50145600 | 5.49063300 | 1.43794900 |
| H | 2.61939300 | 4.24290700 | 2.02327600 |
| H | 1.11978600 | 2.70226600 | 1.30628900 |
| H | -0.77367800 | 2.04229400 | 0.49516700 |
| H | -2.59210200 | 0.97303300 | -0.92354900 |
| H | -2.13522200 | 1.86435100 | -2.38625700 |
| H | 3.53413900 | 5.96883100 | 0.35157400 |
| H | 2.53043900 | 5.20493500 | -0.89169100 |
| H | 4.00429900 | -4.04561500 | 1.43794900 |
| H | 2.36476900 | -4.38991500 | 2.02327600 |
| H | 1.78033800 | -2.32089600 | 1.30628900 |
| H | 2.15551700 | -0.35112200 | 0.49516700 |
| H | 4.30157000 | 0.93093200 | 0.22135300 |
| H | 4.59236900 | -0.09214300 | -1.19198000 |
| H | 3.40209000 | -6.04507000 | 0.35157400 |
| H | 3.24238600 | -4.79389200 | -0.89169100 |
| H | 2.13872300 | 1.75830900 | -0.92354900 |
| H | 2.68218600 | 0.91698100 | -2.38625700 |
| H | -1.34457500 | -4.19073500 | 0.22135300 |
| H | -2.37598300 | -3.93103600 | -1.19198000 |
| H | -1.38183900 | -1.69117200 | 0.49516700 |
| H | -2.90012400 | -0.38137000 | 1.30628900 |
| H | -4.98416200 | 0.14700700 | 2.02327600 |
| H | -5.50575500 | -1.44501800 | 1.43794900 |
| H | 0.45337900 | -2.73134300 | -0.92354900 |
| H | -0.54696400 | -2.78133200 | -2.38625700 |
| H | -6.93622900 | 0.07623900 | 0.35157400 |
| H | -5.77282500 | -0.41104300 | -0.89169100 |
| I | 0.00000000 | 0.00000000 | 2.23373200 |

1- NO₃⁻ (model) B3LYP/6-31(1)++G(d,p)

| | | | |
|---|-------------|-------------|-------------|
| C | -3.94111200 | 0.37717100 | -0.35224700 |
| C | -2.16274700 | 4.63179500 | 1.29413400 |
| N | -2.01393500 | 3.23143000 | 0.94682300 |
| C | -3.02844100 | 2.58678500 | 0.26825100 |
| N | -2.90353900 | 1.22062300 | 0.21822200 |
| O | -3.95439500 | 3.21273700 | -0.26601800 |
| C | -3.31737200 | -0.72895300 | -1.20988400 |
| C | -1.80837900 | 5.62477700 | 0.17584900 |
| C | 5.09262500 | -0.44290400 | 1.29413400 |
| N | 3.80546700 | 0.12840400 | 0.94682300 |
| C | 3.75444200 | 1.32931400 | 0.26825100 |
| N | 2.50886000 | 1.90422700 | 0.21822200 |
| C | 2.29719600 | 3.22451700 | -0.35224700 |
| O | 4.75950900 | 1.81823800 | -0.26601800 |
| C | 5.77539000 | -1.24628600 | 0.17584900 |
| C | 1.02739400 | 3.23740500 | -1.20988400 |
| C | 1.64391600 | -3.60168800 | -0.35224700 |
| N | 0.39467900 | -3.12485000 | 0.21822200 |
| C | -0.72600100 | -3.91609900 | 0.26825100 |
| N | -1.79153300 | -3.35983300 | 0.94682300 |
| C | -2.92987900 | -4.18889100 | 1.29413400 |
| O | -0.80511500 | -5.03097500 | -0.26601800 |
| C | 2.28997800 | -2.50845200 | -1.20988400 |
| C | -3.96701100 | -4.37849100 | 0.17584900 |
| S | 0.00000000 | 5.93912400 | -0.06958700 |
| S | 0.55197000 | 4.91493500 | -1.80161200 |
| S | 5.14343200 | -2.96956200 | -0.06958700 |
| S | 3.98047400 | -2.93548800 | -1.80161200 |
| S | -5.14343200 | -2.96956200 | -0.06958700 |
| S | -4.53244400 | -1.97944800 | -1.80161200 |
| H | -4.54651600 | -0.07887300 | 0.44257000 |
| H | -4.59790100 | 1.01187100 | -0.94988900 |
| H | -3.20969300 | 4.82054000 | 1.56647700 |
| H | -1.54429000 | 4.82682600 | 2.17619000 |
| H | -1.32633700 | 2.67017900 | 1.43735700 |
| H | -2.27619400 | 0.76994900 | 0.87931100 |
| H | -2.52297900 | -1.25304700 | -0.67270900 |
| H | -2.88820200 | -0.31234500 | -2.12888400 |
| H | -2.22310200 | 6.60840600 | 0.42805300 |
| H | -2.24541400 | 5.30720300 | -0.77305100 |
| H | 5.77955700 | 0.36940600 | 1.56647700 |
| H | 4.95229900 | -1.07601900 | 2.17619000 |
| H | 2.97561100 | -0.18644800 | 1.43735700 |
| H | 1.80489200 | 1.58626700 | 0.87931100 |
| H | 2.20495200 | 3.97683500 | 0.44257000 |
| H | 3.17525700 | 3.47596300 | -0.94988900 |
| H | 6.83459900 | -1.37894000 | 0.42805300 |
| H | 5.71888000 | -0.70901600 | -0.77305100 |
| H | 0.17631900 | 2.81148700 | -0.67270900 |
| H | 1.17360200 | 2.65742900 | -2.12888400 |
| H | 2.34156400 | -3.89796200 | 0.44257000 |
| H | 1.42264400 | -4.48783500 | -0.94988900 |
| H | 0.47130100 | -2.35621600 | 0.87931100 |
| H | -1.64927500 | -2.48373100 | 1.43735700 |
| H | -3.40800900 | -3.75080800 | 2.17619000 |
| H | -2.56986300 | -5.18994600 | 1.56647700 |
| H | 2.34666000 | -1.55844000 | -0.67270900 |
| H | 1.71460000 | -2.34508400 | -2.12888400 |
| H | -4.61149700 | -5.22946600 | 0.42805300 |
| H | -3.47346600 | -4.59818700 | -0.77305100 |
| N | 0.00000000 | 0.00000000 | 1.98324000 |

| | | | |
|---|-------------|-------------|-------------|
| O | -1.15746600 | -0.48825400 | 1.97780000 |
| O | 1.00157300 | -0.75826800 | 1.97780000 |
| O | 0.15589300 | 1.24652200 | 1.97780000 |
| 1-F⁻ (model) B3LYP/6-31(1)++G(d,p) | | | |
| C | -3.10316500 | -1.05198000 | -1.96224400 |
| C | -2.38777500 | 2.92048300 | 0.73547300 |
| N | -1.90633400 | 1.67002100 | 0.17846700 |
| C | -2.66183000 | 1.06984000 | -0.80205800 |
| N | -2.27830500 | -0.20666900 | -1.12457000 |
| O | -3.60684200 | 1.64587500 | -1.36874400 |
| C | -4.48257100 | -1.39973500 | -1.37989300 |
| C | -1.55371100 | 3.42309200 | 1.90641100 |
| C | 3.72310000 | 0.60763200 | 0.73547300 |
| N | 2.39944700 | 0.81592300 | 0.17846700 |
| C | 2.25742400 | 1.77029300 | -0.80205800 |
| N | 0.96017200 | 2.07640400 | -1.12457000 |
| C | 0.64054100 | 3.21341000 | -1.96224400 |
| O | 3.22879100 | 2.30067900 | -1.36874400 |
| C | 3.74134000 | -0.36599300 | 1.90641100 |
| C | 1.02908000 | 4.58188800 | -1.37989300 |
| C | 2.46262400 | -2.16142900 | -1.96224400 |
| N | 1.31813300 | -1.86973600 | -1.12457000 |
| C | 0.40440700 | -2.84013300 | -0.80205800 |
| N | -0.49311400 | -2.48594400 | 0.17846700 |
| C | -1.33532500 | -3.52811500 | 0.73547300 |
| O | 0.37805100 | -3.94655400 | -1.36874400 |
| C | 3.45349100 | -3.18215300 | -1.37989300 |
| C | -2.18762900 | -3.05709900 | 1.90641100 |
| S | 0.17137300 | 4.03796000 | 1.60387400 |
| S | 0.00000000 | 5.33409900 | -0.03823900 |
| S | 3.41128900 | -2.16739300 | 1.60387400 |
| S | 4.61946600 | -2.66705000 | -0.03823900 |
| S | -3.58266200 | -1.87056700 | 1.60387400 |
| S | -4.61946600 | -2.66705000 | -0.03823900 |
| H | -3.28682700 | -0.53537600 | -2.91311100 |
| H | -2.53218100 | -1.95979800 | -2.17656900 |
| H | -3.41932600 | 2.80540400 | 1.10490700 |
| H | -2.43197800 | 3.68492200 | -0.04760200 |
| H | -1.28205300 | 1.06464000 | 0.74003200 |
| H | -1.60208900 | -0.66960100 | -0.53122900 |
| H | -5.10206400 | -1.85715500 | -2.16300000 |
| H | -4.98219200 | -0.48582600 | -1.05323600 |
| H | -2.10355000 | 4.22960400 | 2.39960600 |
| H | -1.39005500 | 2.62631500 | 2.64249000 |
| H | 4.13921400 | 1.55852100 | 1.10490700 |
| H | 4.40722500 | 0.26369400 | -0.04760200 |
| H | 1.56303200 | 0.57797100 | 0.74003200 |
| H | 0.22115300 | 1.72225000 | -0.53122900 |
| H | -0.43114400 | 3.17283200 | -2.17656900 |
| H | 1.17976400 | 3.11416300 | -2.91311100 |
| H | 4.71472000 | -0.29307400 | 2.39960600 |
| H | 2.96948300 | -0.10933400 | 2.64249000 |
| H | 2.07035800 | 4.55761800 | -1.05323600 |
| H | 0.94268900 | 5.34709400 | -2.16300000 |
| H | 2.96332500 | -1.21303400 | -2.17656900 |
| H | 2.10706200 | -2.57878800 | -2.91311100 |
| H | 1.38093600 | -1.05265000 | -0.53122900 |
| H | -0.28097900 | -1.64261100 | 0.74003200 |
| H | -1.97524700 | -3.94861600 | -0.04760200 |
| H | -0.71988800 | -4.36392500 | 1.10490700 |
| H | 4.15937500 | -3.48993900 | -2.16300000 |
| H | 2.91183400 | -4.07179200 | -1.05323600 |
| H | -2.61116900 | -3.93653000 | 2.39960600 |
| H | -1.57942800 | -2.51698100 | 2.64249000 |
| F | 0.00000000 | 0.00000000 | 1.17802800 |

1-Cl (model) B3LYP/6-31(1)++G(d,p)

| | | | |
|----|-------------|-------------|-------------|
| C | -2.98257500 | 0.79185400 | -1.96000200 |
| C | -0.33148000 | 3.89490600 | 0.69318800 |
| N | -0.62357800 | 2.54045500 | 0.25211200 |
| C | -1.50084500 | 2.37482100 | -0.80548700 |
| N | -1.94868000 | 1.09602100 | -0.99136700 |
| O | -1.82236300 | 3.31143800 | -1.55354500 |
| C | -4.38950600 | 1.26673900 | -1.56439500 |
| C | 0.70081600 | 3.95152700 | 1.81316000 |
| C | 3.53882800 | -1.66038300 | 0.69318800 |
| N | 2.51188700 | -0.73019300 | 0.25211200 |
| C | 2.80707800 | 0.11236000 | -0.80548700 |
| N | 1.92352200 | 1.13959600 | -0.99136700 |
| C | 2.17705300 | 2.18705900 | -1.96000200 |
| O | 3.77897100 | -0.07750700 | -1.55354500 |
| C | 3.07171500 | -2.58268700 | 1.81316000 |
| C | 3.29178100 | 3.16805400 | -1.56439500 |
| C | 0.80552200 | -2.97891300 | -1.96000200 |
| N | 0.02515800 | -2.23561700 | -0.99136700 |
| C | -1.30623200 | -2.48718000 | -0.80548700 |
| N | -1.88831000 | -1.81026200 | 0.25211200 |
| C | -3.20734700 | -2.23452300 | 0.69318800 |
| O | -1.95660800 | -3.23393200 | -1.55354500 |
| C | 1.09772500 | -4.43479300 | -1.56439500 |
| C | -3.77253000 | -1.36883900 | 1.81316000 |
| S | 2.46573200 | 3.50442300 | 1.45302200 |
| S | 2.93589200 | 4.50181800 | -0.33200400 |
| S | 1.80205400 | -3.88759800 | 1.45302200 |
| S | 2.43074200 | -4.79346600 | -0.33200400 |
| S | -4.26778500 | 0.38317400 | 1.45302200 |
| S | -5.36663400 | 0.29164800 | -0.33200400 |
| H | -2.72744100 | 1.29367600 | -2.90050600 |
| H | -2.97098800 | -0.28707700 | -2.13670600 |
| H | -1.24111400 | 4.38805000 | 1.07412700 |
| H | 0.00000000 | 4.48428300 | -0.16586200 |
| H | -0.61196300 | 1.81289600 | 0.97322400 |
| H | -1.76857400 | 0.39321600 | -0.28609900 |
| H | -5.04973500 | 1.22106500 | -2.44070100 |
| H | -4.34790300 | 2.30760300 | -1.23624000 |
| H | 0.69873800 | 4.96223800 | 2.23087700 |
| H | 0.44856900 | 3.24852000 | 2.61661100 |
| H | 4.42072000 | -1.11918900 | 1.07412700 |
| H | 3.88350300 | -2.24214100 | -0.16586200 |
| H | 1.87599500 | -0.37647200 | 0.97322400 |
| H | 1.22482200 | 1.33502200 | -0.28609900 |
| H | 1.23687800 | 2.71649000 | -2.13670600 |
| H | 2.48407600 | 1.71519500 | -2.90050600 |
| H | 3.94805600 | -3.08624400 | 2.23087700 |
| H | 2.58901600 | -2.01273200 | 2.61661100 |
| H | 4.17239400 | 2.61159300 | -1.23624000 |
| H | 3.58234100 | 3.76266600 | -2.44070100 |
| H | 1.73411100 | -2.42941300 | -2.13670600 |
| H | 0.24336400 | -3.00887100 | -2.90050600 |
| H | 0.54375200 | -1.72823800 | -0.28609900 |
| H | -1.26403200 | -1.43642300 | 0.97322400 |
| H | -3.88350300 | -2.24214100 | -0.16586200 |
| H | -3.17960600 | -3.26886100 | 1.07412700 |
| H | 1.46739400 | -4.98373100 | -2.44070100 |
| H | 0.17550900 | -4.91919500 | -1.23624000 |
| H | -4.64679300 | -1.87599500 | 2.23087700 |
| H | -3.03758600 | -1.23578800 | 2.61661100 |
| Cl | 0.00000000 | 0.00000000 | 2.27282800 |

1-Br⁻ (model) B3LYP/6-31(1)++G(d,p)

| | | | |
|----|-------------|-------------|-------------|
| C | -2.66123600 | 1.40868400 | -2.06082000 |
| C | 0.60728400 | 3.92588300 | 0.53415300 |
| N | 0.00000000 | 2.66071200 | 0.15232000 |
| C | -0.87634800 | 2.65587800 | -0.92080600 |
| N | -1.62881000 | 1.52296700 | -1.05041900 |
| O | -0.93819700 | 3.59609400 | -1.72833400 |
| C | -3.94084400 | 2.20334100 | -1.75585400 |
| C | 1.65234100 | 3.78814700 | 1.63536300 |
| C | 3.09627200 | -2.48886500 | 0.53415300 |
| N | 2.30424400 | -1.33035600 | 0.15232000 |
| C | 2.73823200 | -0.56899900 | -0.92080600 |
| N | 2.13333300 | 0.64910700 | -1.05041900 |
| C | 2.55057400 | 1.60035500 | -2.06082000 |
| O | 3.58340700 | -0.98554500 | -1.72833400 |
| C | 2.45446100 | -3.32504300 | 1.63536300 |
| C | 3.87857100 | 2.31120100 | -1.75585400 |
| C | 0.11066100 | -3.00904000 | -2.06082000 |
| N | -0.50452300 | -2.17207400 | -1.05041900 |
| C | -1.86188300 | -2.08687900 | -0.92080600 |
| N | -2.30424400 | -1.33035600 | 0.15232000 |
| C | -3.70355600 | -1.43701800 | 0.53415300 |
| O | -2.64521000 | -2.61054900 | -1.72833400 |
| C | 0.06227300 | -4.51454100 | -1.75585400 |
| C | -4.10680200 | -0.46310500 | 1.63536300 |
| S | 3.25871000 | 2.93543300 | 1.26606100 |
| S | 3.89615400 | 3.73022000 | -0.56772900 |
| S | 0.91280500 | -4.28984300 | 1.26606100 |
| S | 1.28238900 | -5.23927800 | -0.56772900 |
| S | -4.17151500 | 1.35440900 | 1.26606100 |
| S | -5.17854300 | 1.50905800 | -0.56772900 |
| H | -2.25825400 | 1.79666900 | -3.00318800 |
| H | -2.88496200 | 0.34735400 | -2.19730900 |
| H | -0.15447800 | 4.63133300 | 0.90595400 |
| H | 1.04541600 | 4.38623200 | -0.35505900 |
| H | -0.17918400 | 1.99562000 | 0.90863500 |
| H | -1.62919900 | 0.82763000 | -0.31604600 |
| H | -4.54661100 | 2.28503600 | -2.66804500 |
| H | -3.67966400 | 3.21576600 | -1.44010100 |
| H | 1.89077300 | 4.78879500 | 2.00690000 |
| H | 1.26711700 | 3.19599000 | 2.47469200 |
| H | 4.08809100 | -2.18188400 | 0.90595400 |
| H | 3.27588100 | -3.09847300 | -0.35505900 |
| H | 1.81784900 | -0.84263200 | 0.90863500 |
| H | 1.53134800 | 0.99711200 | -0.31604600 |
| H | 1.74329800 | 2.32477400 | -2.19730900 |
| H | 2.68508800 | 1.05737000 | -3.00318800 |
| H | 3.20183200 | -4.03185500 | 2.00690000 |
| H | 2.13425000 | -2.69535000 | 2.47469200 |
| H | 4.62476700 | 1.57880000 | -1.44010100 |
| H | 4.25220500 | 2.79496200 | -2.66804500 |
| H | 1.14166400 | -2.67212700 | -2.19730900 |
| H | -0.42683400 | -2.85403900 | -3.00318800 |
| H | 0.09785100 | -1.82474200 | -0.31604600 |
| H | -1.63866500 | -1.15298800 | 0.90863500 |
| H | -4.32129700 | -1.28775900 | -0.35505900 |
| H | -3.93361300 | -2.44944800 | 0.90595400 |
| H | 0.29440600 | -5.07999800 | -2.66804500 |
| H | -0.94510200 | -4.79456600 | -1.44010100 |
| H | -5.09260500 | -0.75694000 | 2.00690000 |
| H | -3.40136700 | -0.50064000 | 2.47469200 |
| Br | 0.00000000 | 0.00000000 | 2.40269300 |

1-I (model) B3LYP/6-31(1)++G(d,p)

| | | | |
|---|-------------|-------------|-------------|
| C | -2.62991400 | 1.37147900 | -2.23831000 |
| C | 0.60447600 | 3.94448900 | 0.34698700 |
| N | 0.00000000 | 2.66916000 | -0.00964900 |
| C | -0.85618800 | 2.63671000 | -1.10186300 |
| N | -1.62208200 | 1.51138500 | -1.20536000 |
| O | -0.88353000 | 3.54548300 | -1.94537300 |
| C | -3.91993500 | 2.16429000 | -1.97638600 |
| C | 1.66845500 | 3.83068100 | 1.43275700 |
| C | 3.11379000 | -2.49573700 | 0.34698700 |
| N | 2.31156100 | -1.33458000 | -0.00964900 |
| C | 2.71155200 | -0.57687400 | -1.10186300 |
| N | 2.11993900 | 0.64907200 | -1.20536000 |
| C | 2.50269300 | 1.59183200 | -2.23831000 |
| O | 3.51224300 | -1.00758200 | -1.94537300 |
| C | 2.48324000 | -3.36026500 | 1.43275700 |
| C | 3.83429800 | 2.31261900 | -1.97638600 |
| C | 0.12722100 | -2.96331200 | -2.23831000 |
| N | -0.49785600 | -2.16045700 | -1.20536000 |
| C | -1.85536400 | -2.05983600 | -1.10186300 |
| N | -2.31156100 | -1.33458000 | -0.00964900 |
| C | -3.71826600 | -1.44875300 | 0.34698700 |
| O | -2.62871300 | -2.53790100 | -1.94537300 |
| C | 0.08563800 | -4.47690800 | -1.97638600 |
| C | -4.15169500 | -0.47041600 | 1.43275700 |
| S | 3.26831600 | 2.97346200 | 1.04943800 |
| S | 3.87380400 | 3.74541700 | -0.80535200 |
| S | 0.94093600 | -4.31717600 | 1.04943800 |
| S | 1.30672500 | -5.22752100 | -0.80535200 |
| S | -4.20925200 | 1.34371300 | 1.04943800 |
| S | -5.18052800 | 1.48210400 | -0.80535200 |
| H | -2.20496800 | 1.74633400 | -3.17600100 |
| H | -2.84472500 | 0.30708600 | -2.36328700 |
| H | -0.15680700 | 4.64937500 | 0.72061700 |
| H | 1.02369900 | 4.39179100 | -0.55731600 |
| H | -0.22000700 | 2.04805600 | 0.76998800 |
| H | -1.64692500 | 0.83955300 | -0.44977900 |
| H | -4.50481700 | 2.22735800 | -2.90348300 |
| H | -3.67173300 | 3.18342000 | -1.67140100 |
| H | 1.91063900 | 4.83913500 | 1.78015200 |
| H | 1.30034200 | 3.25402300 | 2.29064600 |
| H | 4.10488000 | -2.18888800 | 0.72061700 |
| H | 3.29155400 | -3.08244500 | -0.55731600 |
| H | 1.88367200 | -0.83349600 | 0.76998800 |
| H | 1.55053600 | 1.00650200 | -0.44977900 |
| H | 1.68830700 | 2.31006100 | -2.36328700 |
| H | 2.61485300 | 1.03639100 | -3.17600100 |
| H | 3.23549500 | -4.07422900 | 1.78015200 |
| H | 2.16789500 | -2.75314100 | 2.29064600 |
| H | 4.59278900 | 1.58810500 | -1.67140100 |
| H | 4.18135700 | 2.78760700 | -2.90348300 |
| H | 1.15641800 | -2.61714800 | -2.36328700 |
| H | -0.40988600 | -2.78272500 | -3.17600100 |
| H | 0.09638800 | -1.84605500 | -0.44977900 |
| H | -1.66366500 | -1.21456000 | 0.76998800 |
| H | -4.31525200 | -1.30934700 | -0.55731600 |
| H | -3.94807300 | -2.46048600 | 0.72061700 |
| H | 0.32346000 | -5.01496500 | -2.90348300 |
| H | -0.92105500 | -4.77152400 | -1.67140100 |
| H | -5.14613400 | -0.76490600 | 1.78015200 |
| H | -3.46823700 | -0.50088200 | 2.29064600 |
| I | 0.00000000 | 0.00000000 | 2.65717600 |

1- NO₃⁻ (model) B3LYP/6-31(1)++G(d,p)

| | | | |
|---|-------------|-------------|-------------|
| C | -2.67524300 | 1.45936200 | -1.68202800 |
| C | 0.74559000 | 4.35241400 | 0.27797200 |
| N | 0.00000000 | 3.11103500 | 0.22000400 |
| C | -0.87543100 | 2.89309900 | -0.82042000 |
| N | -1.70747200 | 1.81612700 | -0.66478600 |
| O | -0.88543500 | 3.60870600 | -1.83539300 |
| C | -3.97981400 | 2.27233400 | -1.63564600 |
| C | 1.77620100 | 4.37785500 | 1.40026700 |
| C | 3.39650700 | -2.82190700 | 0.27797200 |
| N | 2.69423600 | -1.55551800 | 0.22000400 |
| C | 2.94321300 | -0.68840400 | -0.82042000 |
| N | 2.42654800 | 0.57065000 | -0.66478600 |
| C | 2.60146600 | 1.58714700 | -1.68202800 |
| O | 3.56794900 | -1.03754400 | -1.83539300 |
| C | 2.90323300 | -3.72716300 | 1.40026700 |
| C | 3.95780600 | 2.31045300 | -1.63564600 |
| C | 0.07377700 | -3.04650900 | -1.68202800 |
| N | -0.71907700 | -2.38677800 | -0.66478600 |
| C | -2.06778200 | -2.20469500 | -0.82042000 |
| N | -2.69423600 | -1.55551800 | 0.22000400 |
| C | -4.14209600 | -1.53050800 | 0.27797200 |
| O | -2.68251400 | -2.57116200 | -1.83539300 |
| C | 0.02200800 | -4.58278700 | -1.63564600 |
| C | -4.67943400 | -0.65069200 | 1.40026700 |
| S | 3.22050800 | 3.22431700 | 1.31194000 |
| S | 4.17362700 | 3.74772600 | -0.47789900 |
| S | 1.18208700 | -4.40120000 | 1.31194000 |
| S | 1.15881200 | -5.48833000 | -0.47789900 |
| S | -4.40259500 | 1.17688300 | 1.31194000 |
| S | -5.33243900 | 1.74060400 | -0.47789900 |
| H | -2.21502900 | 1.65006200 | -2.65672000 |
| H | -2.87718400 | 0.38906400 | -1.60779300 |
| H | 0.07227900 | 5.21138400 | 0.43932400 |
| H | 1.23233300 | 4.52676000 | -0.68667500 |
| H | -0.11428300 | 2.55779600 | 1.06675100 |
| H | -1.74717500 | 1.34741300 | 0.23130600 |
| H | -4.48511300 | 2.21263900 | -2.60774600 |
| H | -3.74901700 | 3.32117900 | -1.43824000 |
| H | 2.16548500 | 5.39556700 | 1.49565800 |
| H | 1.32036000 | 4.10680000 | 2.36139500 |
| H | 4.47705100 | -2.66828700 | 0.43932400 |
| H | 3.30412300 | -3.33061200 | -0.68667500 |
| H | 2.27225700 | -1.17992600 | 1.06675100 |
| H | 2.04048100 | 0.83939100 | 0.23130600 |
| H | 1.77553100 | 2.29718200 | -1.60779300 |
| H | 2.53651000 | 1.09324000 | -2.65672000 |
| H | 3.58995500 | -4.57314800 | 1.49565800 |
| H | 2.89641300 | -3.19686600 | 2.36139500 |
| H | 4.75073400 | 1.58615500 | -1.43824000 |
| H | 4.15875800 | 2.77790300 | -2.60774600 |
| H | 1.10165200 | -2.68624600 | -1.60779300 |
| H | -0.32148100 | -2.74330200 | -2.65672000 |
| H | -0.29330700 | -2.18680400 | 0.23130600 |
| H | -2.15797500 | -1.37786900 | 1.06675100 |
| H | -4.53645600 | -1.19614900 | -0.68667500 |
| H | -4.54933000 | -2.54309600 | 0.43932400 |
| H | 0.32635500 | -4.99054100 | -2.60774600 |
| H | -1.00171700 | -4.90733400 | -1.43824000 |
| H | -5.75544000 | -0.82241800 | 1.49565800 |
| H | -4.21677300 | -0.90993400 | 2.36139500 |
| N | 0.00000000 | 0.00000000 | 2.19178500 |

| | | | |
|---|-------------|-------------|------------|
| O | -0.50760800 | -1.14959200 | 2.18745700 |
| O | 1.24938000 | 0.13519400 | 2.18745700 |
| O | -0.74177100 | 1.01439800 | 2.18745700 |