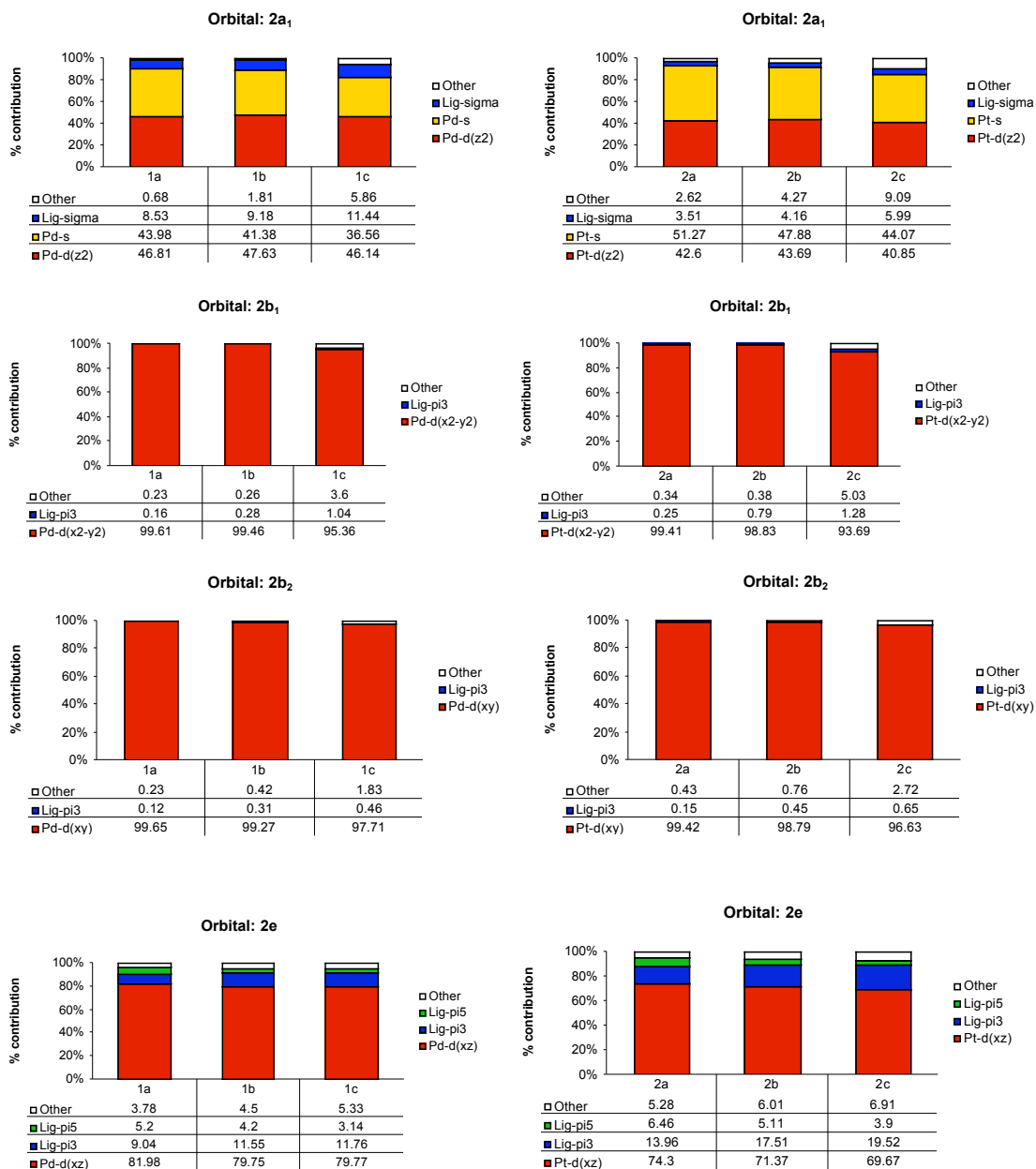
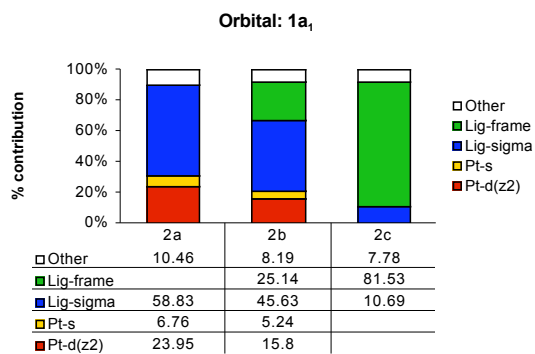
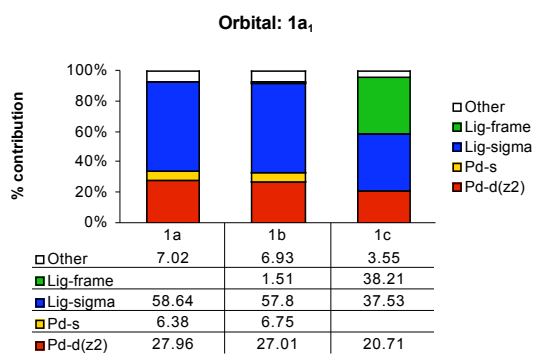
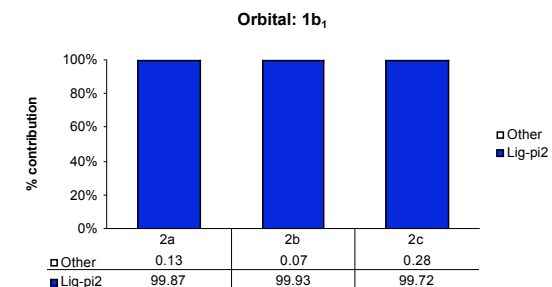
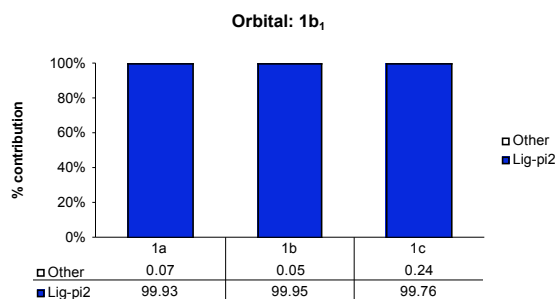
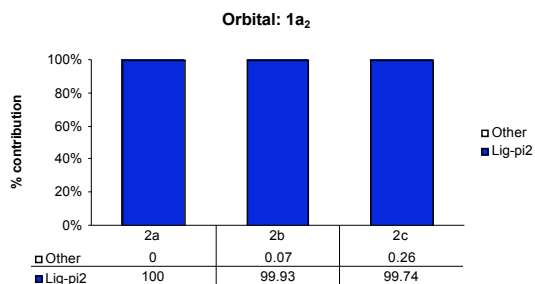
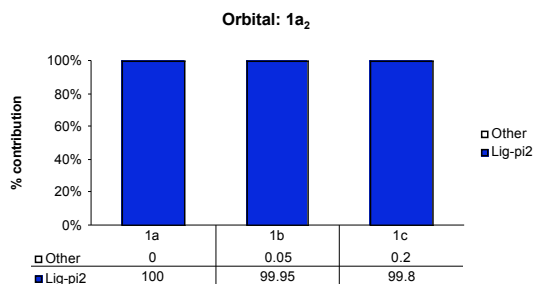
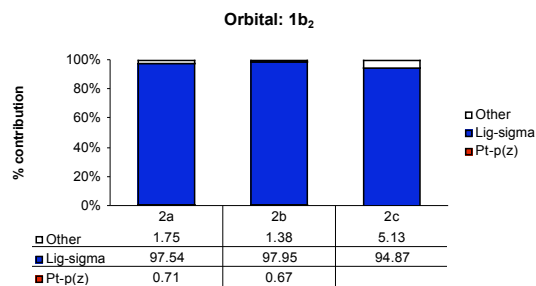
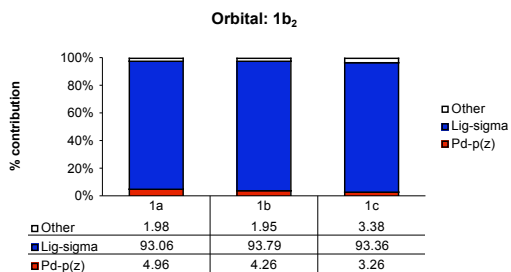
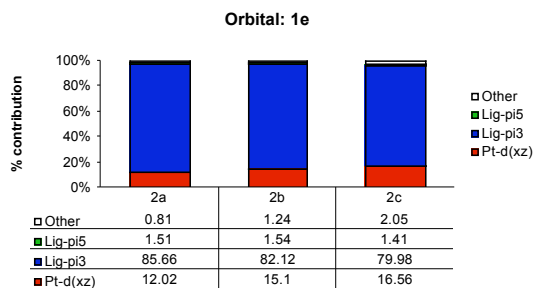
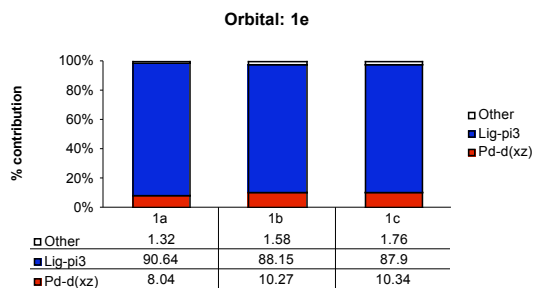
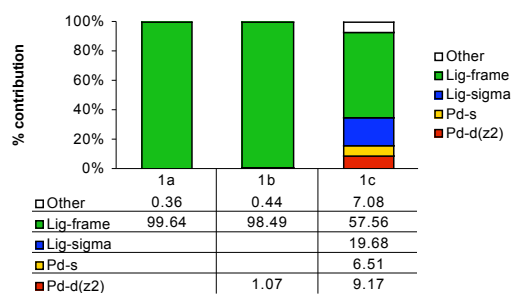
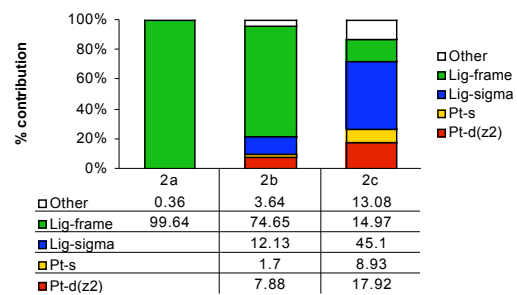


Supplementary information

The graphs below contain the orbital compositions obtained from fragment calculations carried out on complexes **1a-c** and **2a-c**. Metal based orbitals are shown in red and yellow, ligand based orbitals are shown in blue and green. Orbitals contributing less than 1% are not stated in the output of a fragment calculation. Therefore, orbitals with no composition stated are accounted for in the contribution from “Other” orbitals. Plots on the left side of the page correspond to palladium, those on the right of the page to platinum





Orbital: 0a₁Orbital: 0a₁

The tables below present the xyz coordinates optimised with gradient corrections applies both during and after SCF convergence.

1a during

```
C 0.481186 0.481186 -4.216267
N 0.751548 0.751548 -2.879426
C 0.000000 0.000000 -2.008285
N -0.751548 -0.751548 -2.879426
C -0.481186 -0.481186 -4.216267
H -0.980084 -0.980084 -5.036730
H 0.980084 0.980084 -5.036730
H -1.425072 -1.425072 -2.537693
H 1.425072 1.425072 -2.537693
C 0.481186 -0.481186 4.216267
N 0.751548 -0.751548 2.879426
C 0.000000 0.000000 2.008285
N -0.751548 0.751548 2.879426
C -0.481186 0.481186 4.216267
H -0.980084 0.980084 5.036730
H 0.980084 -0.980084 5.036730
H -1.425072 1.425072 2.537693
H 1.425072 -1.425072 2.537693
Pd 0.000000 0.000000 0.000000
```

1a post

```
C 0.478490 0.478490 -4.147166
N 0.744989 0.744989 -2.826321
C 0.000000 0.000000 -1.968618
N -0.744989 -0.744989 -2.826321
C -0.478490 -0.478490 -4.147166
H -0.976524 -0.976524 -4.973425
H 0.976524 0.976524 -4.973425
H -1.418642 -1.418642 -2.473700
H 1.418642 1.418642 -2.473700
C 0.478490 -0.478490 4.147166
N 0.744989 -0.744989 2.826321
C 0.000000 0.000000 1.968618
N -0.744989 0.744989 2.826321
C -0.478490 0.478490 4.147166
H -0.976524 0.976524 4.973425
H 0.976524 -0.976524 4.973425
H -1.418642 1.418642 2.473700
H 1.418642 -1.418642 2.473700
Pd 0.000000 0.000000 0.000000
```

1b during

31

C 0.481796 0.481796 -4.212772
N 0.760384 0.760384 -2.880637
C 0.000000 0.000000 -2.020372
N -0.760384 -0.760384 -2.880637
C -0.481796 -0.481796 -4.212772
H -0.979779 -0.979779 -5.035418
H 0.979779 0.979779 -5.035418
C -1.739291 -1.739291 -2.419808
C 1.739291 1.739291 -2.419808
C 0.481796 -0.481796 4.212772
N 0.760384 -0.760384 2.880637
C 0.000000 0.000000 2.020372
N -0.760384 0.760384 2.880637
C -0.481796 0.481796 4.212772
H -0.979779 0.979779 5.035418
H 0.979779 -0.979779 5.035418
C -1.739291 1.739291 2.419808
C 1.739291 -1.739291 2.419808
Pd 0.000000 0.000000 0.000000
H 1.244303 2.500662 -1.805443
H 2.500662 1.244303 -1.805443
H 2.210309 2.210309 -3.290795
H -1.244303 -2.500662 -1.805443
H -2.500662 -1.244303 -1.805443
H -2.210309 -2.210309 -3.290795
H -2.210309 2.210309 3.290795
H -1.244303 2.500662 1.805443
H -2.500662 1.244303 1.805443
H 2.210309 -2.210309 3.290795
H 1.244303 -2.500662 1.805443
H 2.500662 -1.244303 1.805443

1b post 31

C 0.479428 0.479428 -4.141338
N 0.752261 0.752261 -2.824972
C 0.000000 0.000000 -1.979430
N -0.752261 -0.752261 -2.824972
C -0.479428 -0.479428 -4.141338
H -0.981154 -0.981154 -4.964448
H 0.981154 0.981154 -4.964448
C -1.711260 -1.711260 -2.355476
C 1.711260 1.711260 -2.355476
C 0.479428 -0.479428 4.141338

N 0.752261 -0.752261 2.824972
C 0.000000 0.000000 1.979430
N -0.752261 0.752261 2.824972
C -0.479428 0.479428 4.141338
H -0.981154 0.981154 4.964448
H 0.981154 -0.981154 4.964448
C -1.711260 1.711260 2.355476
C 1.711260 -1.711260 2.355476
Pd 0.000000 0.000000 0.000000
H 1.209743 2.465128 -1.730287
H 2.465128 1.209743 -1.730287
H 2.194678 2.194678 -3.216794
H -1.209743 -2.465128 -1.730287
H -2.465128 -1.209743 -1.730287
H -2.194678 -2.194678 -3.216794
H -2.194678 2.194678 3.216794
H -1.209743 2.465128 1.730287
H -2.465128 1.209743 1.730287
H 2.194678 -2.194678 3.216794
H 1.209743 -2.465128 1.730287
H 2.465128 -1.209743 1.730287

1c during

67

C 0.479819 0.479819 -4.265486
N 0.766961 0.766961 -2.936783
C 0.000000 0.000000 -2.071783
N -0.766961 -0.766961 -2.936783
C -0.479819 -0.479819 -4.265486
H -0.961638 -0.961638 -5.103415
H 0.961638 0.961638 -5.103415
C -1.788196 -1.788196 -2.513867
C 1.788196 1.788196 -2.513867
C 0.479819 -0.479819 4.265486
N 0.766961 -0.766961 2.936783
C 0.000000 0.000000 2.071783
N -0.766961 0.766961 2.936783
C -0.479819 0.479819 4.265486
H -0.961638 0.961638 5.103415
H 0.961638 -0.961638 5.103415
C -1.788196 1.788196 2.513867
C 1.788196 -1.788196 2.513867
Pd 0.000000 0.000000 0.000000
C 1.086271 2.868634 -1.682711
C 2.868634 1.086271 -1.682711
C 2.430570 2.430570 -3.750542

C -1.086271 -2.868634 -1.682711
C -2.868634 -1.086271 -1.682711
C -2.430570 -2.430570 -3.750542
C -2.430570 2.430570 3.750542
C -1.086271 2.868634 1.682711
C -2.868634 1.086271 1.682711
C 2.430570 -2.430570 3.750542
C 1.086271 -2.868634 1.682711
C 2.868634 -1.086271 1.682711
H 1.821319 3.605386 -1.326692
H 0.321136 3.387296 -2.278634
H 0.603017 2.389468 -0.816839
H 3.167850 3.167850 -3.405330
H 2.962003 1.694012 -4.370324
H 1.694012 2.962003 -4.370324
H 3.605386 1.821319 -1.326692
H 2.389468 0.603017 -0.816839
H 3.387296 0.321136 -2.278634
H -0.321136 -3.387296 -2.278634
H -0.603017 -2.389468 -0.816839
H -1.821319 -3.605386 -1.326692
H -3.167850 -3.167850 -3.405330
H -2.962003 -1.694012 -4.370324
H -1.694012 -2.962003 -4.370324
H -3.387296 -0.321136 -2.278634
H -3.605386 -1.821319 -1.326692
H -2.389468 -0.603017 -0.816839
H -0.321136 3.387296 2.278634
H -0.603017 2.389468 0.816839
H -1.821319 3.605386 1.326692
H -3.605386 1.821319 1.326692
H -2.389468 0.603017 0.816839
H -3.387296 0.321136 2.278634
H -1.694012 2.962003 4.370324
H -3.167850 3.167850 3.405330
H -2.962003 1.694012 4.370324
H 3.387296 -0.321136 2.278634
H 3.605386 -1.821319 1.326692
H 2.389468 -0.603017 0.816839
H 2.962003 -1.694012 4.370324
H 1.694012 -2.962003 4.370324
H 3.167850 -3.167850 3.405330
H 1.821319 -3.605386 1.326692
H 0.321136 -3.387296 2.278634
H 0.603017 -2.389468 0.816839

C 0.478017 0.478017 -4.190562
N 0.756205 0.756205 -2.876273
C 0.000000 0.000000 -2.026918
N -0.756205 -0.756205 -2.876273
C -0.478017 -0.478017 -4.190562
H -0.969701 -0.969701 -5.023169
H 0.969701 0.969701 -5.023169
C -1.751312 -1.751312 -2.437624
C 1.751312 1.751312 -2.437624
C 0.478017 -0.478017 4.190562
N 0.756205 -0.756205 2.876273
C 0.000000 0.000000 2.026918
N -0.756205 0.756205 2.876273
C -0.478017 0.478017 4.190562
H -0.969701 0.969701 5.023169
H 0.969701 -0.969701 5.023169
C -1.751312 1.751312 2.437624
C 1.751312 -1.751312 2.437624
Pd 0.000000 0.000000 0.000000
C 1.046165 2.794807 -1.605430
C 2.794807 1.046165 -1.605430
C 2.395548 2.395548 -3.640049
C -1.046165 -2.794807 -1.605430
C -2.794807 -1.046165 -1.605430
C -2.395548 -2.395548 -3.640049
C -2.395548 2.395548 3.640049
C -1.046165 2.794807 1.605430
C -2.794807 1.046165 1.605430
C 2.395548 -2.395548 3.640049
C 1.046165 -2.794807 1.605430
C 2.794807 -1.046165 1.605430
H 1.777212 3.512128 -1.198156
H 0.295297 3.337686 -2.203752
H 0.534534 2.271664 -0.770196
H 3.131012 3.131012 -3.279499
H 2.932189 1.659359 -4.261683
H 1.659359 2.932189 -4.261683
H 3.512128 1.777212 -1.198156
H 2.271664 0.534534 -0.770196
H 3.337686 0.295297 -2.203752
H -0.295297 -3.337686 -2.203752
H -0.534534 -2.271664 -0.770196
H -1.777212 -3.512128 -1.198156
H -3.131012 -3.131012 -3.279499
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H -1.659359 -2.932189 -4.261683
H -3.337686 -0.295297 -2.203752
H -3.512128 -1.777212 -1.198156

H -2.271664 -0.534534 -0.770196
H -0.295297 3.337686 2.203752
H -0.534534 2.271664 0.770196
H -1.777212 3.512128 1.198156
H -3.512128 1.777212 1.198156
H -2.271664 0.534534 0.770196
H -3.337686 0.295297 2.203752
H -1.659359 2.932189 4.261683
H -3.131012 3.131012 3.279499
H -2.932189 1.659359 4.261683
H 3.337686 -0.295297 2.203752
H 3.512128 -1.777212 1.198156
H 2.271664 -0.534534 0.770196
H 2.932189 -1.659359 4.261683
H 1.659359 -2.932189 4.261683
H 3.131012 -3.131012 3.279499
H 1.777212 -3.512128 1.198156
H 0.295297 -3.337686 2.203752
H 0.534534 -2.271664 0.770196

2a during

19

C 0.481126 0.481126 -4.186884
N 0.754053 0.754053 -2.852291
C 0.000000 0.000000 -1.981916
N -0.754053 -0.754053 -2.852291
C -0.481126 -0.481126 -4.186884
H -0.979250 -0.979250 -5.008027
H 0.979250 0.979250 -5.008027
H -1.427085 -1.427085 -2.507669
H 1.427085 1.427085 -2.507669
C 0.481126 -0.481126 4.186884
N 0.754053 -0.754053 2.852291
C 0.000000 0.000000 1.981916
N -0.754053 0.754053 2.852291
C -0.481126 0.481126 4.186884
H -0.979250 0.979250 5.008027
H 0.979250 -0.979250 5.008027
H -1.427085 1.427085 2.507669
H 1.427085 -1.427085 2.507669
Pt 0.000000 0.000000 0.000000

2a post

19

C 0.478424 0.478424 -4.128979
N 0.747310 0.747310 -2.810178
C 0.000000 0.000000 -1.952799
N -0.747310 -0.747310 -2.810178
C -0.478424 -0.478424 -4.128979
H -0.975546 -0.975546 -4.956018
H 0.975546 0.975546 -4.956018
H -1.420409 -1.420409 -2.454133
H 1.420409 1.420409 -2.454133
C 0.478424 -0.478424 4.128979
N 0.747310 -0.747310 2.810178
C 0.000000 0.000000 1.952799
N -0.747310 0.747310 2.810178
C -0.478424 0.478424 4.128979
H -0.975546 0.975546 4.956018
H 0.975546 -0.975546 4.956018
H -1.420409 1.420409 2.454133
H 1.420409 -1.420409 2.454133
Pt 0.000000 0.000000 0.000000

2b during

31

C 0.481705 0.481705 -4.184459
N 0.762884 0.762884 -2.854433
C 0.000000 0.000000 -1.994449
N -0.762884 -0.762884 -2.854433
C -0.481705 -0.481705 -4.184459
H -0.979329 -0.979329 -5.007363
H 0.979329 0.979329 -5.007363
C -1.741300 -1.741300 -2.392613
C 1.741300 1.741300 -2.392613
C 0.481705 -0.481705 4.184459
N 0.762884 -0.762884 2.854433
C 0.000000 0.000000 1.994449
N -0.762884 0.762884 2.854433
C -0.481705 0.481705 4.184459
H -0.979329 0.979329 5.007363
H 0.979329 -0.979329 5.007363
C -1.741300 1.741300 2.392613
C 1.741300 -1.741300 2.392613
Pt 0.000000 0.000000 0.000000
H 1.246112 2.502126 -1.777720
H 2.502126 1.246112 -1.777720
H 2.211990 2.211990 -3.264103
H -1.246112 -2.502126 -1.777720

H -2.502126 -1.246112 -1.777720
H -2.211990 -2.211990 -3.264103
H -2.211990 2.211990 3.264103
H -1.246112 2.502126 1.777720
H -2.502126 1.246112 1.777720
H 2.211990 -2.211990 3.264103
H 1.246112 -2.502126 1.777720
H 2.502126 -1.246112 1.777720

2b post

31

C 0.479365 0.479365 -4.123351
N 0.754535 0.754535 -2.808894
C 0.000000 0.000000 -1.963529
N -0.754535 -0.754535 -2.808894
C -0.479365 -0.479365 -4.123351
H -0.980523 -0.980523 -4.946807
H 0.980523 0.980523 -4.946807
C -1.712036 -1.712036 -2.334600
C 1.712036 1.712036 -2.334600
C 0.479365 -0.479365 4.123351
N 0.754535 -0.754535 2.808894
C 0.000000 0.000000 1.963529
N -0.754535 0.754535 2.808894
C -0.479365 0.479365 4.123351
H -0.980523 0.980523 4.946807
H 0.980523 -0.980523 4.946807
C -1.712036 1.712036 2.334600
C 1.712036 -1.712036 2.334600
Pt 0.000000 0.000000 0.000000
H 1.208676 2.463393 -1.707618
H 2.463393 1.208676 -1.707618
H 2.197338 2.197338 -3.193774
H -1.208676 -2.463393 -1.707618
H -2.463393 -1.208676 -1.707618
H -2.197338 -2.197338 -3.193774
H -2.197338 2.197338 3.193774
H -1.208676 2.463393 1.707618
H -2.463393 1.208676 1.707618
H 2.197338 -2.197338 3.193774
H 1.208676 -2.463393 1.707618
H 2.463393 -1.208676 1.707618

2c during

67

C 0.479422 0.479422 -4.225980
N 0.770635 0.770635 -2.900010
C 0.000000 0.000000 -2.033738
N -0.770635 -0.770635 -2.900010
C -0.479422 -0.479422 -4.225980
H -0.960199 -0.960199 -5.064657
H 0.960199 0.960199 -5.064657
C -1.795432 -1.795432 -2.489908
C 1.795432 1.795432 -2.489908
C 0.479422 -0.479422 4.225980
N 0.770635 -0.770635 2.900010
C 0.000000 0.000000 2.033738
N -0.770635 0.770635 2.900010
C -0.479422 0.479422 4.225980
H -0.960199 0.960199 5.064657
H 0.960199 -0.960199 5.064657
C -1.795432 1.795432 2.489908
C 1.795432 -1.795432 2.489908
Pt 0.000000 0.000000 0.000000
C 1.101477 2.884132 -1.662387
C 2.884132 1.101477 -1.662387
C 2.429704 2.429704 -3.735773
C -1.101477 -2.884132 -1.662387
C -2.884132 -1.101477 -1.662387
C -2.429704 -2.429704 -3.735773
C -2.429704 2.429704 3.735773
C -1.101477 2.884132 1.662387
C -2.884132 1.101477 1.662387
C 2.429704 -2.429704 3.735773
C 1.101477 -2.884132 1.662387
C 2.884132 -1.101477 1.662387
H 1.840818 3.624769 -1.323348
H 0.329946 3.396775 -2.255387
H 0.629574 2.411813 -0.786620
H 3.168787 3.168787 -3.398397
H 2.958390 1.690267 -4.354457
H 1.690267 2.958390 -4.354457
H 3.624769 1.840818 -1.323348
H 2.411813 0.629574 -0.786620
H 3.396775 0.329946 -2.255387
H -0.329946 -3.396775 -2.255387
H -0.629574 -2.411813 -0.786620
H -1.840818 -3.624769 -1.323348
H -3.168787 -3.168787 -3.398397

H -2.958390 -1.690267 -4.354457
H -1.690267 -2.958390 -4.354457
H -3.396775 -0.329946 -2.255387
H -3.624769 -1.840818 -1.323348
H -2.411813 -0.629574 -0.786620
H -0.329946 3.396775 2.255387
H -0.629574 2.411813 0.786620
H -1.840818 3.624769 1.323348
H -3.624769 1.840818 1.323348
H -2.411813 0.629574 0.786620
H -3.396775 0.329946 2.255387
H -1.690267 2.958390 4.354457
H -3.168787 3.168787 3.398397
H -2.958390 1.690267 4.354457
H 3.396775 -0.329946 2.255387
H 3.624769 -1.840818 1.323348
H 2.411813 -0.629574 0.786620
H 2.958390 -1.690267 4.354457
H 1.690267 -2.958390 4.354457
H 3.168787 -3.168787 3.398397
H 1.840818 -3.624769 1.323348
H 0.329946 -3.396775 2.255387
H 0.629574 -2.411813 0.786620

2c post

67

C 0.477655 0.477655 -4.166139
N 0.759211 0.759211 -2.854190
C 0.000000 0.000000 -2.003687
N -0.759211 -0.759211 -2.854190
C -0.477655 -0.477655 -4.166139
H -0.968670 -0.968670 -4.999160
H 0.968670 0.968670 -4.999160
C -1.756597 -1.756597 -2.424969
C 1.756597 1.756597 -2.424969
C 0.477655 -0.477655 4.166139
N 0.759211 -0.759211 2.854190
C 0.000000 0.000000 2.003687
N -0.759211 0.759211 2.854190
C -0.477655 0.477655 4.166139
H -0.968670 0.968670 4.999160
H 0.968670 -0.968670 4.999160
C -1.756597 1.756597 2.424969
C 1.756597 -1.756597 2.424969
Pt 0.000000 0.000000 0.000000

C 1.056593 2.806919 -1.596073
C 2.806919 1.056593 -1.596073
C 2.394576 2.394576 -3.634772
C -1.056593 -2.806919 -1.596073
C -2.806919 -1.056593 -1.596073
C -2.394576 -2.394576 -3.634772
C -2.394576 2.394576 3.634772
C -1.056593 2.806919 1.596073
C -2.806919 1.056593 1.596073
C 2.394576 -2.394576 3.634772
C 1.056593 -2.806919 1.596073
C 2.806919 -1.056593 1.596073
H 1.792318 3.521568 -1.192368
H 0.309074 3.352390 -2.196473
H 0.544140 2.287307 -0.758528
H 3.131582 3.131582 -3.280144
H 2.928898 1.655787 -4.255494
H 1.655787 2.928898 -4.255494
H 3.521568 1.792318 -1.192368
H 2.287307 0.544140 -0.758528
H 3.352390 0.309074 -2.196473
H -0.309074 -3.352390 -2.196473
H -0.544140 -2.287307 -0.758528
H -1.792318 -3.521568 -1.192368
H -3.131582 -3.131582 -3.280144
H -2.928898 -1.655787 -4.255494
H -1.655787 -2.928898 -4.255494
H -3.352390 -0.309074 -2.196473
H -3.521568 -1.792318 -1.192368
H -2.287307 -0.544140 -0.758528
H -0.309074 3.352390 2.196473
H -0.544140 2.287307 0.758528
H -1.792318 3.521568 1.192368
H -3.521568 1.792318 1.192368
H -2.287307 0.544140 0.758528
H -3.352390 0.309074 2.196473
H -1.655787 2.928898 4.255494
H -3.131582 3.131582 3.280144
H -2.928898 1.655787 4.255494
H 3.352390 -0.309074 2.196473
H 3.521568 -1.792318 1.192368
H 2.287307 -0.544140 0.758528
H 2.928898 -1.655787 4.255494
H 1.655787 -2.928898 4.255494
H 3.131582 -3.131582 3.280144
H 1.792318 -3.521568 1.192368
H 0.309074 -3.352390 2.196473
H 0.544140 -2.287307 0.758528

a during

C 0.000000 0.680460 -4.165103
N 0.000000 1.051166 -2.820825
C 0.000000 0.000000 -1.939273
N 0.000000 -1.051166 -2.820825
C 0.000000 -0.680460 -4.165103
H 0.000000 -1.386223 -4.986586
H 0.000000 1.386223 -4.986586
H 0.000000 -2.010458 -2.498028
H 0.000000 2.010458 -2.498028

a post

9

C 0.000000 0.676348 -4.152802
N 0.000000 1.040968 -2.824121
C 0.000000 0.000000 -1.957565
N 0.000000 -1.040968 -2.824121
C 0.000000 -0.676348 -4.152802
H 0.000000 -1.381905 -4.979179
H 0.000000 1.381905 -4.979179
H 0.000000 -2.002659 -2.497200
H 0.000000 2.002659 -2.497200

b during

15

C 0.681328 0.000000 -4.157539
N 1.063234 0.000000 -2.817672
C 0.000000 0.000000 -1.950672
N -1.063234 0.000000 -2.817672
C -0.681328 0.000000 -4.157539
H -1.385491 0.000000 -4.981507
H 1.385491 0.000000 -4.981507
C -2.448114 0.000000 -2.357117
C 2.448114 0.000000 -2.357117
H 2.641984 0.891151 -1.748869
H 2.641984 -0.891151 -1.748869
H 3.119831 0.000000 -3.222769
H -2.641984 -0.891151 -1.748869
H -2.641984 0.891151 -1.748869
H -3.119831 0.000000 -3.222769

b post

15

C 0.677375 0.000000 -4.142024
N 1.051457 0.000000 -2.817835
C 0.000000 0.000000 -1.965365
N -1.051457 0.000000 -2.817835
C -0.677375 0.000000 -4.142024
H -1.386953 0.000000 -4.966452
H 1.386953 0.000000 -4.966452
C -2.414222 0.000000 -2.364951
C 2.414222 0.000000 -2.364951
H 2.610442 0.891861 -1.752903
H 2.610442 -0.891861 -1.752903
H 3.089962 0.000000 -3.231480
H -2.610442 -0.891861 -1.752903
H -2.610442 0.891861 -1.752903
H -3.089962 0.000000 -3.231480

c during

33

C 0.000000 0.681280 -4.271396
N 0.000000 1.069004 -2.932039
C 0.000000 0.000000 -2.074998
N 0.000000 -1.069004 -2.932039
C 0.000000 -0.681280 -4.271396
H 0.000000 -1.368102 -5.107653
H 0.000000 1.368102 -5.107653
C 0.000000 -2.474733 -2.421053
C 0.000000 2.474733 -2.421053
C -1.260863 2.671724 -1.565042
C 1.260863 2.671724 -1.565042
C 0.000000 3.462850 -3.592684
C 1.260863 -2.671724 -1.565042
C -1.260863 -2.671724 -1.565042
C 0.000000 -3.462850 -3.592684
H -1.270712 3.682605 -1.131386
H -2.167198 2.541777 -2.174044
H -1.276434 1.928914 -0.757728
H 0.000000 4.485934 -3.193074
H 0.894664 3.349174 -4.221354
H -0.894664 3.349174 -4.221354
H 1.270712 3.682605 -1.131386
H 1.276434 1.928914 -0.757728

H 2.167198 2.541777 -2.174044
H 2.167198 -2.541777 -2.174044
H 1.276434 -1.928914 -0.757728
H 1.270712 -3.682605 -1.131386
H 0.000000 -4.485934 -3.193074
H -0.894664 -3.349174 -4.221354
H 0.894664 -3.349174 -4.221354
H -2.167198 -2.541777 -2.174044
H -1.270712 -3.682605 -1.131386
H -1.276434 -1.928914 -0.757728

c post

67

C 0.477655 0.477655 -4.166139
N 0.759211 0.759211 -2.854190
C 0.000000 0.000000 -2.003687
N -0.759211 -0.759211 -2.854190
C -0.477655 -0.477655 -4.166139
H -0.968670 -0.968670 -4.999160
H 0.968670 0.968670 -4.999160
C -1.756597 -1.756597 -2.424969
C 1.756597 1.756597 -2.424969
C 0.477655 -0.477655 4.166139
N 0.759211 -0.759211 2.854190
C 0.000000 0.000000 2.003687
N -0.759211 0.759211 2.854190
C -0.477655 0.477655 4.166139
H -0.968670 0.968670 4.999160
H 0.968670 -0.968670 4.999160
C -1.756597 1.756597 2.424969
C 1.756597 -1.756597 2.424969
Pt 0.000000 0.000000 0.000000
C 1.056593 2.806919 -1.596073
C 2.806919 1.056593 -1.596073
C 2.394576 2.394576 -3.634772
C -1.056593 -2.806919 -1.596073
C -2.806919 -1.056593 -1.596073
C -2.394576 -2.394576 -3.634772
C -2.394576 2.394576 3.634772
C -1.056593 2.806919 1.596073
C -2.806919 1.056593 1.596073
C 2.394576 -2.394576 3.634772
C 1.056593 -2.806919 1.596073
C 2.806919 -1.056593 1.596073
H 1.792318 3.521568 -1.192368

H 0.309074 3.352390 -2.196473
H 0.544140 2.287307 -0.758528
H 3.131582 3.131582 -3.280144
H 2.928898 1.655787 -4.255494
H 1.655787 2.928898 -4.255494
H 3.521568 1.792318 -1.192368
H 2.287307 0.544140 -0.758528
H 3.352390 0.309074 -2.196473
H -0.309074 -3.352390 -2.196473
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H -1.792318 -3.521568 -1.192368
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H 3.352390 -0.309074 2.196473
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H 1.655787 -2.928898 4.255494
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H 0.544140 -2.287307 0.758528