OM 9909946

Supporting Information

# A Comparative Density Functional Study of the Associative and the Dissociative Mechanism in the Rhodium(I)-Catalyzed Olefin Hydroboration Reactions

Christoph Widauer, Hansjörg Grützmacher and Tom Ziegler

ZORA single point energetics

Table 1. Relative energies for species involved in the associative mechanism according to the Equations (1) and (2), respectively. The energies given in *italics* letters are obtained by single point calculations of the optimized structures (See section „Compuational Details") using the ZORA scalar relativistic approach (ADF99).

| | **a** R = OH | | **b** 2R = $O_2(CH)_2$ | |
|---|---|---|---|---|
| **0** | 0.0 | | 0.0 | |
| **1** + $C_2H_4$ | –43.9 | *–44.1* | –45.8 | *–45.6* |
| **2**[c] | –35.5 | *–35.3* | –37.3 | *–36.4* |
| **3** | –49.0 | *–49.4* | | |
| **4** | –49.4 | *–49.0* | | |
| **TS-5** | – | – | –36.9 | *–36.8* |
| **6** | –53.7 | *–52.4* | –52.1 | *–51.4* |
| **7** | –52.2 | *–52.0* | | |
| **TS-8** | –44.1 | *–43.5* | | |
| **9** | –45.9 | *–46.2* | | |
| **TS-10** | –35.2 | *–34.4* | | |
| **11** + $[RhClH_2(PH_3)_2]$ | –39.5 | *–39.1* | | |
| **TS-12** | –32.0 | *–31.7* | –34.5 | *–34.0* |
| **13** | –59.1 | *–59.8* | –60.2 | *–60.3* |
| **TS-14** | –50.2 | *–50.5* | | |
| **15** | –56.2 | *–56.5* | | |
| **16** + $[RhCl(PH_3)_2]$ | –31.0 | *–31.1* | –31.9 | *–32.4* |
| **17** | –50.0 | *–49.3* | | |
| **18**[a] | –57.4 | *–57.4* | | |
| **TS-19** | –48.3 | *–48.0* | | |
| **20** | –48.4 | *–48.8* | | |
| **TS-21** | –45.3 | *–45.0* | | |
| **22** + $HBR_2$ | –45.6 | *–46.3* | | |

[a] The relative energies for **18a** indeed coincide accidentally.

Table 4. Relative Energies for species involved in the dissociative mechanism according to Equation (1). The energies given in *italics* letters are obtained by single point calculations of the optimized structures (See section „Compuational Details“) using the ZORA scalar relativistic approach (ADF99).

| | **a** R = OH | |
|---|---|---|
| **0** | 0.0 | |
| **23** + $PH_3$ | –37.6 | *–38.0* |
| **TS-24** + $PH_3$ | –18.4 | *–18.6* |
| **25** + $PH_3$ | –36.7 | *–36.0* |
| **26** + $PH_3$[a] | –26.0 | *–26.0* |
| **TS-27** + $PH_3$ | –30.2 | *–29.8* |
| **TS-28** + $PH_3$ | –29.5 | *–29.7* |
| **29** + $PH_3$ | –29.4 | *–29.5* |
| **TS-30** + $PH_3$ | –13.6 | *–14.5* |
| **31** + $PH_3$ | –31.2 | *–31.5* |

[a] The relative energies for **26a** + $PH_3$ (relative to **a0**) indeed coincide accidentally.

Supporting Information

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XYZ Coordinates of all optimized species

[$RhCl(PH_3)_2$]
11

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| XX | 1.02230 | 0.00000 | 0.00000 |
| Cl | -0.31375 | 2.29970 | 0.00000 |
| P | -0.00180 | -0.00269 | -2.30020 |
| P | 0.00079 | -0.00048 | 2.30000 |
| H | -1.10518 | 0.51817 | 3.04000 |
| H | 0.07849 | -1.26885 | 2.96965 |
| H | 1.03817 | 0.64632 | 3.03899 |
| H | -1.11685 | 0.49855 | -3.03856 |
| H | 0.09258 | -1.27109 | -2.96636 |
| H | 1.02508 | 0.65735 | -3.04232 |

[$RhClH_2(PH_3)_2$]
12

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.41490 | 0.00000 | 0.00000 |
| P | 0.01013 | 2.30598 | 0.00000 |
| P | 0.01983 | -2.30547 | 0.03381 |
| H | -1.35513 | -0.00904 | -0.77858 |
| H | 0.82125 | -2.98629 | -0.92995 |
| H | -1.17089 | -3.08001 | -0.10566 |
| H | 0.53247 | -2.94382 | 1.20270 |
| H | 0.80503 | 2.97420 | -0.97816 |
| H | -1.18380 | 3.07363 | -0.15072 |
| H | 0.52279 | 2.96750 | 1.15581 |
| H | -1.37061 | 0.00110 | 0.75748 |

$C_2H_4$
6

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.33210 | 0.00000 | 0.00000 |
| H | -0.57238 | 0.92974 | 0.00000 |
| H | -0.57238 | -0.92974 | 0.00000 |
| H | 1.90446 | -0.92975 | 0.00000 |
| H | 1.90446 | 0.92975 | 0.00000 |

$HB(OH)_2$
6

| | | | |
|---|---|---|---|
| H | 0.00000 | 0.00000 | 0.00000 |
| B | 1.19570 | 0.00000 | 0.00000 |
| O | 1.82605 | 1.22335 | 0.00000 |
| O | 1.82825 | -1.22255 | 0.00000 |
| H | 2.80835 | -1.16821 | 0.00000 |
| H | 2.80624 | 1.17073 | 0.00000 |

HB[O–CH=CH–O]
8

| | | | |
|---|---|---|---|
| H | 0.00000 | 0.00000 | 0.00000 |
| B | 1.18550 | 0.00000 | 0.00000 |
| O | 1.97912 | 1.14263 | 0.00000 |
| O | 1.98042 | -1.14124 | 0.00000 |
| C | 3.28755 | -0.66761 | 0.00000 |
| C | 3.28682 | 0.67055 | 0.00000 |
| H | 4.08819 | 1.39874 | 0.00000 |
| H | 4.08984 | -1.39465 | 0.00000 |

**1a**
16

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.41180 | 0.00000 | 0.00000 |
| P | 0.08679 | 2.31768 | 0.00000 |
| B | -1.61178 | -0.00422 | -1.24788 |
| O | -2.09050 | -1.22036 | -1.73100 |
| H | -2.76435 | -1.13420 | -2.43956 |
| O | -2.11180 | 1.21027 | -1.71234 |
| H | -2.77630 | 1.13511 | -2.43062 |
| H | 0.55156 | 2.95411 | -1.18893 |
| H | -1.06965 | 3.12361 | 0.21778 |
| H | 0.97049 | 2.94207 | 0.92928 |
| H | -1.53317 | 0.00057 | 0.47612 |
| P | 0.08334 | -2.31679 | 0.03802 |
| H | 0.55957 | -2.97599 | -1.13360 |
| H | -1.07526 | -3.11792 | 0.26198 |
| H | 0.95702 | -2.92291 | 0.98877 |

**1b**
18

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.39210 | 0.00000 | 0.00000 |
| P | 0.14189 | 2.31686 | 0.00000 |
| B | -1.75614 | 0.00695 | -1.05678 |
| O | -2.37328 | -1.13379 | -1.62652 |
| C | -3.28230 | -0.65004 | -2.55169 |
| O | -2.36302 | 1.15775 | -1.61876 |
| C | -3.27609 | 0.68876 | -2.54739 |
| H | 0.69798 | 2.93067 | -1.16093 |
| H | -0.99608 | 3.16424 | 0.15359 |
| H | 0.99146 | 2.91113 | 0.97891 |
| H | -1.61167 | -0.00084 | 0.37928 |
| P | 0.14698 | -2.31403 | -0.00590 |
| H | 0.72426 | -2.92296 | -1.15904 |
| H | -0.99026 | -3.16536 | 0.12918 |
| H | 0.98346 | -2.90611 | 0.98553 |
| H | -3.84046 | 1.41592 | -3.11782 |
| H | -3.85274 | -1.36793 | -3.12743 |

**2a**
23

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.46070 | 0.00000 | 0.00000 |
| P | 0.23280 | 2.30236 | 0.00000 |
| B | 0.14721 | -0.08749 | -2.17457 |
| O | 0.23582 | -1.32049 | -2.80862 |
| H | 0.39232 | -1.26175 | -3.77902 |
| O | 0.20147 | 1.09113 | -2.90924 |
| H | 0.37363 | 0.95687 | -3.86964 |
| H | 0.85652 | 2.93080 | 1.11514 |
| H | 0.99435 | 2.88552 | -1.05100 |
| H | -0.92402 | 3.14325 | -0.08872 |
| H | 0.13461 | 0.06993 | 1.66400 |
| P | 0.24585 | -2.28978 | 0.20223 |
| H | 0.98379 | -2.96553 | -0.80942 |
| H | 0.90349 | -2.80414 | 1.35530 |
| H | -0.90692 | -3.14073 | 0.22449 |
| C | -2.06771 | -0.02202 | -0.79752 |
| C | -2.06402 | 0.01446 | 0.61935 |
| H | -2.30707 | -0.95335 | -1.31417 |
| H | -2.30256 | 0.88200 | -1.36248 |
| H | -2.31526 | 0.94218 | 1.13517 |
| H | -2.31594 | -0.88511 | 1.18251 |

**2b**
24

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.46470 | 0.00000 | 0.00000 |
| P | 0.22436 | 2.30772 | 0.00000 |
| B | 0.34079 | -0.19672 | -2.11643 |
| O | 0.44301 | -1.40735 | -2.83298 |
| C | 0.79609 | -1.06106 | -4.13074 |
| O | 0.60302 | 0.85745 | -3.01253 |
| C | 0.89022 | 0.26792 | -4.23540 |
| H | 0.80833 | 2.93140 | -1.14082 |
| H | -0.92800 | 3.14974 | 0.12526 |
| H | 1.02847 | 2.89292 | 1.01736 |
| H | 0.05623 | 0.14414 | 1.66211 |
| P | 0.24574 | -2.27262 | 0.37049 |
| H | 0.89625 | -3.03847 | -0.63867 |
| H | -0.89810 | -3.11224 | 0.56360 |
| H | 1.00799 | -2.68201 | 1.49960 |
| H | 1.13812 | 0.91635 | -5.06638 |
| H | 0.94363 | -1.85715 | -4.84942 |
| C | -2.13440 | 0.02518 | 0.36835 |
| C | -1.94729 | -0.07697 | -1.03372 |
| H | -2.44446 | 0.97453 | 0.80752 |
| H | -2.44388 | -0.85153 | 0.93882 |
| H | -2.13235 | 0.79489 | -1.66414 |
| H | -2.12920 | -1.03087 | -1.53119 |

**3a**
22

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.55850 | 0.00000 | 0.00000 |
| P | 0.10231 | 2.31484 | 0.00000 |
| B | -2.03991 | 0.05000 | 0.41552 |
| O | -2.72713 | -1.13457 | 0.66656 |
| H | -3.68640 | -1.01036 | 0.84387 |
| O | -2.71494 | 1.26828 | 0.41148 |
| H | -3.67542 | 1.19444 | 0.61019 |
| H | -0.36020 | 3.04431 | -1.14244 |
| H | -0.57753 | 3.08326 | 0.98748 |
| H | 1.40698 | 2.87724 | 0.10363 |
| H | 0.01694 | 0.16199 | 1.58164 |
| P | 0.09297 | -2.26720 | 0.44898 |
| H | -0.35044 | -3.20236 | -0.54129 |
| H | -0.60735 | -2.83316 | 1.55152 |
| H | 1.39460 | -2.79870 | 0.67987 |
| C | -0.97562 | -0.20316 | -2.15129 |
| C | 0.38539 | -0.22442 | -2.32451 |
| H | -1.54876 | 0.71181 | -2.31231 |
| H | -1.55471 | -1.12838 | -2.13642 |
| H | 0.94357 | 0.67246 | -2.59108 |
| H | 0.93783 | -1.15936 | -2.41347 |

**4a**
22

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.52580 | 0.00000 | 0.00000 |
| P | 0.02362 | 2.31798 | 0.00000 |
| B | 0.12553 | 0.10277 | -2.06724 |
| O | 0.16786 | -1.06866 | -2.81130 |
| H | 0.30349 | -0.93408 | -3.77535 |
| O | 0.18078 | 1.34246 | -2.68951 |
| H | 0.31942 | 1.30458 | -3.66164 |
| H | 1.19595 | 2.95181 | -0.49884 |
| H | -0.96380 | 3.09587 | -0.67099 |
| H | -0.04836 | 2.97618 | 1.27041 |
| H | -1.55266 | 0.01431 | -0.36738 |
| P | 0.03295 | -2.30393 | -0.22573 |
| H | 1.20300 | -2.88140 | -0.79331 |
| H | -0.95816 | -3.01750 | -0.96020 |
| H | -0.02622 | -3.08168 | 0.97591 |
| C | -0.96537 | -0.11061 | 2.26540 |
| C | 0.38507 | -0.11531 | 2.41822 |
| H | -1.54216 | -1.03558 | 2.25785 |
| H | -1.54601 | 0.80847 | 2.34703 |
| H | 0.95260 | -1.03965 | 2.51532 |
| H | 0.94790 | 0.79829 | 2.60448 |

**TS-5b**
24

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.49330 | 0.00000 | 0.00000 |
| P | 0.24555 | 2.30647 | 0.00000 |
| B | 0.40096 | -0.25461 | -2.09708 |
| O | 0.70441 | -1.48094 | -2.71854 |
| C | 1.20391 | -1.15615 | -3.97238 |
| O | 0.67260 | 0.78632 | -3.00778 |
| C | 1.18568 | 0.17027 | -4.14118 |
| H | 0.83791 | 2.90758 | -1.14920 |
| H | -0.88447 | 3.17834 | 0.12232 |
| H | 1.07065 | 2.87775 | 1.00715 |
| H | 0.05572 | 0.19489 | 1.64063 |
| P | 0.20520 | -2.24381 | 0.55366 |
| H | 0.76695 | -3.12288 | -0.41867 |
| H | -0.93972 | -3.03261 | 0.89822 |
| H | 1.03404 | -2.57145 | 1.66170 |
| H | 1.49245 | 0.79915 | -4.96728 |
| H | 1.52691 | -1.96476 | -4.61586 |
| C | -2.13263 | 0.00808 | -0.06716 |
| C | -1.69245 | -0.15480 | -1.42800 |
| H | -2.55430 | 0.96686 | 0.23886 |
| H | -2.56890 | -0.84684 | 0.45218 |
| H | -1.84201 | 0.68469 | -2.11321 |
| H | -1.86002 | -1.12646 | -1.90242 |

**6a**
22

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.51270 | 0.00000 | 0.00000 |
| P | 0.07977 | 2.30502 | 0.00000 |
| H | 0.54875 | 2.99545 | 1.16201 |
| H | 0.95785 | 2.90621 | -0.94652 |
| H | -1.07367 | 3.12008 | -0.23998 |
| P | 0.16344 | -2.25178 | -0.46554 |
| H | 0.95946 | -2.62598 | -1.58528 |
| H | 0.76996 | -3.11695 | 0.49775 |
| H | -0.98483 | -3.06273 | -0.74413 |
| H | -0.30061 | 0.14830 | -1.51537 |
| C | -2.09370 | -0.05870 | 0.34720 |
| C | -2.37642 | 0.37208 | 1.79727 |
| B | -1.31129 | -0.08021 | 2.86305 |
| O | -1.64267 | -0.24526 | 4.18717 |
| O | -0.01995 | -0.24552 | 2.36525 |
| H | -2.63838 | 0.57644 | -0.36395 |
| H | -2.44415 | -1.08904 | 0.18930 |
| H | -2.39230 | 1.48135 | 1.85525 |
| H | -3.39326 | 0.06710 | 2.11354 |
| H | -0.88995 | -0.47889 | 4.77028 |
| H | 0.73712 | -0.44308 | 2.95567 |

**6b**

24

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.50000 | 0.00000 | 0.00000 |
| P | 0.09432 | 2.30567 | 0.00000 |
| H | 0.51126 | 2.98860 | 1.18507 |
| H | 1.02415 | 2.89332 | -0.90420 |
| H | -1.03957 | 3.12888 | -0.29589 |
| P | 0.19456 | -2.26376 | -0.40888 |
| H | 1.02183 | -2.65220 | -1.50000 |
| H | 0.78788 | -3.08511 | 0.59779 |
| H | -0.93735 | -3.09549 | -0.69108 |
| H | -0.32732 | 0.13310 | -1.50426 |
| C | -2.10802 | -0.05943 | 0.28327 |
| C | -2.47115 | 0.40630 | 1.70759 |
| B | -1.46019 | -0.05945 | 2.79887 |
| O | -1.64562 | -0.28809 | 4.16123 |
| O | -0.10576 | -0.26109 | 2.48891 |
| H | -2.62977 | 0.55400 | -0.46384 |
| H | -2.44617 | -1.09563 | 0.13884 |
| H | -2.48844 | 1.51501 | 1.74279 |
| H | -3.50333 | 0.10329 | 1.97218 |
| C | -0.38988 | -0.61733 | 4.66195 |
| C | 0.52224 | -0.60209 | 3.68266 |
| H | 1.58749 | -0.79026 | 3.65460 |
| H | -0.31233 | -0.83358 | 5.72000 |

**6c**

22

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.53790 | 0.00000 | 0.00000 |
| B | 2.23342 | 1.40988 | 0.00000 |
| S | 1.25525 | 2.66895 | 0.86706 |
| RH | -0.91120 | 1.26066 | 1.47628 |
| P | -2.26421 | 2.38405 | -0.03294 |
| Cl | -1.94130 | 2.75795 | 3.19064 |
| P | -0.00175 | 0.14325 | 3.28333 |
| S | 3.85660 | 1.65020 | -0.76962 |
| H | 1.04912 | 0.78188 | 4.00909 |
| H | -0.89284 | -0.09587 | 4.36658 |
| H | 0.58996 | -1.15806 | 3.19743 |
| H | -3.66205 | 2.41094 | 0.23533 |
| H | -2.05115 | 3.78791 | -0.17376 |
| H | -2.31824 | 2.05079 | -1.42498 |
| H | -1.98929 | 0.14729 | 1.47912 |
| H | -0.36372 | -1.02852 | 0.13287 |
| H | -0.35578 | 0.34379 | -0.98246 |
| H | 1.91206 | -0.51161 | 0.91136 |
| H | 1.91032 | -0.62205 | -0.83893 |
| H | 4.05398 | 2.95978 | -0.44033 |
| H | 2.06173 | 3.77497 | 0.90671 |

**7a**
22

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.44070 | 0.00000 | 0.00000 |
| P | 0.05753 | 2.31138 | 0.00000 |
| H | 0.97735 | 2.99205 | 0.85395 |
| H | 0.42693 | 2.94506 | -1.22360 |
| H | -1.10331 | 3.09968 | 0.28380 |
| P | 0.05987 | -2.28170 | -0.36001 |
| H | 0.44716 | -2.71979 | -1.66126 |
| H | 0.96669 | -3.08942 | 0.39129 |
| H | -1.10496 | -3.10187 | -0.21773 |
| H | -1.18511 | 0.07962 | -1.00762 |
| C | -1.79036 | -0.09155 | 1.12790 |
| C | -1.35999 | -0.20001 | 2.59201 |
| B | -2.64783 | -0.28229 | 3.51230 |
| O | -3.17914 | -1.53116 | 3.77824 |
| O | -3.19953 | 0.90098 | 3.96858 |
| H | -2.40075 | 0.80773 | 0.96041 |
| H | -2.39186 | -0.96155 | 0.82720 |
| H | -0.74177 | -1.10069 | 2.75068 |
| H | -0.75783 | 0.67628 | 2.88659 |
| H | -3.99724 | -1.51560 | 4.31847 |
| H | -4.01701 | 0.78711 | 4.49785 |

**7c**
22

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.53450 | 0.00000 | 0.00000 |
| B | 2.04757 | 1.50452 | 0.00000 |
| S | 2.27310 | 2.31818 | -1.61151 |
| RH | -0.60832 | -2.02568 | 0.11371 |
| P | -0.77944 | -1.99722 | 2.41980 |
| Cl | -0.00937 | -4.38211 | 0.26231 |
| P | -0.76348 | -2.28194 | -2.17970 |
| S | 2.30535 | 2.30163 | 1.61539 |
| H | 0.22445 | -3.04752 | -2.86854 |
| H | -1.91546 | -2.96703 | -2.66748 |
| H | -0.81318 | -1.16147 | -3.06908 |
| H | -1.93194 | -2.61709 | 2.98709 |
| H | 0.20730 | -2.66844 | 3.20310 |
| H | -0.83241 | -0.77263 | 3.15923 |
| H | -1.89324 | -1.14983 | 0.05346 |
| H | -0.38747 | 0.47830 | -0.91080 |
| H | -0.38952 | 0.56957 | 0.85589 |
| H | 1.92352 | -0.53116 | 0.88633 |
| H | 1.92141 | -0.53676 | -0.88300 |
| H | 2.62535 | 3.55907 | 1.19151 |
| H | 2.61441 | 3.56749 | -1.18251 |

**TS-8a**

22

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.40080 | 0.00000 | 0.00000 |
| P | 0.13875 | 2.30974 | 0.00000 |
| H | 0.94413 | 2.95887 | 0.98475 |
| H | 0.71412 | 2.92608 | -1.15138 |
| H | -1.00878 | 3.16239 | 0.10790 |
| P | 0.13183 | -2.27887 | -0.32426 |
| H | 0.65947 | -2.71698 | -1.57691 |
| H | 0.98048 | -3.05803 | 0.51847 |
| H | -1.01681 | -3.13182 | -0.29010 |
| H | -1.43819 | 0.05408 | -0.66758 |
| C | -2.13325 | -0.06176 | 0.65320 |
| C | -1.97831 | 0.24434 | 2.15019 |
| B | -1.12219 | -0.76678 | 3.00554 |
| O | -0.41859 | -0.26109 | 4.08167 |
| O | -1.19094 | -2.11856 | 2.69997 |
| H | -2.86083 | 0.64749 | 0.22453 |
| H | -2.54895 | -1.06975 | 0.51551 |
| H | -1.61156 | 1.26959 | 2.31786 |
| H | -3.00524 | 0.23784 | 2.58703 |
| H | 0.07776 | -0.93482 | 4.59169 |
| H | -0.66960 | -2.68685 | 3.30467 |

**9a**

22

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.36060 | 0.00000 | 0.00000 |
| P | 0.19069 | 2.29900 | 0.00000 |
| H | 1.01659 | 2.91639 | 0.98615 |
| H | 0.77977 | 2.89844 | -1.15461 |
| H | -0.92644 | 3.19021 | 0.10874 |
| P | 0.18030 | -2.28667 | -0.22631 |
| H | 0.73847 | -2.79506 | -1.43934 |
| H | 1.01409 | -3.01497 | 0.67614 |
| H | -0.95311 | -3.16297 | -0.17193 |
| H | -1.76960 | 0.19775 | -0.37851 |
| C | -2.56470 | -0.16492 | 0.38004 |
| C | -2.54540 | 0.46650 | 1.77310 |
| B | -1.31854 | 0.00435 | 2.66227 |
| O | -0.59060 | 0.98105 | 3.32114 |
| O | -1.15713 | -1.36046 | 2.87042 |
| H | -3.45047 | 0.15276 | -0.19786 |
| H | -2.57591 | -1.25902 | 0.42316 |
| H | -2.55951 | 1.56540 | 1.69459 |
| H | -3.48815 | 0.18660 | 2.28657 |
| H | 0.16983 | 0.63263 | 3.83197 |
| H | -0.37639 | -1.58221 | 3.41967 |

**TS-10a**
22

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.47960 | 0.00000 | 0.00000 |
| P | 0.30595 | 2.29177 | 0.00000 |
| P | 0.19425 | -2.24241 | -0.53406 |
| H | 0.02415 | 0.15472 | -1.63411 |
| H | 1.11793 | -2.53510 | -1.57593 |
| H | -0.91924 | -3.01091 | -0.99407 |
| H | 0.67678 | -3.16368 | 0.44292 |
| H | 1.04552 | 2.87025 | -1.06766 |
| H | -0.80023 | 3.20461 | 0.00404 |
| H | 1.02747 | 2.86098 | 1.09088 |
| C | -1.72621 | 0.00715 | 1.44080 |
| C | -2.14995 | 0.02191 | 0.06992 |
| H | -2.57843 | -0.88683 | -0.35591 |
| H | -2.55364 | 0.94612 | -0.34593 |
| H | -1.76303 | 0.96571 | 1.97257 |
| B | -1.87713 | -1.22988 | 2.38417 |
| O | -1.96973 | -2.49281 | 1.82274 |
| H | -2.06821 | -3.21767 | 2.47397 |
| O | -1.94032 | -0.96872 | 3.73929 |
| H | -1.99484 | -1.76543 | 4.30596 |
| H | 0.03984 | -0.16085 | 1.67949 |

**11a**
10

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.34170 | 0.00000 | 0.00000 |
| B | 2.20179 | 1.29836 | 0.00000 |
| O | 1.55618 | 2.52153 | 0.00107 |
| H | 2.15631 | 3.29528 | 0.00117 |
| O | 3.57676 | 1.14497 | -0.00126 |
| H | 4.07767 | 1.98705 | -0.00124 |
| H | 1.86227 | -0.96550 | -0.00081 |
| H | -0.58244 | -0.92477 | -0.00023 |
| H | -0.56314 | 0.93676 | 0.00071 |

**TS-12a**
22

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.47420 | 0.00000 | 0.00000 |
| P | 0.27180 | 2.30282 | 0.00000 |
| B | -0.06456 | 0.11308 | -2.16549 |
| O | -0.05798 | -1.04855 | -2.93117 |
| H | -0.07049 | -0.88778 | -3.90349 |
| O | -0.15488 | 1.35016 | -2.79771 |
| H | -0.16795 | 1.29813 | -3.78195 |
| H | 0.74802 | 2.91221 | 1.19960 |
| H | 1.20593 | 2.85052 | -0.91860 |
| H | -0.82524 | 3.18899 | -0.24747 |
| P | 0.26745 | -2.29190 | -0.23010 |
| H | 1.20504 | -2.74424 | -1.19588 |
| H | 0.73906 | -3.01873 | 0.90401 |
| H | -0.82886 | -3.14915 | -0.56711 |
| C | -2.15919 | 0.01030 | -0.09460 |
| C | -1.80146 | -0.05388 | 1.28577 |
| H | -2.54798 | -0.88392 | -0.58464 |
| H | -2.53984 | 0.94787 | -0.50301 |
| H | -1.94047 | -0.99043 | 1.82924 |
| H | -1.93009 | 0.83139 | 1.91151 |
| H | 0.03380 | -0.08655 | 1.68751 |

**TS-12b**
24

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.47140 | 0.00000 | 0.00000 |
| P | 0.27075 | 2.30213 | 0.00000 |
| B | -0.04801 | 0.12375 | -2.13808 |
| O | 0.15770 | -0.92792 | -3.05694 |
| C | 0.01214 | -0.38102 | -4.32431 |
| O | -0.32976 | 1.28897 | -2.88907 |
| C | -0.27384 | 0.92055 | -4.22736 |
| H | 1.10097 | 2.87746 | -0.99906 |
| H | -0.85243 | 3.18228 | -0.11899 |
| H | 0.86448 | 2.88788 | 1.15666 |
| H | 0.04977 | -0.08941 | 1.68289 |
| P | 0.26135 | -2.29242 | -0.22176 |
| H | 1.04452 | -2.77352 | -1.30521 |
| H | -0.86941 | -3.15973 | -0.36935 |
| H | 0.90043 | -2.97907 | 0.85188 |
| H | -0.45493 | 1.68214 | -4.97502 |
| H | 0.14092 | -1.03416 | -5.17778 |
| C | -1.79808 | -0.05362 | 1.30220 |
| C | -2.16537 | 0.00853 | -0.07250 |
| H | -1.91461 | 0.83348 | 1.92808 |
| H | -1.92768 | -0.98982 | 1.84879 |
| H | -2.54263 | 0.94504 | -0.48484 |
| H | -2.55639 | -0.88589 | -0.55952 |

**13a**
22

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.45280 | 0.00000 | 0.00000 |
| P | 0.13916 | 2.31883 | 0.00000 |
| B | -1.13528 | 0.05915 | -1.66672 |
| O | -1.51461 | -1.13254 | -2.27684 |
| H | -2.02077 | -1.02111 | -3.11105 |
| O | -1.49780 | 1.28843 | -2.21022 |
| H | -2.00515 | 1.21744 | -3.04801 |
| H | 0.90297 | 2.93189 | 1.03948 |
| H | 0.77727 | 2.92993 | -1.11612 |
| H | -1.01989 | 3.15384 | 0.06742 |
| P | 0.13332 | -2.31430 | -0.16500 |
| H | 0.75847 | -2.84790 | -1.32736 |
| H | 0.90286 | -3.00357 | 0.82114 |
| H | -1.02835 | -3.14804 | -0.14743 |
| C | -1.97886 | -0.02742 | 0.78839 |
| C | -1.81845 | -0.09998 | 2.30259 |
| H | -2.80989 | -0.11570 | 2.79569 |
| H | -2.55195 | -0.89366 | 0.42498 |
| H | -2.54439 | 0.87383 | 0.50727 |
| H | -1.27263 | 0.76600 | 2.70962 |
| H | -1.28659 | -1.00908 | 2.62538 |

**13b**
24

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.44510 | 0.00000 | 0.00000 |
| P | 0.11823 | 2.32099 | 0.00000 |
| B | -1.28431 | 0.07191 | -1.53133 |
| O | -1.78955 | -1.03856 | -2.24339 |
| C | -2.59536 | -0.51667 | -3.24692 |
| O | -1.81432 | 1.24316 | -2.11746 |
| C | -2.61002 | 0.81807 | -3.17350 |
| H | 0.91907 | 2.94115 | 1.00589 |
| H | 0.69715 | 2.94402 | -1.14201 |
| H | -1.04932 | 3.13714 | 0.12038 |
| P | 0.12123 | -2.31238 | -0.21909 |
| H | 0.70929 | -2.82030 | -1.41228 |
| H | 0.91749 | -3.02430 | 0.72796 |
| H | -1.04479 | -3.13848 | -0.18518 |
| C | -1.91080 | -0.04835 | 0.94284 |
| C | -1.60730 | -0.11650 | 2.43353 |
| H | -2.55173 | -0.15253 | 3.01106 |
| H | -2.50269 | -0.92056 | 0.62973 |
| H | -2.50816 | 0.84551 | 0.71199 |
| H | -1.04641 | 0.76139 | 2.79070 |
| H | -1.03121 | -1.01459 | 2.70631 |
| H | -3.09229 | -1.21188 | -3.91142 |
| H | -3.12293 | 1.57058 | -3.75832 |

**TS-14a**
22

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.38560 | 0.00000 | 0.00000 |
| P | 0.17274 | 2.31978 | 0.00000 |
| B | -1.54036 | 0.02890 | -1.42792 |
| O | -1.76658 | -1.17527 | -2.11495 |
| H | -2.14856 | -1.04664 | -3.00833 |
| O | -1.78511 | 1.26299 | -2.07044 |
| H | -1.78515 | 1.19219 | -3.04738 |
| H | 0.98185 | 2.94475 | 0.99711 |
| H | 0.76411 | 2.92081 | -1.14927 |
| H | -0.97356 | 3.16937 | 0.10114 |
| P | 0.25566 | -2.29685 | -0.18470 |
| H | 0.92144 | -2.75167 | -1.35988 |
| H | 1.06494 | -2.96242 | 0.78489 |
| H | -0.84058 | -3.21356 | -0.20747 |
| C | -2.27978 | 0.03855 | 0.31032 |
| C | -3.18307 | -1.17566 | 0.51621 |
| H | -3.97833 | -0.92891 | 1.24052 |
| H | -2.86555 | 0.94300 | 0.08344 |
| H | -1.77960 | 0.27840 | 1.26969 |
| H | -2.62736 | -2.03213 | 0.92406 |
| H | -3.66014 | -1.50556 | -0.41774 |

**15a**
22

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.36910 | 0.00000 | 0.00000 |
| P | 0.20093 | 2.30646 | 0.00000 |
| B | -1.61510 | 0.04051 | -1.76828 |
| O | -1.58982 | -1.20232 | -2.42243 |
| H | -1.28302 | -1.14439 | -3.34989 |
| O | -1.45633 | 1.25034 | -2.47021 |
| H | -1.04568 | 1.13410 | -3.35129 |
| H | 0.88048 | 2.93804 | 1.08480 |
| H | 0.93062 | 2.89896 | -1.07184 |
| H | -0.94657 | 3.16008 | -0.04539 |
| P | 0.20326 | -2.30867 | 0.02092 |
| H | 0.91647 | -2.90153 | -1.06268 |
| H | 0.93080 | -2.90807 | 1.09278 |
| H | -0.91678 | -3.19837 | 0.02218 |
| C | -2.34628 | 0.11055 | -0.35395 |
| C | -3.40712 | -0.97498 | -0.12426 |
| H | -3.82489 | -0.93634 | 0.89335 |
| H | -2.78333 | 1.11588 | -0.24220 |
| H | -1.69037 | 0.06524 | 0.62772 |
| H | -2.99860 | -1.97967 | -0.29673 |
| H | -4.23436 | -0.83785 | -0.83899 |

**16a**
12

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.54460 | 0.00000 | 0.00000 |
| B | 2.14543 | 1.45578 | 0.00000 |
| H | -0.39542 | -1.02741 | -0.00628 |
| H | 1.90177 | -0.54748 | -0.88954 |
| H | 1.90353 | -0.55043 | 0.88664 |
| H | -0.39723 | 0.51794 | -0.88714 |
| H | -0.39766 | 0.50711 | 0.89319 |
| O | 2.41949 | 2.05446 | 1.21837 |
| H | 2.75753 | 2.97202 | 1.14767 |
| O | 2.34236 | 2.08436 | -1.21822 |
| H | 2.68325 | 3.00079 | -1.14647 |

**16b**
14

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.54470 | 0.00000 | 0.00000 |
| B | 2.17329 | 1.42972 | 0.00000 |
| H | -0.39037 | -1.02882 | -0.00517 |
| H | 1.90276 | -0.55280 | -0.88626 |
| H | 1.90513 | -0.55544 | 0.88327 |
| H | -0.39820 | 0.51597 | -0.88687 |
| H | -0.39899 | 0.50730 | 0.89162 |
| O | 2.53350 | 2.15625 | 1.14098 |
| C | 3.02022 | 3.36799 | 0.66848 |
| O | 2.44269 | 2.19471 | -1.14126 |
| C | 2.96685 | 3.39038 | -0.66842 |
| H | 3.36340 | 4.09458 | 1.39396 |
| H | 3.25186 | 4.14171 | -1.39388 |

**17a**
22

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.44550 | 0.00000 | 0.00000 |
| P | 0.10665 | 2.30904 | 0.00000 |
| P | 0.14212 | -2.29316 | 0.30491 |
| C | -1.71621 | 0.02565 | -1.24603 |
| C | -2.68255 | -1.15268 | -1.24567 |
| B | -3.55504 | -1.31242 | 0.05727 |
| O | -3.70520 | -2.57877 | 0.59972 |
| O | -4.15189 | -0.18121 | 0.58343 |
| H | -4.67952 | -0.33938 | 1.39373 |
| H | -4.29418 | -2.61029 | 1.38335 |
| H | -2.16646 | -2.09933 | -1.47970 |
| H | -3.39259 | -1.00049 | -2.08993 |
| H | -1.17333 | 0.09319 | -2.20392 |
| H | -2.27739 | 0.95571 | -1.08510 |
| H | 0.96599 | 2.95337 | -0.94104 |
| H | 1.03696 | -2.72647 | 1.32646 |
| H | -1.05002 | 3.12962 | -0.19261 |
| H | 0.60397 | 2.94130 | 1.17770 |
| H | -0.97697 | -3.12276 | 0.62248 |
| H | 0.67195 | -3.08090 | -0.76316 |
| H | -1.27288 | 0.05917 | 0.89867 |

**18a**
22

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| B | 2.01190 | 0.00000 | 0.00000 |
| P | -0.04916 | 2.32788 | 0.00000 |
| Cl | -1.28264 | 0.21706 | -2.08719 |
| H | 0.65373 | 3.14585 | 0.93735 |
| H | 0.38559 | 2.94840 | -1.20488 |
| H | -1.33143 | 2.94849 | 0.10469 |
| P | -0.00241 | -2.28783 | -0.41405 |
| H | 0.63615 | -2.73675 | -1.60446 |
| H | 0.56429 | -3.22818 | 0.50219 |
| H | -1.27182 | -2.91382 | -0.60655 |
| C | 0.39798 | -0.30927 | 2.07476 |
| C | 0.78872 | 0.85339 | 2.97470 |
| H | 0.03711 | 1.65810 | 2.96141 |
| O | 2.69963 | -1.21070 | -0.00165 |
| O | 2.68834 | 1.21430 | -0.04726 |
| H | 3.66404 | 1.13284 | -0.12140 |
| H | 3.67601 | -1.12204 | -0.05946 |
| H | 0.87641 | 0.51375 | 4.02391 |
| H | 1.75726 | 1.29410 | 2.69320 |
| H | -0.60487 | -0.67923 | 2.35914 |
| H | 1.10547 | -1.13898 | 2.22206 |

**TS-19a**
22

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.54980 | 0.00000 | 0.00000 |
| P | 0.20879 | 2.30948 | 0.00000 |
| B | -1.78037 | 0.07400 | 1.09163 |
| O | -2.40088 | -1.11537 | 1.46984 |
| H | -3.25867 | -0.99241 | 1.93286 |
| O | -2.37843 | 1.30739 | 1.34410 |
| H | -3.23791 | 1.24968 | 1.81640 |
| H | -0.85568 | 3.15494 | -0.44451 |
| H | 0.48195 | 2.96613 | 1.23183 |
| H | 1.26996 | 2.84677 | -0.78439 |
| H | -0.11495 | 0.09443 | 1.62872 |
| P | 0.17049 | -2.29724 | 0.25195 |
| H | -0.87731 | -3.17142 | -0.17632 |
| H | 0.35021 | -2.83248 | 1.55771 |
| H | 1.27149 | -2.91901 | -0.40452 |
| C | -1.27212 | -0.08779 | -1.86009 |
| C | 0.06198 | -0.12172 | -2.26509 |
| H | -1.85410 | 0.83434 | -1.93199 |
| H | -1.87087 | -1.00148 | -1.83445 |
| H | 0.56116 | 0.77285 | -2.63834 |
| H | 0.54304 | -1.05996 | -2.54266 |

**20a**
22

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.52020 | 0.00000 | 0.00000 |
| P | 0.28328 | 2.30385 | 0.00000 |
| B | -1.19342 | -0.04321 | 1.94141 |
| O | -1.77349 | -1.27198 | 2.25086 |
| H | -2.65426 | -1.19926 | 2.67506 |
| O | -1.74516 | 1.17940 | 2.32095 |
| H | -2.63021 | 1.10596 | 2.73602 |
| H | -0.82248 | 3.20625 | -0.12256 |
| H | 0.90385 | 2.89390 | 1.13589 |
| H | 1.11302 | 2.84672 | -1.02275 |
| H | 0.08475 | -0.05400 | 1.85556 |
| P | 0.26809 | -2.29509 | -0.15673 |
| H | -0.83732 | -3.17909 | -0.37600 |
| H | 0.85402 | -2.97016 | 0.95008 |
| H | 1.12657 | -2.76472 | -1.19194 |
| C | -1.89876 | 0.04842 | -1.01824 |
| C | -0.84387 | 0.07526 | -1.97963 |
| H | -2.46529 | 0.96106 | -0.81149 |
| H | -2.47828 | -0.86838 | -0.87743 |
| H | -0.60368 | 1.00355 | -2.50404 |
| H | -0.61601 | -0.81520 | -2.57052 |

**TS-21a**
22

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.51800 | 0.00000 | 0.00000 |
| P | 0.17870 | 2.31040 | 0.00000 |
| B | -0.21537 | 0.06764 | -2.12786 |
| O | -0.15432 | -1.12600 | -2.84375 |
| H | 0.02141 | -1.01423 | -3.80279 |
| O | -0.15908 | 1.30397 | -2.76786 |
| H | 0.02129 | 1.25275 | -3.73118 |
| H | 1.29176 | 2.86630 | -0.68693 |
| H | -0.85850 | 3.14408 | -0.51584 |
| H | 0.34073 | 2.96271 | 1.26219 |
| H | -1.27752 | 0.03359 | -1.08345 |
| P | 0.16901 | -2.30658 | -0.14008 |
| H | 1.28627 | -2.82327 | -0.85001 |
| H | -0.86611 | -3.10238 | -0.71589 |
| H | 0.31654 | -3.03600 | 1.08102 |
| C | -1.26342 | -0.05288 | 1.92574 |
| C | 0.07370 | -0.06752 | 2.30043 |
| H | -1.85484 | -0.97059 | 1.91828 |
| H | -1.84897 | 0.86722 | 1.97182 |
| H | 0.57495 | -0.99511 | 2.57731 |
| H | 0.58029 | 0.83956 | 2.63041 |

**22a**
16

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.37940 | 0.00000 | 0.00000 |
| P | 0.09235 | 2.31476 | 0.00000 |
| P | 0.09014 | -2.31403 | 0.00686 |
| C | -2.05245 | 0.00396 | 0.70481 |
| C | -2.05382 | -0.00078 | -0.70145 |
| H | 1.35242 | -2.97354 | 0.01493 |
| H | -0.53249 | -3.04345 | 1.07218 |
| H | -0.52470 | -3.04954 | -1.05854 |
| H | 1.35567 | 2.97166 | -0.00255 |
| H | -0.53201 | 3.05561 | -1.05652 |
| H | -0.51638 | 3.03984 | 1.07639 |
| H | -2.27543 | 0.92057 | 1.25666 |
| H | -2.27904 | -0.90873 | 1.26224 |
| H | -2.27770 | 0.91265 | -1.25778 |
| H | -2.28153 | -0.91698 | -1.25145 |

**23a**
18

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.38550 | 0.00000 | 0.00000 |
| P | 0.24773 | 2.30895 | 0.00000 |
| B | -1.83144 | 0.11157 | -1.04226 |
| C | -0.24293 | -2.08187 | 0.79529 |
| C | 0.14074 | -2.20057 | -0.52281 |
| O | -2.51042 | -1.04990 | -1.39204 |
| H | -3.17742 | -0.92931 | -2.10011 |
| O | -2.16129 | 1.35466 | -1.58079 |
| H | -2.85547 | 1.31986 | -2.27365 |
| H | 1.17332 | 2.87204 | 0.92519 |
| H | 0.76271 | 2.87689 | -1.20119 |
| H | -0.85025 | 3.19959 | 0.19525 |
| H | -1.28447 | -2.22526 | 1.08593 |
| H | 0.50104 | -2.11218 | 1.59448 |
| H | -0.59865 | -2.41633 | -1.29210 |
| H | 1.19415 | -2.31353 | -0.78536 |
| H | -1.60279 | 0.13112 | 0.37328 |

**TS-24a**
18

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.45040 | 0.00000 | 0.00000 |
| P | 0.08901 | 2.30879 | 0.00000 |
| B | -1.08162 | -1.71599 | -0.70454 |
| C | -0.14004 | -0.93229 | 1.83904 |
| C | -0.08499 | -2.01196 | 0.85583 |
| O | -2.45150 | -1.92730 | -0.52707 |
| H | -2.83268 | -2.54449 | -1.18525 |
| O | -0.38009 | -2.16914 | -1.81830 |
| H | -0.95580 | -2.35899 | -2.58945 |
| H | 1.08293 | 2.90554 | 0.82570 |
| H | 0.41311 | 2.97832 | -1.22095 |
| H | -1.02732 | 3.11525 | 0.37424 |
| H | -1.07927 | -0.75655 | 2.36763 |
| H | 0.76571 | -0.70329 | 2.40518 |
| H | -0.87133 | -2.76909 | 1.00020 |
| H | 0.89841 | -2.45468 | 0.66393 |
| H | -1.56414 | 0.24545 | 0.05393 |

**25a**
18

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| P | 2.21540 | 0.00000 | 0.00000 |
| Cl | -0.55470 | 2.39521 | 0.00000 |
| H | 0.18187 | -1.37430 | 0.71739 |
| C | -0.10876 | -1.47250 | -1.48329 |
| C | -1.56951 | -1.93384 | -1.57128 |
| B | -2.52823 | -0.72636 | -1.26666 |
| O | -3.57583 | -0.37566 | -2.07027 |
| O | -2.20076 | -0.02054 | -0.09103 |
| H | -2.27728 | 0.98164 | -0.08742 |
| H | -4.07338 | 0.40714 | -1.74810 |
| H | 0.18752 | -0.89095 | -2.36886 |
| H | 0.58383 | -2.31412 | -1.36091 |
| H | -1.76929 | -2.39175 | -2.55723 |
| H | -1.74985 | -2.72086 | -0.81397 |
| H | 2.89629 | -0.94691 | -0.82917 |
| H | 2.91693 | -0.26481 | 1.21693 |
| H | 2.93068 | 1.17287 | -0.39087 |

**25c**
18

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.53800 | 0.00000 | 0.00000 |
| B | 2.10023 | 1.45827 | 0.00000 |
| S | 1.26479 | 2.53560 | -1.26883 |
| RH | -0.89326 | 1.47756 | -1.22852 |
| Cl | -2.08093 | 3.58317 | -1.37502 |
| P | -2.87613 | 0.40537 | -1.23635 |
| S | 3.43323 | 2.00267 | 1.08216 |
| H | -0.34515 | 0.32922 | -2.12496 |
| H | 1.22845 | 3.72352 | -0.59018 |
| H | 3.56765 | 3.28106 | 0.61997 |
| H | -0.37948 | 0.34181 | 0.97628 |
| H | -0.37915 | -1.01360 | -0.18623 |
| H | 1.92681 | -0.61207 | 0.83552 |
| H | 1.90369 | -0.49234 | -0.92471 |
| H | -2.95658 | -0.95537 | -0.80346 |
| H | -3.58746 | 0.26714 | -2.46626 |
| H | -3.93475 | 0.94736 | -0.44939 |

**26a**
18

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| P | 2.18710 | 0.00000 | 0.00000 |
| Cl | -0.28145 | 2.36813 | 0.00000 |
| H | 0.20141 | -1.18744 | 0.98169 |
| C | -0.42993 | -1.73245 | -1.04798 |
| C | -1.90452 | -1.40210 | -0.98379 |
| B | -2.73409 | -1.58700 | -2.32910 |
| O | -4.10323 | -1.69708 | -2.20789 |
| O | -2.04464 | -1.62185 | -3.52114 |
| H | -2.60633 | -1.70890 | -4.31971 |
| H | -4.57601 | -1.79740 | -3.06032 |
| H | 0.01918 | -1.61866 | -2.04245 |
| H | -0.17886 | -2.71014 | -0.62152 |
| H | -2.05522 | -0.29667 | -0.76165 |
| H | -2.40609 | -1.92494 | -0.15318 |
| H | 2.85529 | -0.67134 | -1.07225 |
| H | 2.90367 | -0.59426 | 1.08298 |
| H | 2.86896 | 1.25218 | -0.05614 |

**26c**
18

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.51920 | 0.00000 | 0.00000 |
| B | 2.22297 | 1.43468 | 0.00000 |
| S | 1.20940 | 2.90752 | -0.34619 |
| RH | -0.42426 | -2.00030 | -0.40849 |
| Cl | -0.12342 | -3.59139 | -2.13000 |
| P | -2.58708 | -1.80211 | -0.36114 |
| S | 4.01310 | 1.44688 | 0.34441 |
| H | -0.58127 | -1.79211 | 1.12936 |
| H | 2.19675 | 3.84566 | -0.26000 |
| H | 4.23515 | 2.78688 | 0.22506 |
| H | -0.41927 | 0.53438 | -0.86512 |
| H | -0.40772 | 0.42724 | 0.92399 |
| H | 1.91078 | -0.51348 | -0.90431 |
| H | 1.91094 | -0.56339 | 0.86790 |
| H | -3.15968 | -0.49508 | -0.27926 |
| H | -3.30065 | -2.42460 | 0.70586 |
| H | -3.32927 | -2.31875 | -1.46438 |

**TS-27a**
18

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| P | 2.20860 | 0.00000 | 0.00000 |
| Cl | -0.22756 | 2.37563 | 0.00000 |
| C | -0.28378 | -2.00525 | -0.80809 |
| C | -1.80031 | -2.25435 | -0.88155 |
| B | -2.60847 | -0.90425 | -0.96284 |
| O | -3.63008 | -0.69918 | -1.84770 |
| O | -2.19534 | 0.05737 | -0.02549 |
| H | -2.34786 | 1.02626 | -0.17397 |
| H | -4.05134 | 0.18428 | -1.77714 |
| H | 0.12949 | -1.71818 | -1.78693 |
| H | 0.25888 | -2.90521 | -0.48179 |
| H | -2.03321 | -2.92374 | -1.72840 |
| H | -2.12883 | -2.78810 | 0.03203 |
| H | 2.91992 | -1.09929 | -0.58032 |
| H | 2.90777 | 0.02398 | 1.24868 |
| H | 2.91719 | 1.06179 | -0.64007 |
| H | 0.06111 | -1.45865 | 0.62270 |

**TS-28a**
18

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.40160 | 0.00000 | 0.00000 |
| P | 0.10436 | 2.34918 | 0.00000 |
| B | -0.33968 | 0.04703 | -1.98074 |
| C | -1.50610 | -1.62666 | 0.28042 |
| C | -0.17323 | -2.12904 | 0.19762 |
| O | -0.75346 | -1.12399 | -2.59008 |
| H | -0.89594 | -1.03873 | -3.55744 |
| O | -0.15626 | 1.22981 | -2.67640 |
| H | -0.23617 | 1.14507 | -3.65116 |
| H | 0.23909 | 2.98328 | 1.27642 |
| H | 1.21911 | 2.95973 | -0.64414 |
| H | -0.92604 | 3.19862 | -0.50925 |
| H | -2.17570 | -1.81639 | -0.56457 |
| H | -2.00969 | -1.63215 | 1.25520 |
| H | 0.15819 | -2.61365 | -0.71873 |
| H | 0.34909 | -2.42338 | 1.11007 |
| H | -1.63664 | -0.10474 | 0.12897 |

**29a**
18

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.36230 | 0.00000 | 0.00000 |
| P | -0.05936 | 2.37346 | 0.00000 |
| B | -0.11099 | 0.00447 | -2.00322 |
| O | -0.61671 | -1.12748 | -2.61947 |
| H | -0.69339 | -1.04690 | -3.59475 |
| O | 0.28742 | 1.12811 | -2.70145 |
| H | 0.29202 | 1.01524 | -3.67693 |
| H | -0.21271 | 3.04483 | 1.25816 |
| H | 1.10049 | 3.08028 | -0.44052 |
| H | -1.03242 | 3.15555 | -0.70049 |
| C | -0.26525 | -2.07197 | 0.19970 |
| C | -1.65657 | -1.59508 | 0.20680 |
| H | -1.74847 | -0.36903 | 0.10020 |
| H | 0.07458 | -2.63370 | -0.66965 |
| H | 0.16039 | -2.41149 | 1.14848 |
| H | -2.25210 | -1.88691 | -0.66842 |
| H | -2.21090 | -1.72879 | 1.14851 |

**TS-30a**
18

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| Cl | 2.35280 | 0.00000 | 0.00000 |
| P | 0.27586 | 2.29921 | 0.00000 |
| B | -0.07277 | -1.27593 | -1.64905 |
| O | 0.98056 | -2.08657 | -2.03157 |
| H | 1.12224 | -2.11199 | -2.99943 |
| O | -1.11447 | -0.92080 | -2.51143 |
| H | -1.08012 | -1.40167 | -3.36763 |
| H | 0.71362 | 2.96504 | 1.19006 |
| H | 1.22570 | 2.87030 | -0.89538 |
| H | -0.82308 | 3.17674 | -0.27939 |
| C | -0.85364 | -1.95557 | 0.05049 |
| C | -2.05234 | -1.08226 | 0.32944 |
| H | -1.84530 | 0.06737 | 0.16601 |
| H | -1.05680 | -2.79139 | -0.63438 |
| H | -0.33921 | -2.36007 | 0.93117 |
| H | -2.85839 | -1.21800 | -0.40653 |
| H | -2.43785 | -1.13260 | 1.35631 |

**31a**
18

| | | | |
|---|---|---|---|
| RH | 0.00000 | 0.00000 | 0.00000 |
| P | 2.19460 | 0.00000 | 0.00000 |
| Cl | -0.08665 | 2.33079 | 0.00000 |
| C | -0.55155 | -2.33432 | -0.47151 |
| C | -2.08425 | -2.36494 | -0.60014 |
| B | -2.73759 | -0.94233 | -0.80264 |
| O | -3.77891 | -0.75709 | -1.67041 |
| O | -2.21218 | 0.07819 | -0.00022 |
| H | -2.37769 | 1.03051 | -0.20672 |
| H | -4.12770 | 0.15982 | -1.69435 |
| H | -0.06869 | -1.98737 | -1.39768 |
| H | -0.12837 | -3.32422 | -0.24130 |
| H | -2.37317 | -3.03815 | -1.42499 |
| H | -2.52013 | -2.80822 | 0.31653 |
| H | 2.90383 | -1.06416 | -0.64833 |
| H | 2.89976 | -0.06497 | 1.24660 |
| H | 2.91518 | 1.09456 | -0.56861 |
| H | -0.20819 | -1.76470 | 0.48205 |