Supplementary Material (ESI) for Dalton Transactions


# Electronic Supplementary Information

## Importance of palladium-carbon bond energies in direct arylation of polyfluorinated benzenes

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**Figure S1**. Correlation between calculated relative Pd-C bond dissociation energies and the calculated relative C-H bond dissociation energies for complexes of type **3**. The individual points represent all $Ar^F$ substituents. Benzene and $Pd(Ph)_2(PMe_3)(AcOH)$ are taken as reference.

**Figure S2.** Fit of the calculated relative Pd-C bond dissociation energies of **3** to eq 1

**Figure S3**. Correlation between calculated relative Pd-C bond dissociation energies for complexes of type **3**and the calculated relative C-C bond dissociation energies for the biaryl products. The individual

**Table S1.** Calculated energies for each reaction

**Fig. S4.** Energy profile (E/kJ $mol^{-1}$) for reaction: above $C_6H_6$, below **1Fm**.

**Fig. S5.** Energy profile (E/kJ $mol^{-1}$) for reaction: above **1Fp**, below **2Fm**.

**Fig. S6.** Energy profile (E/kJ $mol^{-1}$) for reaction: above **1Fo**, below **1Fo-1Fp**

**Fig. S7.** Energy profile (E/kJ $mol^{-1}$) for reaction: above **1Fo-1Fm**, below **2Fo**.

**Fig. S8.** Energy profile (E/kJ $mol^{-1}$) for reaction: above **2Fo**, below **2Fo-1Fp**.

**Fig. S9.** Energy profile (E/kJ $mol^{-1}$) for reaction: above **2Fo-2Fm**, below $C_6F_5$.

**Fig. S10.** Energy profile (G/kJ $mol^{-1}$) for reaction: above $C_6H_6$, below **1Fm**.

**Fig. S11.** Energy profile (G/kJ $mol^{-1}$) for reaction: above **1Fp**, below **2Fm**

**Fig. S12.** Energy profile (G/kJ $mol^{-1}$) for reaction: above **1Fo**, below **1Fo-1Fp**

**Fig. S13.** Energy profile (G/kJ $mol^{-1}$) for reaction: above **1Fo-1Fm**, below **2Fo**

**Fig. S14.** Energy profile (G/kJ $mol^{-1}$) for reaction: above **2Fo-1Fp**, below **2Fo-2Fm**

**Fig. S15.** Energy profile (G/kJ $mol^{-1}$) for reaction: $C_6F_5$

**Table S2.** Coordinates for all extrema

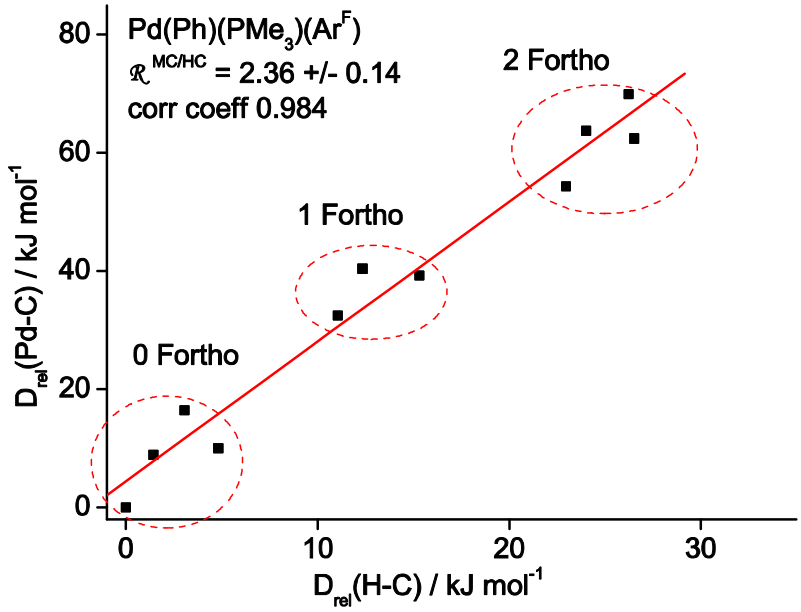


**Figure S1**. Correlation between calculated relative Pd-C bond dissociation energies and the calculated relative C-H bond dissociation energies for complexes of type **3**. The individual points represent all $Ar^F$ substituents. Benzene and $Pd(Ph)_2(PMe_3)(AcOH)$ are taken as reference.

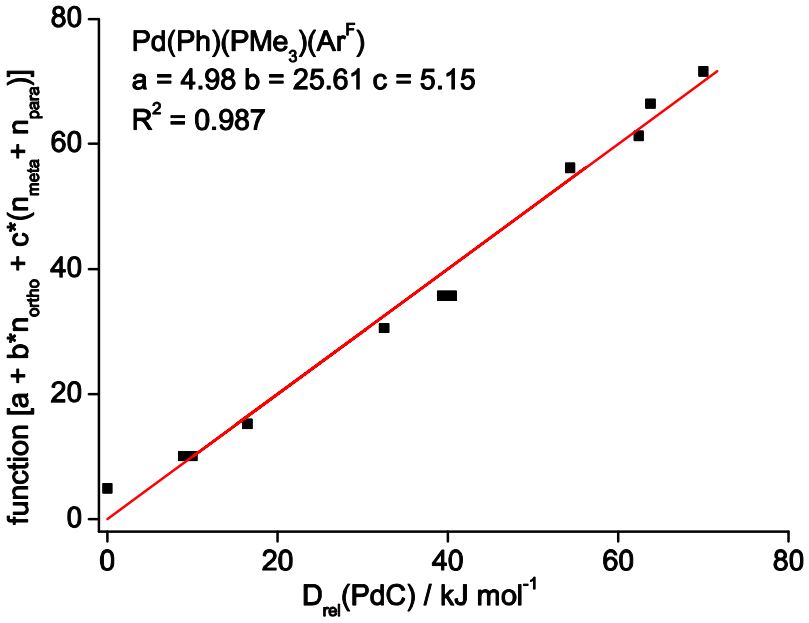


**Figure S2.** Fit of the calculated relative Pd-C bond dissociation energies of **3** to eq 1

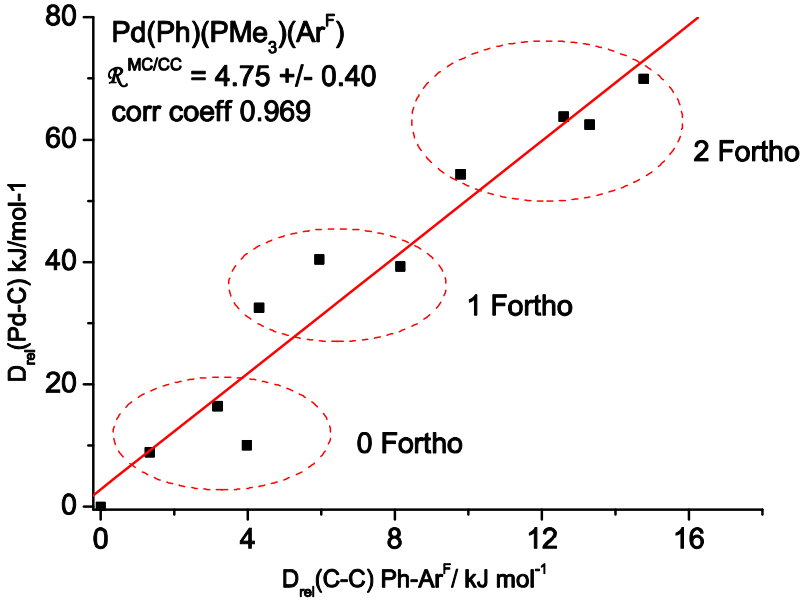


**Figure S3**. Correlation between calculated relative Pd-C bond dissociation energies for complexes of type **3**and the calculated relative C-C bond dissociation energies for the biaryl products. The individual points represent all $Ar^F$ substituents. $Pd(Ph)_2(PMe_3)(AcOH)$ and biphenyl are taken as reference.

**Table S1.** Calculated energies for each reaction

| | E(u.a.) | G(100°C)(u.a.) | ***E(kJ.mol-1)*** | ***G(100°C)(kJ.mol-1)*** |
|---|---|---|---|---|
| **1** | -1336.77 | -1336.48 | ***0*** | ***0*** |
| | | | | |
| **set0Fo** | | | | |
| | | | | |
| C6H6 | | | | |
| | | | | |
| **2** | -1281.19 | -1280.93 | ***30.69*** | ***27.35*** |
| TS-CMD | -1281.16 | -1280.9 | ***106.67*** | ***89.26*** |
| **3** | -1281.17 | -1280.91 | ***78.82*** | ***69.56*** |
| Dissociation of AcOH | -229.01 | -228.99 | | |
| **4** | -1052.13 | -1051.92 | ***147.71*** | ***74.74*** |
| TS-RE | -1052.13 | -1051.91 | ***165.91*** | ***93.13*** |
| Pd0_PMe3 | -589.01 | -588.94 | ***77.97*** | ***-48.56*** |
| Ph-Ph | -463.15 | -463.02 | | |
| | | | | |
| 0Fo-1Fm | | | | |
| | | | | |
| **2** | -1380.39 | -1380.14 | ***30.32*** | ***25.44*** |
| TS-CMD | -1380.37 | -1380.12 | ***103.26*** | ***88.48*** |
| **3** | -1380.38 | -1380.13 | ***71.74*** | ***62.52*** |
| Dissociation of AcOH | -229.01 | -228.99 | | |
| **4** | -1151.34 | -1151.14 | ***140.22*** | ***60.21*** |
| TS-RE | -1151.33 | -1151.13 | ***162.8*** | ***90.4*** |
| Pd0_PMe3 | -589.01 | -588.94 | ***78.06*** | ***-48.42*** |
| Ph-Ph* | -562.35 | -562.23 | | |
| | | | | |
| 0Fo-1Fp | | | | |
| | | | | |
| **2** | -1380.39 | -1380.14 | ***29.24*** | ***27.51*** |
| TS-CMD | -1380.37 | -1380.12 | ***101.25*** | ***81.32*** |
| **3** | -1380.38 | -1380.13 | ***75.65*** | ***60.3*** |
| Dissociation of AcOH | -229.01 | -228.99 | | |
| **4** | -1151.34 | -1151.14 | ***142.55*** | ***63.56*** |
| TS-RE | -1151.33 | -1151.13 | ***164.72*** | ***92.33*** |
| Pd0_PMe3 | -589.01 | -588.94 | ***78.82*** | ***-47.7*** |
| Ph-Ph* | -562.35 | -562.23 | | |
| | | | | |
| 0Fo-2Fm | | | | |
| | | | | |
| **2** | -1479.6 | -1479.35 | ***28.83*** | ***26.83*** |
| TS-CMD | -1479.57 | -1479.33 | ***99.98*** | ***82.90*** |
| **3** | -1479.58 | -1479.34 | ***67.68*** | ***57.60*** |
| Dissociation of AcOH | -229.01 | -228.99 | | |
| **4** | -1250.54 | -1250.35 | ***134.55*** | ***55.84*** |
| TS-RE | -1250.53 | -1250.34 | ***159.61*** | ***87.59*** |
| Pd0_PMe3 | -589.01 | -588.94 | ***78.10*** | ***-48.39*** |
| Ph-Ph* | -661.55 | -661.45 | | |

**set1Fo**

1Fo

| | | | | |
|---|---|---|---|---|
| **2** | -1380.39 | -1380.14 | ***30.23*** | ***26.24*** |
| TS-CMD | -1380.37 | -1380.12 | ***92.18*** | ***77.92*** |
| **3** | -1380.38 | -1380.13 | ***63.15*** | ***54.25*** |
| Dissociation of AcOH | -229.01 | -228.99 | | |
| **4** | -1151.34 | -1151.14 | ***126.21*** | ***50.47*** |
| TS-RE | -1151.33 | -1151.13 | ***162.22*** | ***91.92*** |
| Pd0_PMe3 | -589.01 | -588.94 | ***84.71*** | ***-41.61*** |
| Ph-Ph* | -562.35 | -562.23 | | |

1Fo-1Fp

| | | | | |
|---|---|---|---|---|
| **2** | -1479.6 | -1479.35 | ***29.23*** | ***25.9*** |
| TS-CMD | -1479.57 | -1479.33 | ***86.35*** | ***72.16*** |
| **3** | -1479.58 | -1479.34 | ***59.51*** | ***51.47*** |
| Dissociation of AcOH | -229.01 | -228.99 | | |
| **4** | -1250.55 | -1250.35 | ***123.74*** | ***47.78*** |
| TS-RE | -1250.53 | -1250.34 | ***160.49*** | ***90.39*** |
| Pd0_PMe3 | -589.01 | -588.94 | ***85.17*** | ***-41.34*** |
| Ph-Ph* | -661.55 | -661.44 | | |

1Fo-1Fm

| | | | | |
|---|---|---|---|---|
| **2** | -1479.59 | -1479.35 | ***30.37*** | ***26.88*** |
| TS-CMD | -1479.57 | -1479.33 | ***88.51*** | ***74.16*** |
| **3** | -1479.58 | -1479.34 | ***57.47*** | ***48.26*** |
| Dissociation of AcOH | -229.01 | -228.99 | | |
| **4** | -1250.55 | -1250.35 | ***119.58*** | ***43.76*** |
| TS-RE | -1250.53 | -1250.34 | ***158.3*** | ***88.36*** |
| Pd0_PMe3 | -589.01 | -588.94 | ***84.37*** | ***-41.97*** |
| Ph-Ph* | -661.55 | -661.44 | | |

**set2Fo**

2Fo

| | | | | |
|---|---|---|---|---|
| **2** | -1479.59 | -1479.34 | ***55.67*** | ***47.11*** |
| TS-CMD | -1479.58 | -1479.34 | ***77.43*** | ***62.47*** |
| **3** | -1479.59 | -1479.35 | ***46.86*** | ***40.9*** |
| Dissociation of AcOH | -229.01 | -228.99 | | |
| **4** | -1250.55 | -1250.36 | ***116.31*** | ***40.99*** |
| TS-RE | -1250.53 | -1250.34 | ***158.09*** | ***89.49*** |
| Pd0_PMe3 | -589.01 | -588.94 | ***91.17*** | ***-35.53*** |
| Ph-Ph* | -661.55 | -661.44 | | |

2Fo-1Fp

| | | | | |
|---|---|---|---|---|
| **2** | -1578.79 | -1578.56 | ***51.41*** | ***43.58*** |
| TS-CMD | -1578.78 | -1578.55 | ***71.13*** | ***56.75*** |
| **3** | -1578.79 | -1578.56 | ***42.44*** | ***36.67*** |
| Dissociation of AcOH | -229.01 | -228.99 | | |
| **4** | -1349.75 | -1349.57 | ***111.8*** | ***36.73*** |
| TS-RE | -1349.74 | -1349.55 | ***155.85*** | ***87.52*** |
| Pd0_PMe3 | -589.01 | -588.94 | ***91.23*** | ***-35.63*** |
| Ph-Ph* | -760.75 | -760.65 | | |

2Fo-2Fm

| | | | | |
|---|---|---|---|---|
| **2** | -1677.97 | -1677.75 | ***50.9*** | ***36.05*** |
| TS-CMD | -1677.97 | -1677.75 | ***67.68*** | ***52.03*** |
| **3** | -1677.98 | -1677.76 | ***31.91*** | ***26.13*** |
| Dissociation of AcOH | -229.01 | -228.99 | | |
| **4** | -1448.94 | -1448.77 | ***107.9*** | ***34.2*** |
| TS-RE | -1448.92 | -1448.75 | ***148.55*** | ***80.64*** |
| Pd0_PMe3 | -589.01 | -588.94 | ***89.42*** | ***-37.2*** |
| Ph-Ph* | -859.94 | -859.85 | | |

C6F5H

| | | | | |
|---|---|---|---|---|
| **2** | -1777.16 | -1776.95 | ***45.72*** | ***38.98*** |
| TS-CMD | -1777.16 | -1776.95 | ***60.45*** | ***47.34*** |
| **3** | -1777.17 | -1776.96 | ***26.92*** | ***21.3*** |
| Dissociation of AcOH | -229.01 | -228.99 | | |
| **4** | -1548.13 | -1547.96 | ***103.95*** | ***29.84*** |
| TS-RE | -1548.11 | -1547.95 | ***145.99*** | ***78.05*** |
| Pd0_PMe3 | -589.01 | -588.94 | ***89.51*** | ***-37.44*** |
| Ph-Ph* | -959.12 | -959.04 | | |

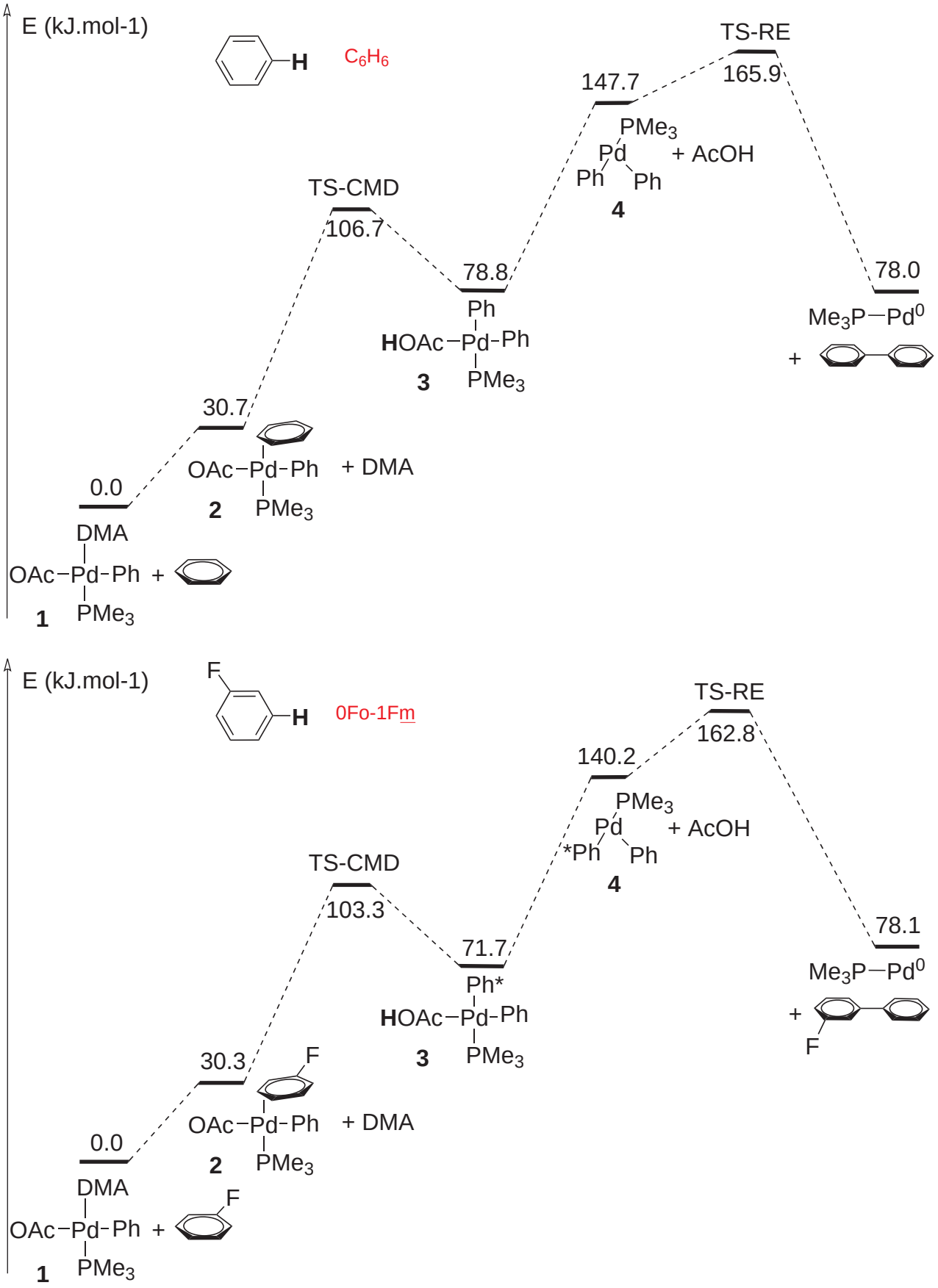


**Fig. S4.** Energy profile (E/kJ mol$^{-1}$) for reaction: above $C_6H_6$, below **1Fm**.

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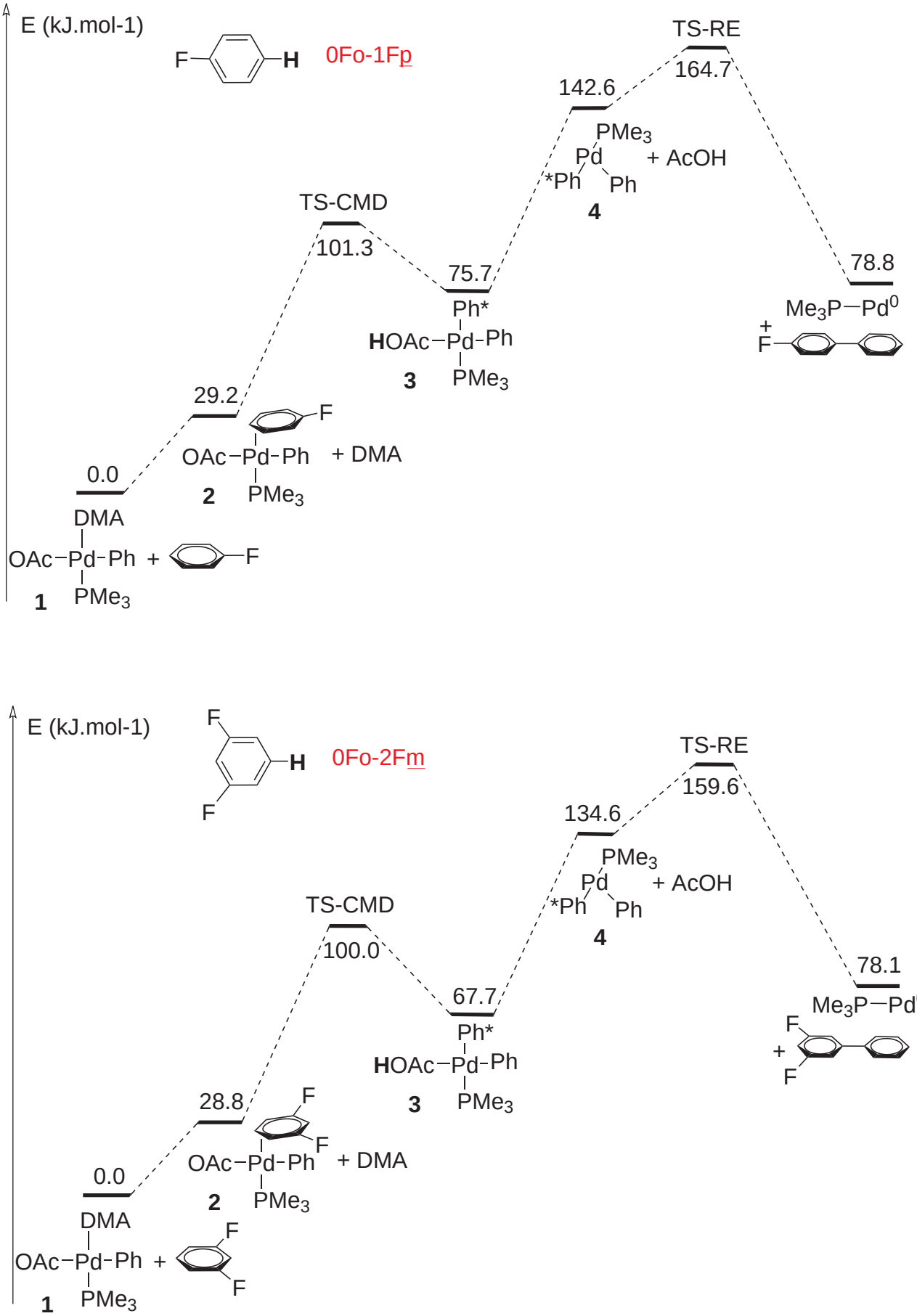
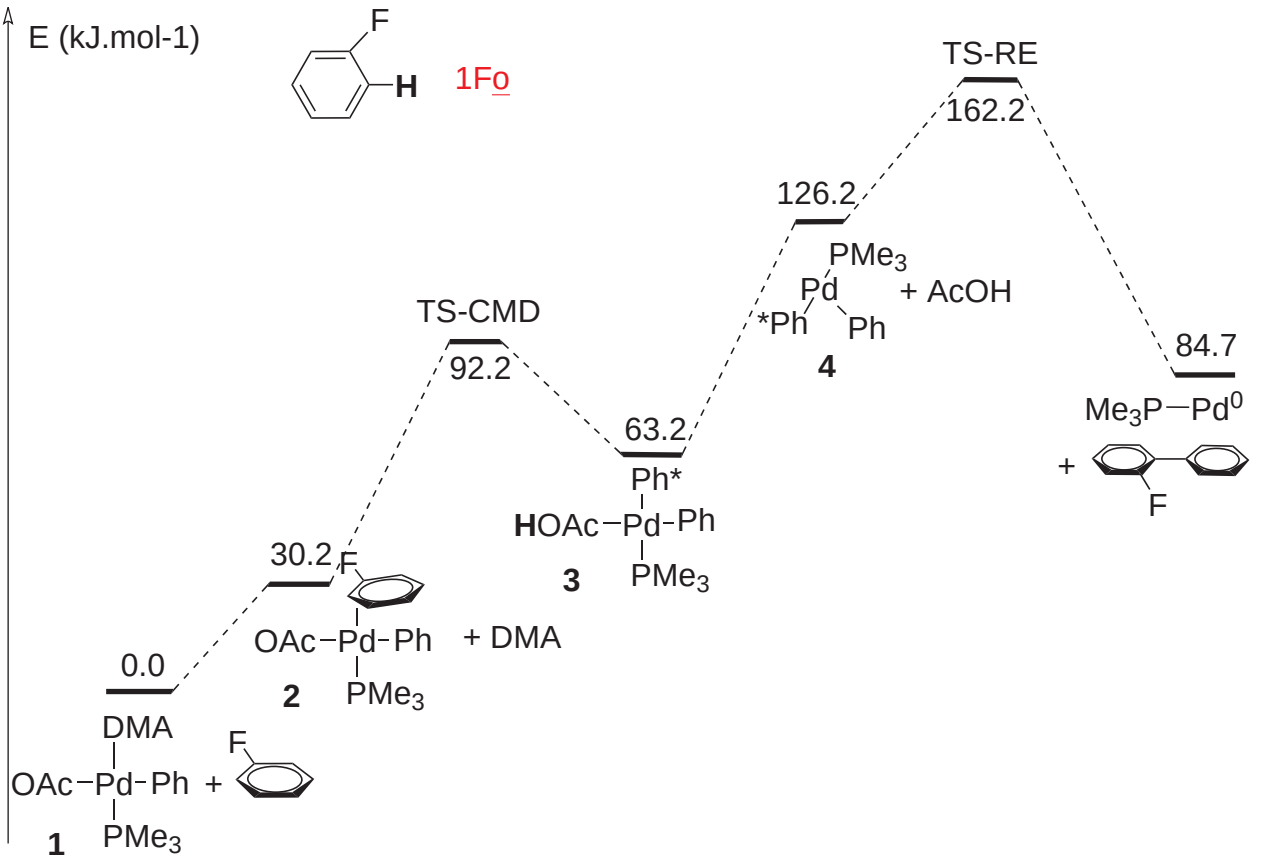



**Fig. S5.** Energy profile (E/kJ mol$^{-1}$) for reaction: above **1Fp**, below **2Fm**.



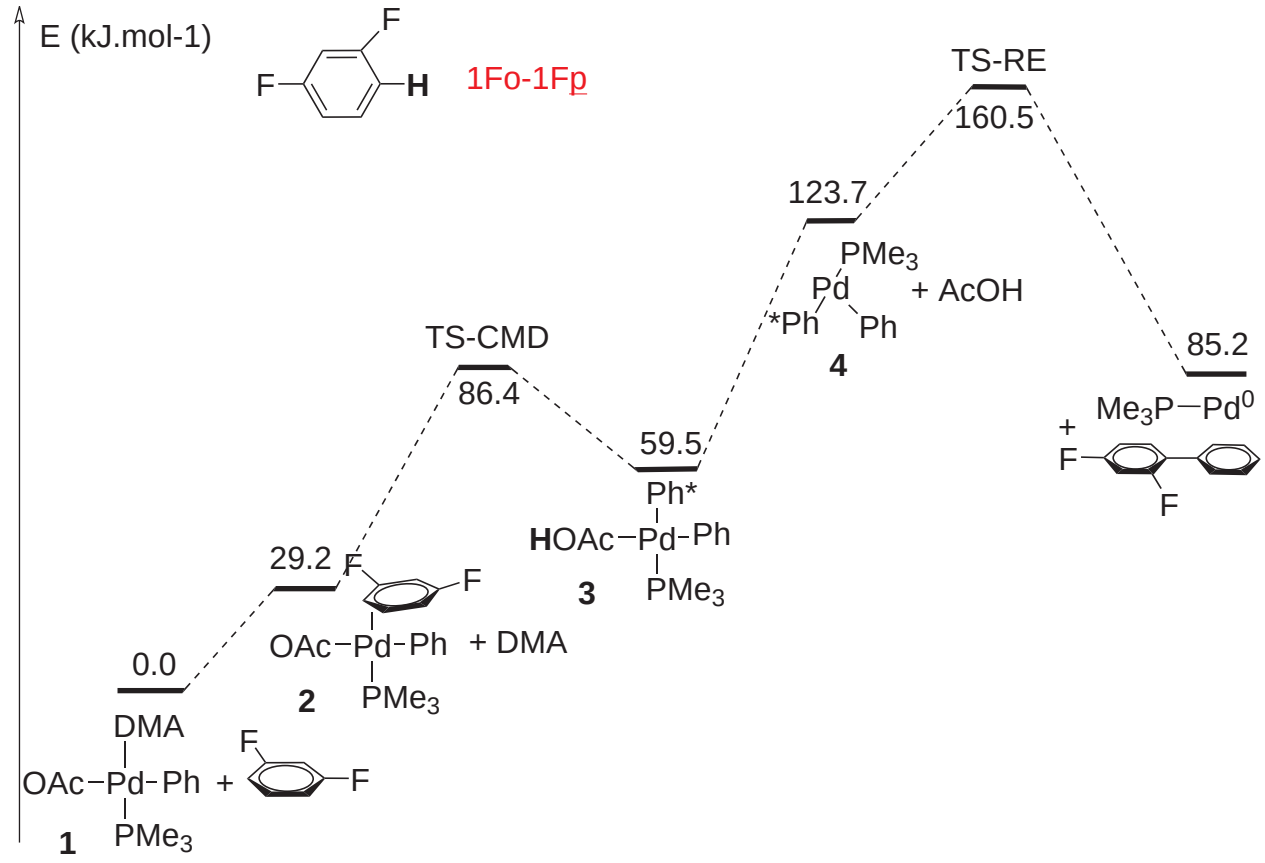




**Fig. S6.** Energy profile (E/kJ mol$^{-1}$) for reaction: above **1Fo**, below **1Fo-1Fp**.

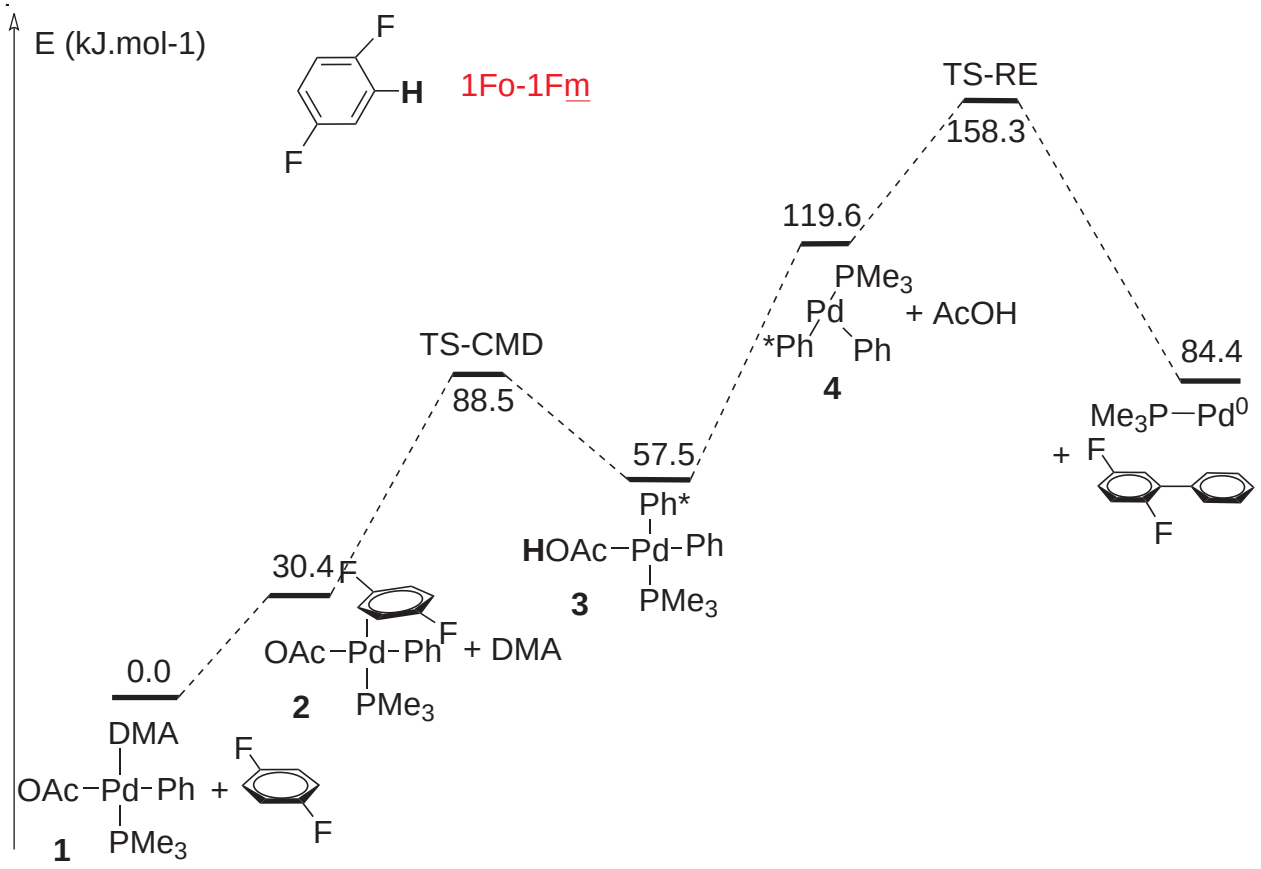
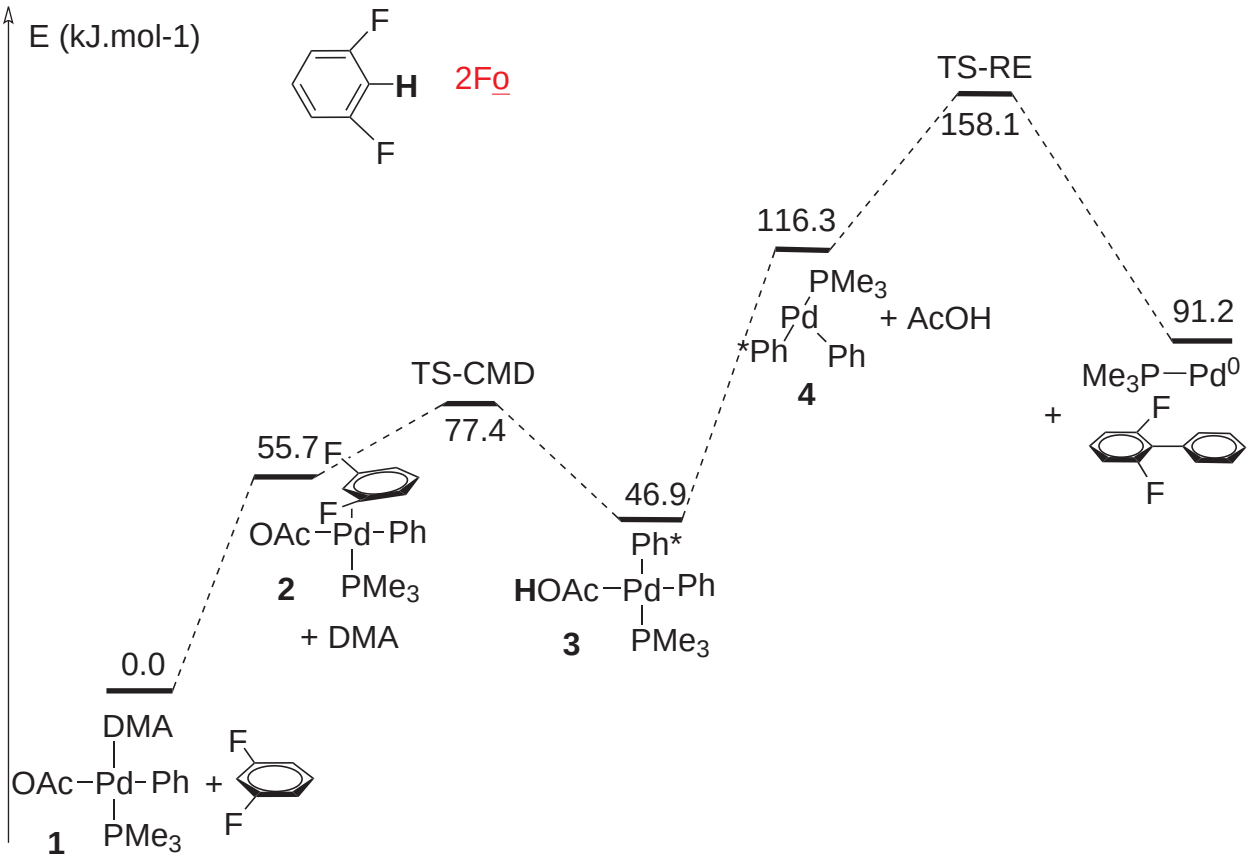



**Fig. S7.** Energy profile (E/kJ mol$^{-1}$) for reaction: above **1Fo-1Fm**.



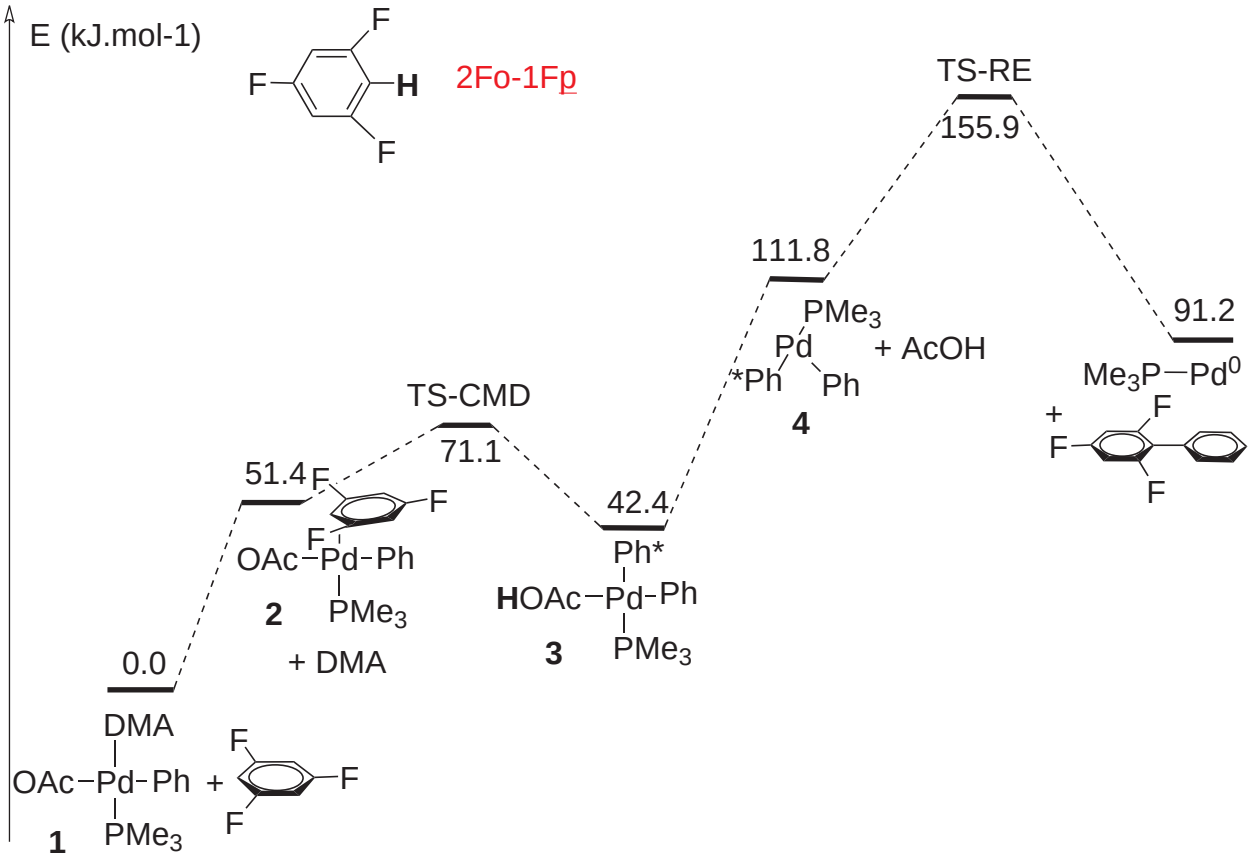
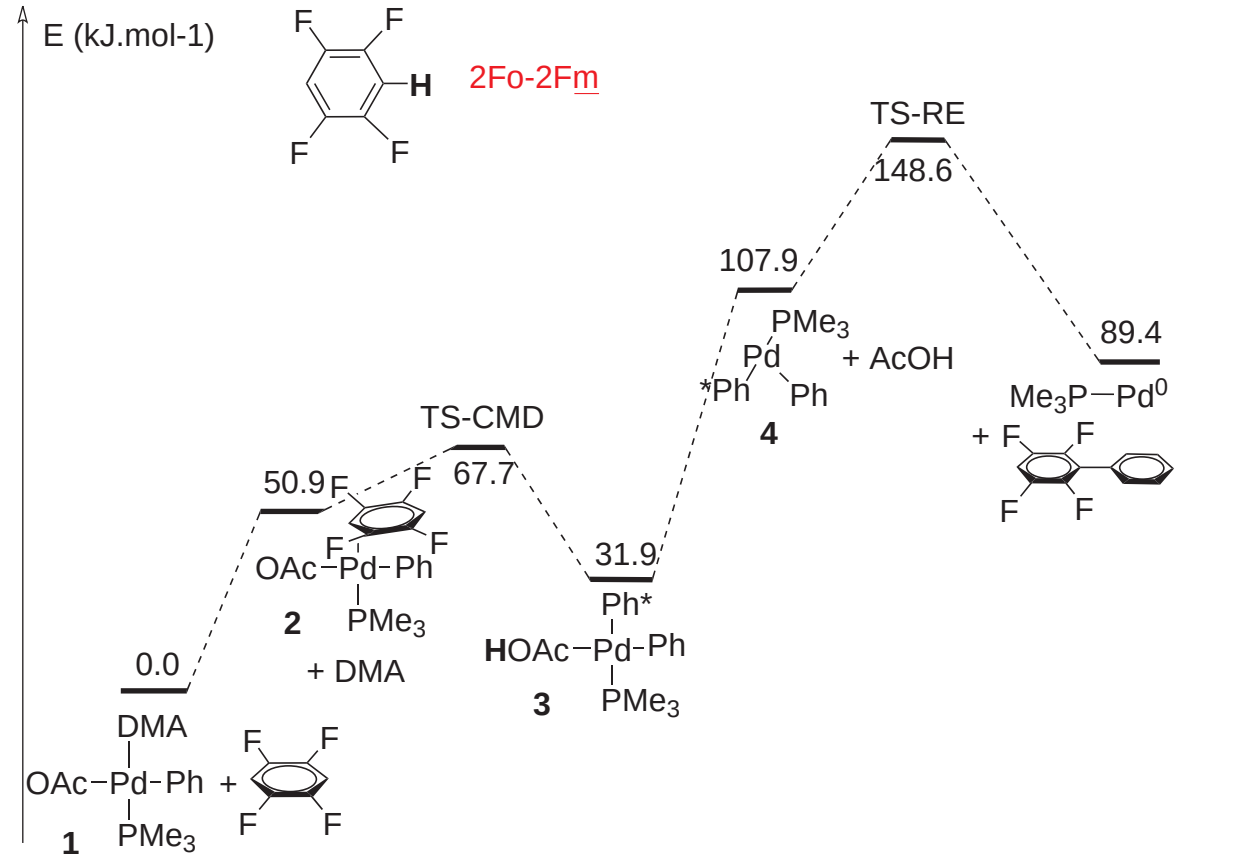




**Fig. S8.** Energy profile (E/kJ mol$^{-1}$) for reaction: above **2Fo**, below **2Fo-1Fp**.



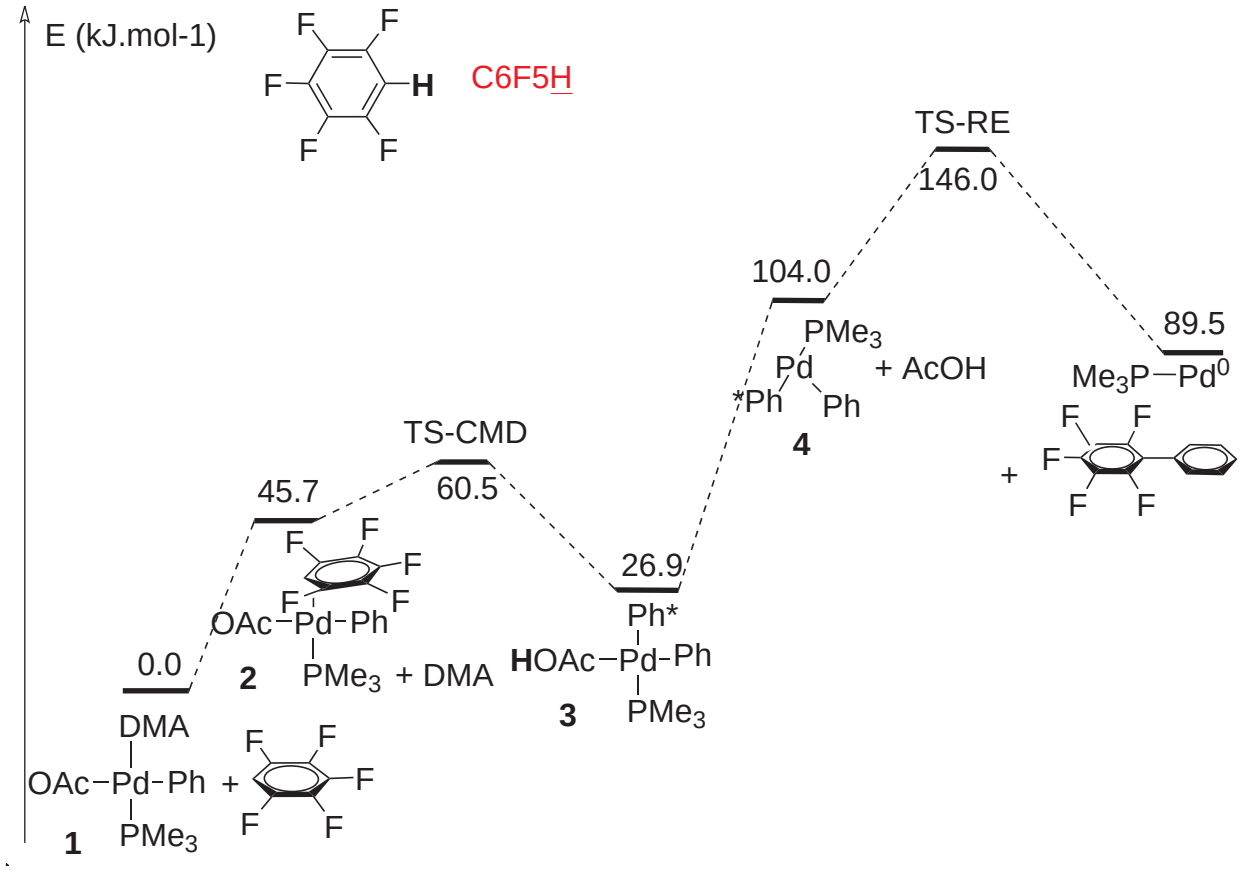




**Fig. S9.** Energy profile (E/kJ mol$^{-1}$) for reaction: above **2Fo-2Fm**, below $C_6F_5$.

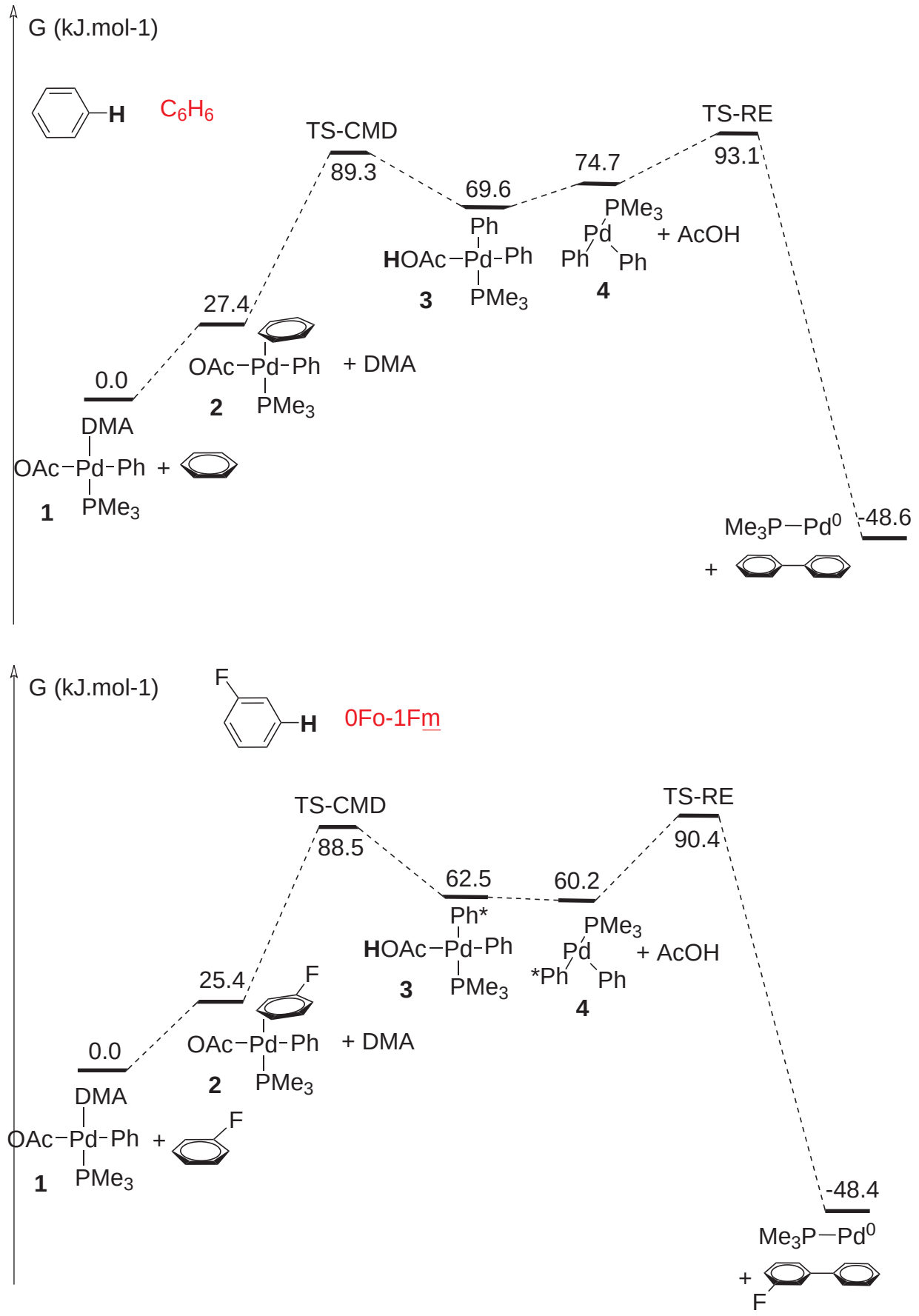



**Fig. S10.** Energy profile (G/kJ mol$^{-1}$) for reaction: above $C_6H_6$, below **1Fm**.

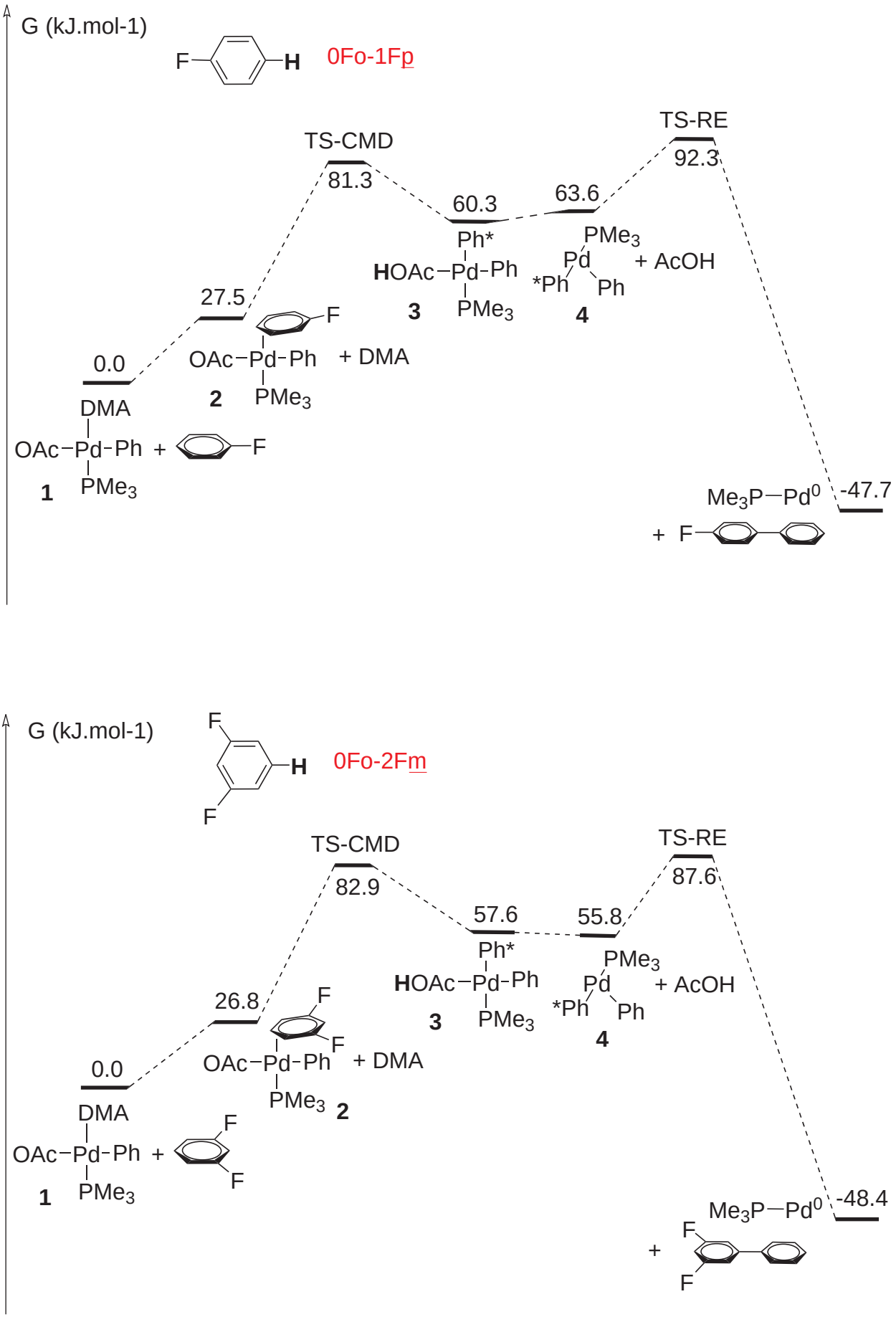
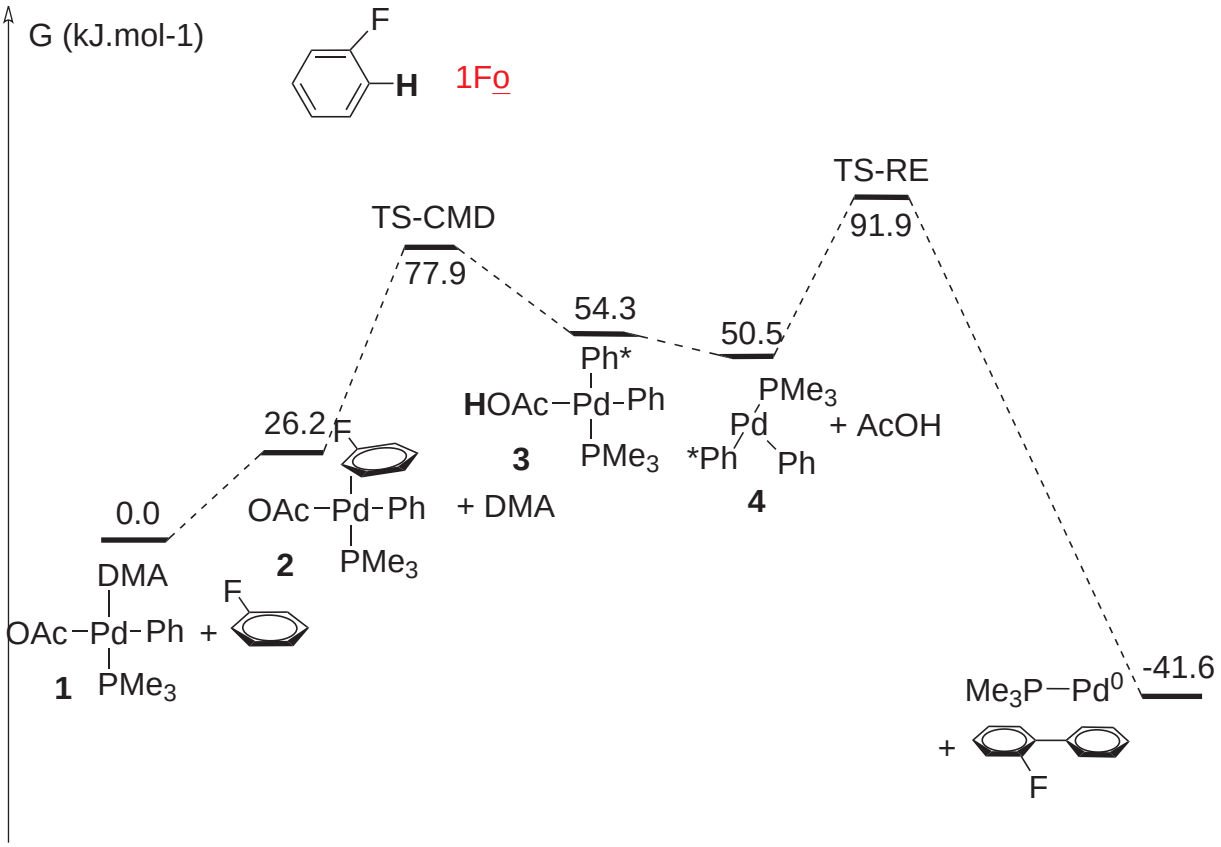



**Fig. S11.** Energy profile (G/kJ mol$^{-1}$) for reaction: above **1Fp**, below **2Fm**



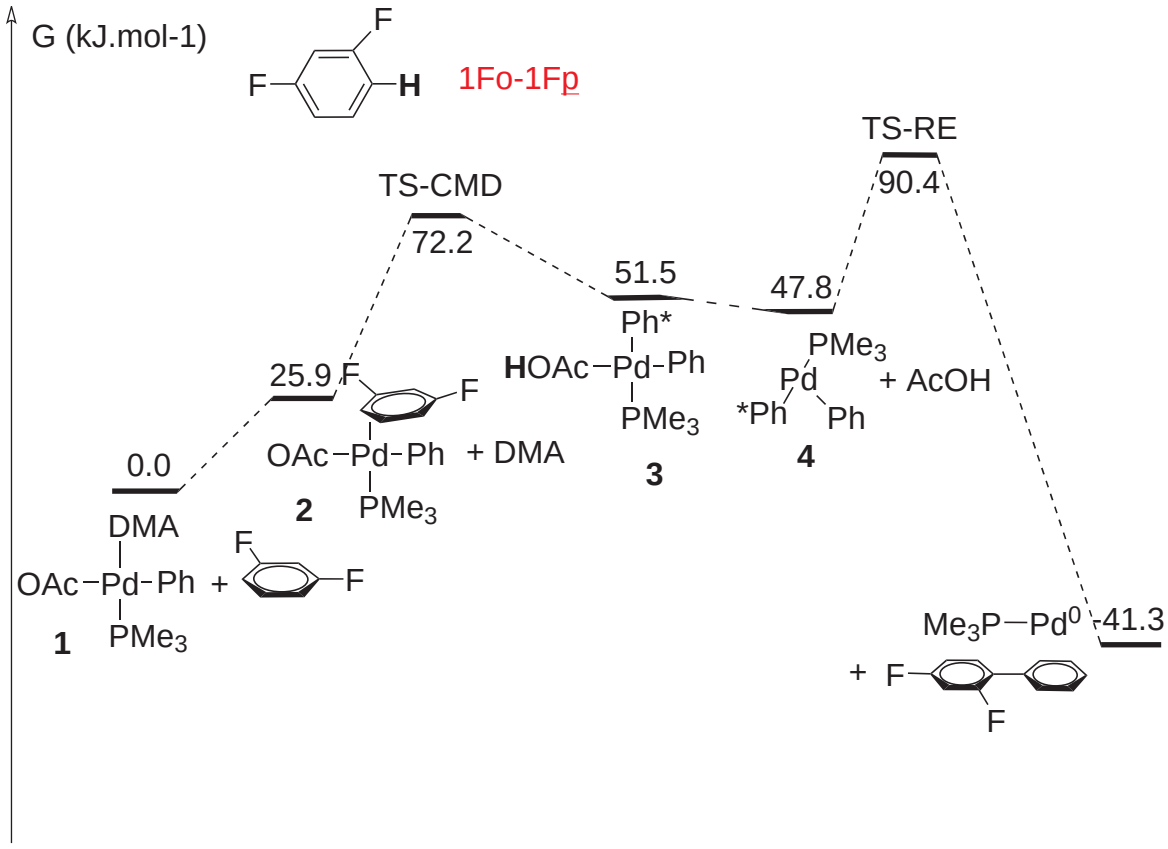




**Fig. S12.** Energy profile (G/kJ mol$^{-1}$) for reaction: above **1Fo**, below **1Fo-1Fp**

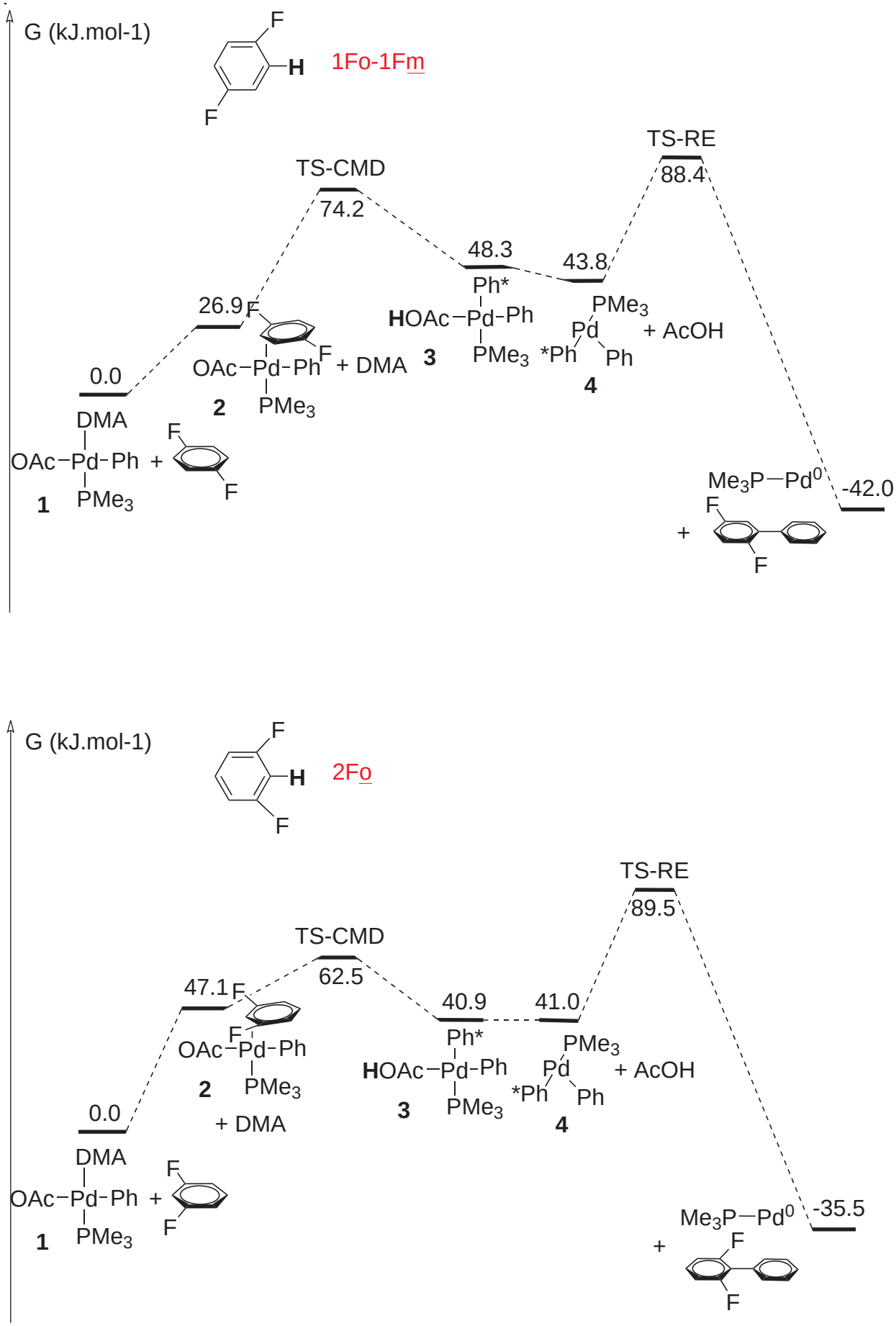



**Fig. S13.** Energy profile (G/kJ mol$^{-1}$) for reaction: above **1Fo-1Fm**, below **2Fo**

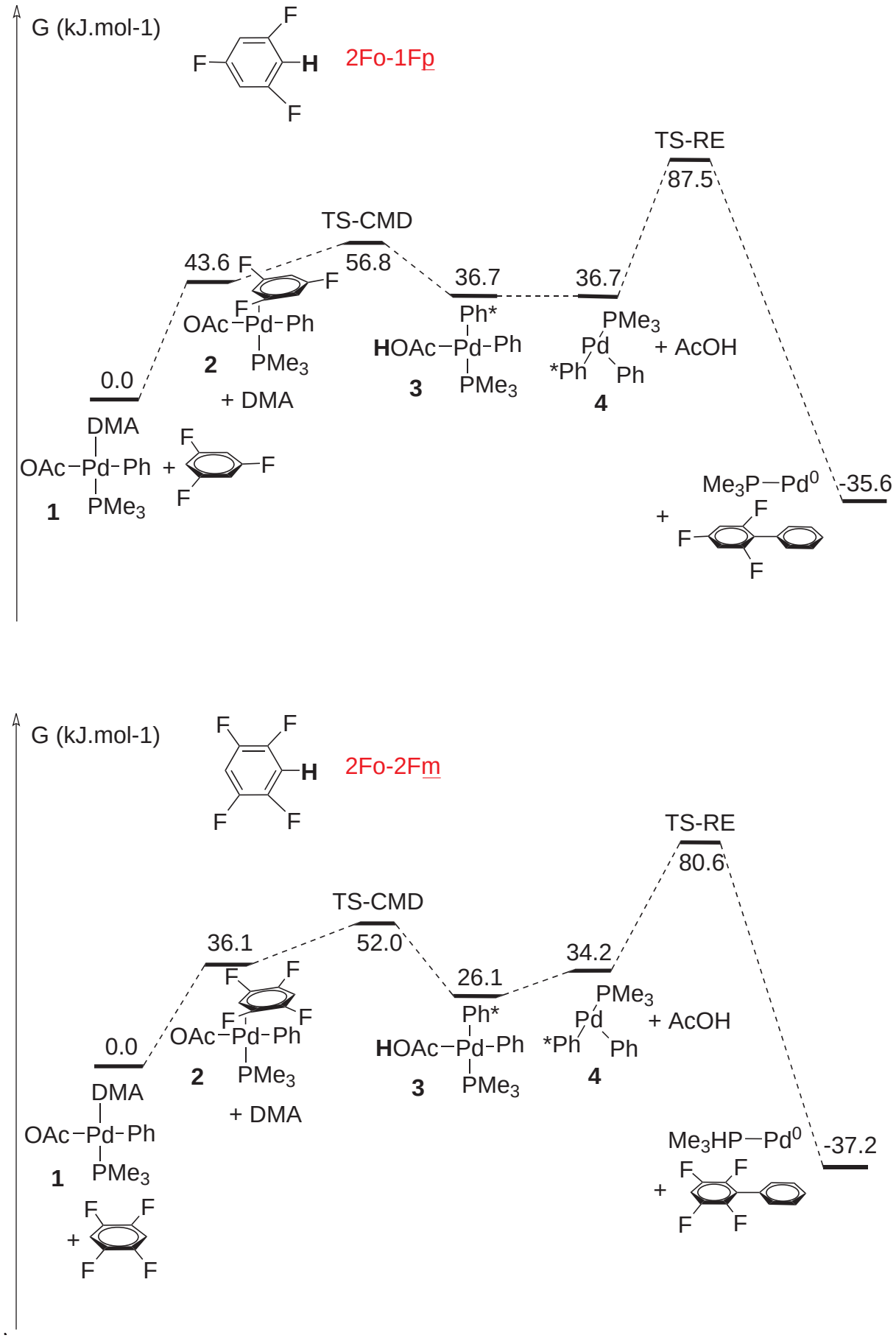



**Fig. S14.** Energy profile (G/kJ mol$^{-1}$) for reaction: above **2Fo-1Fp**, below **2Fo-2Fm**

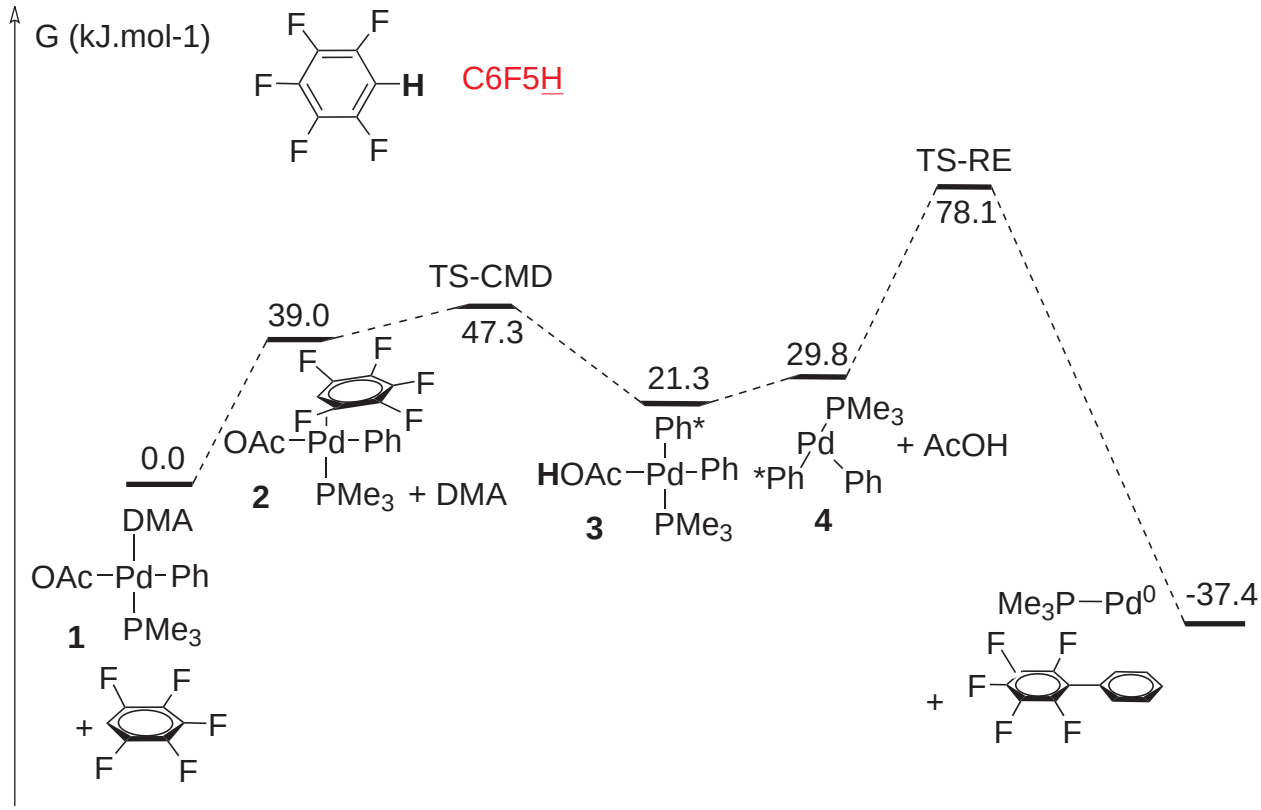



**Fig. S15.** Energy profile (G/kJ mol$^{-1}$) for reaction: $C_6F_5$

**Table S2.** Coordinates for all extrema

**1**

| | | | |
|---|---|---|---|
| C | 0.996680 | 3.649233 | -1.403655 |
| Pd | -0.510103 | 3.501370 | -0.112064 |
| C | 2.216285 | 4.205793 | -0.984828 |
| H | 2.302369 | 4.633877 | 0.011747 |
| C | 0.935678 | 3.102173 | -2.694829 |
| H | 0.009403 | 2.658983 | -3.057068 |
| C | 3.335686 | 4.205419 | -1.821302 |
| H | 4.270779 | 4.636323 | -1.469416 |
| C | 2.055254 | 3.099422 | -3.534836 |
| H | 1.982137 | 2.662638 | -4.528775 |
| C | 3.259814 | 3.653935 | -3.102178 |
| H | 4.129958 | 3.655192 | -3.753660 |
| O | -1.993532 | 3.235700 | 1.387360 |
| P | -1.458628 | 5.252096 | -1.112738 |
| C | -0.359634 | 6.606741 | -1.681679 |
| H | 0.353123 | 6.219774 | -2.413078 |
| H | -0.951564 | 7.411572 | -2.131013 |
| H | 0.205341 | 7.004177 | -0.834174 |
| C | -2.679267 | 6.126478 | -0.062287 |
| H | -3.060347 | 7.010323 | -0.585196 |
| H | -3.504622 | 5.445321 | 0.153048 |
| H | -2.213109 | 6.429303 | 0.878356 |
| C | -2.421005 | 4.808868 | -2.604496 |
| H | -3.163254 | 4.062470 | -2.309662 |
| H | -2.916883 | 5.692647 | -3.020589 |
| H | -1.753960 | 4.382468 | -3.357833 |
| C | -3.206123 | 2.951321 | 1.059465 |
| C | -4.165004 | 2.785095 | 2.232830 |
| H | -4.617747 | 3.758371 | 2.455540 |
| H | -4.971490 | 2.096489 | 1.970737 |
| H | -3.645591 | 2.448666 | 3.133381 |
| O | -3.635138 | 2.842041 | -0.103332 |
| N | -0.929351 | 0.082891 | 0.805675 |
| C | -0.061115 | 0.882378 | 1.451216 |
| C | 0.288886 | 0.597532 | 2.891515 |
| H | -0.521963 | 0.937037 | 3.545346 |
| H | 0.481678 | -0.460345 | 3.088854 |
| H | 1.179462 | 1.178979 | 3.129811 |
| C | -1.208842 | 0.313888 | -0.608023 |
| H | -1.539728 | -0.629806 | -1.050724 |
| H | -1.992675 | 1.071728 | -0.736772 |
| H | -0.298941 | 0.646348 | -1.109439 |
| C | -1.743738 | -0.931668 | 1.451757 |
| H | -2.803222 | -0.725780 | 1.262986 |
| H | -1.506752 | -1.926295 | 1.054811 |
| H | -1.587435 | -0.936876 | 2.528820 |
| O | 0.496372 | 1.848230 | 0.883534 |

**set 0Fo**

C6H6

**2**

| | | | |
|---|---|---|---|
| Pd | 0.355820 | 0.227087 | -0.755096 |
| C | 2.748527 | -0.314665 | -0.261334 |
| C | 3.222042 | 0.207311 | 0.956248 |
| C | 3.032250 | -0.498357 | 2.135890 |
| C | 2.369855 | -1.734714 | 2.119144 |
| C | 1.898687 | -2.260932 | 0.923848 |
| C | 2.081699 | -1.554578 | -0.277589 |
| H | 3.744075 | 1.159921 | 0.965604 |
| H | 3.394638 | -0.093205 | 3.076439 |
| H | 2.226391 | -2.280800 | 3.047502 |
| H | 1.397864 | -3.225114 | 0.909329 |
| H | 1.800754 | -1.995344 | -1.229894 |
| H | 2.989162 | 0.178488 | -1.198836 |
| P | -1.565999 | 1.252917 | -1.364592 |
| C | -1.390043 | 3.062789 | -1.549318 |
| H | -2.329495 | 3.501406 | -1.903069 |
| H | -1.125681 | 3.506014 | -0.585884 |
| H | -0.590704 | 3.241755 | -2.272120 |
| C | -2.211188 | 0.689278 | -2.983135 |
| H | -3.182628 | 1.156959 | -3.177228 |
| H | -1.499988 | 0.978416 | -3.758257 |
| H | -2.324381 | -0.397566 | -2.982697 |
| C | -3.025180 | 1.062624 | -0.267720 |
| H | -3.889873 | 1.563910 | -0.716185 |
| H | -3.255561 | 0.002331 | -0.134180 |
| H | -2.818571 | 1.493607 | 0.713688 |
| C | 1.127099 | 0.558126 | -3.635645 |
| O | 0.771527 | 1.743935 | -3.558028 |
| O | 0.981500 | -0.327639 | -2.704624 |
| C | 1.795700 | 0.032801 | -4.897773 |
| H | 1.331359 | -0.905764 | -5.214250 |
| H | 1.737503 | 0.772651 | -5.697704 |
| H | 2.848967 | -0.183676 | -4.688086 |
| C | -0.140726 | 0.687344 | 1.121790 |
| C | -0.792883 | -0.234566 | 1.955557 |
| C | 0.212373 | 1.930925 | 1.669348 |
| C | -1.066260 | 0.067802 | 3.292955 |
| H | -1.092106 | -1.204124 | 1.563807 |
| C | -0.059245 | 2.236594 | 3.007007 |
| H | 0.718439 | 2.671363 | 1.052855 |
| C | -0.701814 | 1.305874 | 3.824772 |
| H | -1.570075 | -0.666336 | 3.918393 |
| H | 0.231382 | 3.205488 | 3.407615 |
| H | -0.919379 | 1.543751 | 4.862819 |

TS-CMD

| | | | |
|---|---|---|---|
| Pd | 0.181027 | 0.497798 | -0.784736 |
| C | 1.985756 | -0.520503 | -0.067822 |
| C | 2.770785 | -0.030186 | 0.995337 |
| C | 3.393778 | -0.885243 | 1.902364 |
| C | 3.233636 | -2.267596 | 1.778947 |
| C | 2.466804 | -2.788154 | 0.734458 |
| C | 1.864719 | -1.922593 | -0.179211 |
| H | 2.896142 | 1.043843 | 1.112910 |
| H | 3.997308 | -0.478366 | 2.710294 |
| H | 3.711412 | -2.937016 | 2.490317 |
| H | 2.349195 | -3.864269 | 0.628787 |
| H | 1.296502 | -2.345323 | -1.006800 |
| H | 2.308601 | 0.091915 | -1.287798 |
| P | -1.831235 | 1.421115 | -1.390286 |
| C | -1.679837 | 3.151694 | -1.989467 |
| H | -2.646446 | 3.539555 | -2.329014 |
| H | -1.303406 | 3.784152 | -1.180895 |
| H | -0.965323 | 3.185380 | -2.816135 |
| C | -2.606462 | 0.551270 | -2.809376 |
| H | -3.497187 | 1.082928 | -3.161065 |
| H | -1.873984 | 0.470550 | -3.615826 |
| H | -2.889114 | -0.460067 | -2.503958 |
| C | -3.187679 | 1.522970 | -0.162836 |
| H | -4.078332 | 1.977159 | -0.609912 |
| H | -3.431618 | 0.520076 | 0.196862 |
| H | -2.861887 | 2.114260 | 0.696270 |
| C | 1.823165 | 0.284903 | -3.241822 |
| O | 2.783183 | 0.360086 | -2.404261 |
| O | 0.610124 | 0.202735 | -2.905702 |
| C | 2.189403 | 0.285057 | -4.704017 |
| H | 1.296408 | 0.292313 | -5.329561 |
| H | 2.813041 | 1.155808 | -4.925105 |
| H | 2.787419 | -0.604586 | -4.923795 |
| C | -0.235998 | 0.897821 | 1.118844 |
| C | -0.795375 | -0.066672 | 1.970421 |
| C | 0.021653 | 2.172726 | 1.647430 |
| C | -1.089852 | 0.234305 | 3.303335 |
| H | -0.988566 | -1.071030 | 1.600859 |
| C | -0.270643 | 2.474800 | 2.981919 |
| H | 0.466367 | 2.943021 | 1.019705 |
| C | -0.831971 | 1.507059 | 3.815868 |
| H | -1.516450 | -0.533876 | 3.945019 |
| H | -0.055570 | 3.469205 | 3.367838 |
| H | -1.059565 | 1.739164 | 4.853045 |

**3**

| | | | |
|---|---|---|---|
| Pd | 0.189153 | 0.579406 | -0.569103 |
| C | 1.833606 | -0.355809 | 0.227712 |
| C | 3.114098 | 0.176633 | -0.035530 |
| C | 4.276428 | -0.408602 | 0.472578 |
| C | 4.196185 | -1.559915 | 1.259190 |

| | | | |
|---|---|---|---|
| C | 2.945370 | -2.110930 | 1.535683 |
| C | 1.785476 | -1.509470 | 1.034417 |
| H | 5.246114 | 0.034332 | 0.254108 |
| H | 5.098924 | -2.019385 | 1.654048 |
| H | 2.867877 | -3.004098 | 2.152127 |
| H | 1.642359 | -1.558675 | -1.382371 |
| P | -1.677741 | 1.760957 | -1.414338 |
| C | -2.749824 | 2.670384 | -0.235513 |
| H | -3.571909 | 3.174097 | -0.754679 |
| H | -3.151907 | 1.972678 | 0.503591 |
| H | -2.149725 | 3.406617 | 0.305450 |
| C | -1.230437 | 3.057606 | -2.642652 |
| H | -2.118587 | 3.530972 | -3.075461 |
| H | -0.619965 | 3.822667 | -2.154387 |
| H | -0.633559 | 2.603414 | -3.438140 |
| C | -2.891985 | 0.738714 | -2.351658 |
| H | -3.702977 | 1.350540 | -2.762439 |
| H | -2.378123 | 0.228101 | -3.170607 |
| H | -3.318188 | -0.020182 | -1.689245 |
| C | 1.217549 | -0.942602 | -3.118143 |
| O | 1.679975 | -1.882949 | -2.321961 |
| O | 0.704463 | 0.105261 | -2.717777 |
| C | 1.376157 | -1.259226 | -4.575249 |
| H | 2.441956 | -1.300601 | -4.820567 |
| H | 0.955297 | -2.245423 | -4.790039 |
| H | 0.887857 | -0.497044 | -5.181206 |
| C | -0.300154 | 0.982358 | 1.311008 |
| C | -1.218890 | 0.177687 | 2.004275 |
| C | 0.218758 | 2.104585 | 1.976364 |
| C | -1.617531 | 0.491676 | 3.307773 |
| H | -1.631514 | -0.710745 | 1.529688 |
| C | -0.179870 | 2.420797 | 3.278489 |
| H | 0.954748 | 2.735021 | 1.482930 |
| C | -1.102899 | 1.618031 | 3.951029 |
| H | -2.330234 | -0.150777 | 3.821238 |
| H | 0.242139 | 3.294297 | 3.771469 |
| H | -1.409307 | 1.861567 | 4.965095 |
| H | 3.209392 | 1.069906 | -0.651469 |
| H | 0.821515 | -1.943929 | 1.291930 |

**4**

| | | | |
|---|---|---|---|
| C | 2.933767 | -0.626195 | -0.358659 |
| Pd | 0.999381 | -0.295446 | -0.756644 |
| C | 3.903728 | 0.346474 | -0.657208 |
| H | 3.648613 | 1.192682 | -1.292457 |
| C | 3.327332 | -1.725551 | 0.424138 |
| H | 2.615890 | -2.518914 | 0.645816 |
| C | 5.203083 | 0.252036 | -0.150646 |
| H | 5.933815 | 1.022429 | -0.388083 |
| C | 4.625626 | -1.823969 | 0.932558 |
| H | 4.903975 | -2.679817 | 1.544014 |

| | | | |
|---|---|---|---|
| C | 5.567226 | -0.833404 | 0.648178 |
| H | 6.579671 | -0.912344 | 1.036402 |
| P | -1.316730 | 0.171601 | -1.104152 |
| C | -2.499788 | -0.630370 | 0.061511 |
| H | -2.278589 | -0.319766 | 1.086831 |
| H | -3.536862 | -0.367607 | -0.174763 |
| H | -2.385097 | -1.716560 | 0.005480 |
| C | -1.980433 | -0.330892 | -2.741432 |
| H | -3.048087 | -0.102294 | -2.825720 |
| H | -1.430500 | 0.186758 | -3.531751 |
| H | -1.821412 | -1.403212 | -2.882118 |
| C | -1.821292 | 1.942929 | -0.999538 |
| H | -1.261200 | 2.524427 | -1.737333 |
| H | -2.893773 | 2.068723 | -1.185212 |
| H | -1.584269 | 2.338604 | -0.007434 |
| C | 1.333068 | -1.280523 | -2.445972 |
| C | 1.702141 | -0.591453 | -3.608172 |
| C | 1.100307 | -2.659868 | -2.520213 |
| C | 1.799876 | -1.265523 | -4.829716 |
| H | 1.921316 | 0.472378 | -3.570018 |
| C | 1.199082 | -3.329252 | -3.744371 |
| H | 0.846775 | -3.223519 | -1.626159 |
| C | 1.544723 | -2.635423 | -4.904719 |
| H | 2.086486 | -0.714426 | -5.722845 |
| H | 1.013496 | -4.400483 | -3.784137 |
| H | 1.626163 | -3.158461 | -5.853858 |

TS-RE

| | | | |
|---|---|---|---|
| C | 3.305165 | -1.098893 | -0.479884 |
| Pd | 1.407576 | -0.587083 | -0.016024 |
| C | 4.289960 | -0.097385 | -0.450022 |
| H | 4.025765 | 0.933219 | -0.673831 |
| C | 3.694652 | -2.426441 | -0.233599 |
| H | 2.961670 | -3.227866 | -0.286160 |
| C | 5.614509 | -0.407615 | -0.136944 |
| H | 6.360689 | 0.383149 | -0.108198 |
| C | 5.019233 | -2.735611 | 0.080044 |
| H | 5.298981 | -3.767578 | 0.279405 |
| C | 5.983968 | -1.727406 | 0.129933 |
| H | 7.017291 | -1.969906 | 0.363766 |
| P | -0.782230 | 0.004157 | 0.591746 |
| C | -1.007911 | 1.305270 | 1.882258 |
| H | -0.507185 | 2.224515 | 1.565364 |
| H | -2.068549 | 1.517784 | 2.057948 |
| H | -0.550341 | 0.978165 | 2.820527 |
| C | -1.866397 | -1.343022 | 1.234895 |
| H | -2.877605 | -0.979079 | 1.449119 |
| H | -1.924007 | -2.146244 | 0.495090 |
| H | -1.434315 | -1.757516 | 2.150251 |
| C | -1.790264 | 0.670905 | -0.796944 |
| H | -1.834844 | -0.071747 | -1.597988 |

| | | | |
|---|---|---|---|
| H | -2.806679 | 0.921963 | -0.473454 |
| H | -1.305222 | 1.564459 | -1.198961 |
| C | 1.826280 | -0.850627 | -1.986197 |
| C | 2.013084 | 0.285605 | -2.790462 |
| C | 1.458640 | -2.053723 | -2.610459 |
| C | 1.799713 | 0.228204 | -4.169029 |
| H | 2.324863 | 1.225288 | -2.342550 |
| C | 1.245886 | -2.107428 | -3.989304 |
| H | 1.337203 | -2.958796 | -2.021508 |
| C | 1.413455 | -0.967416 | -4.777410 |
| H | 1.942910 | 1.123939 | -4.769433 |
| H | 0.954598 | -3.049604 | -4.448387 |
| H | 1.256109 | -1.012761 | -5.851649 |

Ph*-Ph

| | | | |
|---|---|---|---|
| C | 3.367429 | -1.141178 | -1.541189 |
| C | 4.154194 | -0.011103 | -1.267209 |
| C | 3.230965 | -2.114301 | -0.538694 |
| C | 4.783022 | 0.140833 | -0.032577 |
| C | 3.860737 | -1.963931 | 0.695802 |
| C | 4.639642 | -0.835420 | 0.954667 |
| C | 2.698589 | -1.303914 | -2.854577 |
| C | 2.083025 | -0.214375 | -3.490792 |
| C | 2.663196 | -2.553109 | -3.494271 |
| C | 1.454017 | -0.368350 | -4.725154 |
| H | 2.075787 | 0.755642 | -3.000477 |
| C | 2.033146 | -2.708405 | -4.727846 |
| H | 3.156077 | -3.403957 | -3.031069 |
| C | 1.425719 | -1.616304 | -5.349215 |
| H | 0.976060 | 0.486902 | -5.195728 |
| H | 2.025257 | -3.682895 | -5.209096 |
| H | 0.934764 | -1.736523 | -6.311057 |
| H | 5.130281 | -0.717200 | 1.916981 |
| H | 5.394733 | 1.019454 | 0.155279 |
| H | 4.294152 | 0.741436 | -2.038959 |
| H | 3.734174 | -2.725940 | 1.460515 |
| H | 2.604574 | -2.983833 | -0.720370 |

<u>0Fo-1Fm</u>

**2**

| | | | |
|---|---|---|---|
| Pd | 0.518280 | 0.523018 | -0.754103 |
| C | 2.116459 | -1.390403 | -0.294212 |
| C | 2.840881 | -0.182571 | -0.257559 |
| C | 3.314652 | 0.258764 | 0.983081 |
| C | 3.090981 | -0.434165 | 2.156701 |
| C | 2.362377 | -1.629571 | 2.098863 |
| C | 1.877645 | -2.108528 | 0.888366 |
| H | 3.473481 | -0.045647 | 3.094487 |

| | | | |
|---|---|---|---|
| H | 2.175906 | -2.179627 | 3.016583 |
| H | 1.322593 | -3.040579 | 0.849628 |
| H | 1.825958 | -1.802160 | -1.255671 |
| P | -1.329319 | 1.669219 | -1.371937 |
| C | -1.848449 | 3.083870 | -0.326992 |
| H | -2.724572 | 3.570841 | -0.768758 |
| H | -2.088550 | 2.735977 | 0.679526 |
| H | -1.034499 | 3.810053 | -0.252501 |
| C | -1.184328 | 2.416068 | -3.037087 |
| H | -2.060987 | 3.039817 | -3.242634 |
| H | -0.279028 | 3.024689 | -3.096469 |
| H | -1.123368 | 1.611908 | -3.772332 |
| C | -2.821462 | 0.618722 | -1.477929 |
| H | -3.675210 | 1.204962 | -1.834898 |
| H | -2.602864 | -0.195626 | -2.173056 |
| H | -3.051799 | 0.208851 | -0.491469 |
| C | 0.609572 | -0.405912 | -3.581424 |
| O | -0.562390 | -0.782193 | -3.429947 |
| O | 1.297502 | 0.252791 | -2.705358 |
| C | 1.361900 | -0.713478 | -4.867446 |
| H | 2.110188 | -1.489444 | -4.671126 |
| H | 0.674784 | -1.073211 | -5.635054 |
| H | 1.899908 | 0.170732 | -5.220721 |
| C | -0.099680 | 0.767611 | 1.127410 |
| C | -0.977342 | -0.152638 | 1.721896 |
| C | 0.384030 | 1.820671 | 1.920387 |
| C | -1.343179 | -0.037461 | 3.067332 |
| H | -1.376464 | -0.979237 | 1.137123 |
| C | 0.021929 | 1.936922 | 3.265705 |
| H | 1.055526 | 2.561906 | 1.491678 |
| C | -0.845169 | 1.008602 | 3.845123 |
| H | -2.020952 | -0.767377 | 3.505079 |
| H | 0.417052 | 2.758442 | 3.859584 |
| H | -1.132072 | 1.101996 | 4.889335 |
| F | 4.030603 | 1.402562 | 1.023935 |
| H | 3.134170 | 0.323836 | -1.172435 |

TS-CMD

| | | | |
|---|---|---|---|
| Pd | 0.182716 | 0.485791 | -0.817517 |
| C | 1.931709 | -0.632258 | -0.073741 |
| C | 3.095605 | 0.162893 | -0.137509 |
| C | 4.078593 | 0.031520 | 0.831292 |
| C | 3.984107 | -0.884855 | 1.870132 |
| C | 2.848849 | -1.696271 | 1.930748 |
| C | 1.840236 | -1.565395 | 0.978127 |
| H | 4.783682 | -0.958368 | 2.600565 |
| H | 2.756319 | -2.425482 | 2.731594 |
| H | 0.961393 | -2.200680 | 1.051116 |
| H | 1.572924 | -1.183810 | -1.300492 |
| P | -1.584067 | 1.826412 | -1.394276 |
| C | -2.111303 | 3.141314 | -0.231878 |

| | | | |
|---|---|---|---|
| H | -2.946538 | 3.711748 | -0.651885 |
| H | -2.409182 | 2.694254 | 0.719346 |
| H | -1.273123 | 3.815805 | -0.038067 |
| C | -1.308641 | 2.736521 | -2.963666 |
| H | -2.211453 | 3.276185 | -3.268656 |
| H | -0.490333 | 3.449328 | -2.829876 |
| H | -1.012332 | 2.027561 | -3.739610 |
| C | -3.138197 | 0.898322 | -1.706893 |
| H | -3.941096 | 1.571648 | -2.026146 |
| H | -2.964070 | 0.149211 | -2.483789 |
| H | -3.444006 | 0.384855 | -0.791500 |
| C | 1.193754 | -0.850652 | -3.263083 |
| O | 1.587493 | -1.728083 | -2.424887 |
| O | 0.665237 | 0.245326 | -2.928034 |
| C | 1.396111 | -1.158225 | -4.724620 |
| H | 2.469390 | -1.192675 | -4.936083 |
| H | 0.989728 | -2.147395 | -4.952183 |
| H | 0.924305 | -0.400975 | -5.351326 |
| C | -0.370226 | 0.682217 | 1.085049 |
| C | -1.382888 | -0.129023 | 1.620517 |
| C | 0.237490 | 1.622710 | 1.930372 |
| C | -1.775983 | -0.005053 | 2.957634 |
| H | -1.866420 | -0.879439 | 0.997709 |
| C | -0.155161 | 1.748510 | 3.265762 |
| H | 1.038064 | 2.254695 | 1.553241 |
| C | -1.165943 | 0.937568 | 3.785785 |
| H | -2.559277 | -0.650188 | 3.350219 |
| H | 0.337043 | 2.480176 | 3.902950 |
| H | -1.469135 | 1.035039 | 4.824952 |
| F | 5.183162 | 0.819718 | 0.760842 |
| H | 3.248740 | 0.877350 | -0.942840 |

**3**

| | | | |
|---|---|---|---|
| Pd | 0.208588 | 0.159049 | 0.023828 |
| C | 0.332051 | 0.294880 | 2.071237 |
| C | 1.412391 | -0.357539 | 2.701992 |
| C | 1.558897 | -0.292396 | 4.080773 |
| C | 0.669225 | 0.387501 | 4.901910 |
| C | -0.405776 | 1.032781 | 4.291154 |
| C | -0.565236 | 0.994152 | 2.901774 |
| H | -1.118956 | 1.578876 | 4.904393 |
| H | -1.396312 | 1.537100 | 2.458067 |
| H | -1.046166 | -1.215305 | 1.937376 |
| P | 0.244446 | 0.160838 | -2.338821 |
| C | 1.756197 | 0.913525 | -3.064387 |
| H | 1.717913 | 0.909866 | -4.159072 |
| H | 1.849751 | 1.941458 | -2.704084 |
| H | 2.637230 | 0.355817 | -2.733866 |
| C | 0.180357 | -1.481128 | -3.169682 |
| H | 0.258770 | -1.379630 | -4.257417 |
| H | 0.997578 | -2.107833 | -2.803119 |

| | | | |
|---|---|---|---|
| H | -0.760317 | -1.979807 | -2.921473 |
| C | -1.100153 | 1.085873 | -3.185671 |
| H | -0.964097 | 1.078361 | -4.272516 |
| H | -2.067000 | 0.635573 | -2.942690 |
| H | -1.103334 | 2.118562 | -2.826868 |
| C | -0.740184 | -2.701378 | 0.818998 |
| O | -1.358442 | -2.153083 | 1.845375 |
| O | -0.026178 | -2.071862 | 0.034983 |
| C | -0.978529 | -4.175363 | 0.691112 |
| H | -0.514708 | -4.687372 | 1.540177 |
| H | -2.050728 | -4.385840 | 0.730990 |
| H | -0.550525 | -4.545892 | -0.239437 |
| C | 0.371957 | 2.139043 | 0.023022 |
| C | -0.768567 | 2.952787 | -0.078003 |
| C | 1.622223 | 2.773800 | 0.102916 |
| C | -0.663604 | 4.347298 | -0.112312 |
| H | -1.757584 | 2.500673 | -0.125753 |
| C | 1.729058 | 4.167193 | 0.066835 |
| H | 2.526056 | 2.179214 | 0.211910 |
| C | 0.586967 | 4.962270 | -0.043556 |
| H | -1.564955 | 4.952164 | -0.188960 |
| H | 2.710596 | 4.631509 | 0.136619 |
| H | 0.670130 | 6.045754 | -0.066382 |
| F | 2.616212 | -0.925681 | 4.656159 |
| H | 2.149715 | -0.919130 | 2.133126 |
| H | 0.823101 | 0.406823 | 5.975962 |

**4**

| | | | |
|---|---|---|---|
| C | 3.547291 | -0.964753 | -0.107027 |
| Pd | 1.611466 | -0.471163 | 0.098210 |
| C | 4.506973 | 0.056349 | -0.222283 |
| C | 4.003515 | -2.285167 | 0.054091 |
| H | 3.289844 | -3.103500 | 0.112448 |
| C | 5.857343 | -0.258127 | -0.133951 |
| C | 5.367659 | -2.573550 | 0.139612 |
| H | 5.699109 | -3.600884 | 0.272402 |
| C | 6.317813 | -1.554576 | 0.046732 |
| H | 7.383633 | -1.750974 | 0.102117 |
| P | -0.664194 | 0.146569 | 0.417137 |
| C | -1.165853 | 0.738042 | 2.091237 |
| H | -0.578879 | 1.620337 | 2.362908 |
| H | -2.229820 | 0.996985 | 2.121646 |
| H | -0.970391 | -0.041998 | 2.832991 |
| C | -1.885937 | -1.187111 | 0.086080 |
| H | -2.914126 | -0.823968 | 0.189056 |
| H | -1.734272 | -1.564062 | -0.929180 |
| H | -1.724965 | -2.013950 | 0.783693 |
| C | -1.250112 | 1.503766 | -0.675859 |
| H | -1.076164 | 1.221303 | -1.717817 |
| H | -2.315616 | 1.708923 | -0.526889 |
| H | -0.676894 | 2.412431 | -0.470922 |

| | | | |
|---|---|---|---|
| C | 1.416972 | -0.916819 | -1.822570 |
| C | 1.597993 | 0.065973 | -2.804127 |
| C | 1.012631 | -2.200484 | -2.210990 |
| C | 1.343019 | -0.223800 | -4.148460 |
| H | 1.946913 | 1.058177 | -2.531416 |
| C | 0.759628 | -2.484008 | -3.557217 |
| H | 0.898298 | -2.989343 | -1.472056 |
| C | 0.919062 | -1.497139 | -4.530561 |
| H | 1.489005 | 0.550690 | -4.898198 |
| H | 0.445536 | -3.485803 | -3.842045 |
| H | 0.727451 | -1.721330 | -5.576471 |
| H | 4.226826 | 1.094540 | -0.380456 |
| F | 6.768873 | 0.745816 | -0.236133 |

TS-RE

| | | | |
|---|---|---|---|
| C | 3.300048 | -1.102129 | -0.486866 |
| Pd | 1.403785 | -0.590647 | -0.016794 |
| C | 4.274372 | -0.090501 | -0.449235 |
| C | 3.696043 | -2.429303 | -0.243863 |
| H | 2.968186 | -3.233923 | -0.300145 |
| C | 5.584407 | -0.424553 | -0.137289 |
| C | 5.021880 | -2.731745 | 0.068636 |
| H | 5.309798 | -3.761530 | 0.265247 |
| C | 5.989297 | -1.726597 | 0.124772 |
| H | 7.028708 | -1.937607 | 0.353036 |
| P | -0.786863 | 0.004584 | 0.591590 |
| C | -1.004943 | 1.305340 | 1.882937 |
| H | -0.501997 | 2.223203 | 1.565671 |
| H | -2.064592 | 1.520903 | 2.060547 |
| H | -0.546817 | 0.976244 | 2.820202 |
| C | -1.871907 | -1.341253 | 1.234923 |
| H | -2.882012 | -0.975346 | 1.450698 |
| H | -1.932226 | -2.143876 | 0.494704 |
| H | -1.439538 | -1.757017 | 2.149541 |
| C | -1.792664 | 0.674285 | -0.796818 |
| H | -1.840093 | -0.067973 | -1.598043 |
| H | -2.808094 | 0.927950 | -0.472496 |
| H | -1.305562 | 1.566842 | -1.198500 |
| C | 1.833521 | -0.856304 | -1.985208 |
| C | 2.026063 | 0.278663 | -2.789411 |
| C | 1.459099 | -2.058567 | -2.606759 |
| C | 1.810474 | 0.221124 | -4.167507 |
| H | 2.343952 | 1.216888 | -2.342880 |
| C | 1.244166 | -2.111786 | -3.985190 |
| H | 1.333306 | -2.962148 | -2.016603 |
| C | 1.417022 | -0.973069 | -4.773966 |
| H | 1.958324 | 1.115335 | -4.768798 |
| H | 0.947130 | -3.052542 | -4.443282 |
| H | 1.258500 | -1.018466 | -5.847966 |
| H | 4.034360 | 0.947115 | -0.659743 |
| F | 6.512405 | 0.565046 | -0.089666 |

Ph*-Ph

| | | | |
|---|---|---|---|
| C | 3.369917 | -1.143911 | -1.542405 |
| C | 4.152090 | -0.009488 | -1.277054 |
| C | 3.234604 | -2.117565 | -0.539676 |
| C | 4.765118 | 0.116960 | -0.039820 |
| C | 3.865191 | -1.963278 | 0.693808 |
| C | 4.643863 | -0.837046 | 0.961269 |
| C | 2.700547 | -1.304380 | -2.855813 |
| C | 2.090883 | -0.212058 | -3.492247 |
| C | 2.659116 | -2.554873 | -3.491971 |
| C | 1.459580 | -0.365336 | -4.725375 |
| H | 2.089302 | 0.759029 | -3.004048 |
| C | 2.027677 | -2.708615 | -4.724875 |
| H | 3.148324 | -3.407187 | -3.027797 |
| C | 1.424935 | -1.614327 | -5.346898 |
| H | 0.985641 | 0.491380 | -5.197060 |
| H | 2.014955 | -3.683546 | -5.204874 |
| H | 0.932706 | -1.733658 | -6.308134 |
| F | 5.524037 | 1.212869 | 0.194659 |
| H | 4.309986 | 0.755885 | -2.030143 |
| H | 5.144591 | -0.693466 | 1.912920 |
| H | 2.608885 | -2.986836 | -0.719250 |
| H | 3.742625 | -2.722467 | 1.461321 |

0Fo-1Fp

**2**

| | | | |
|---|---|---|---|
| Pd | 0.287235 | 0.170286 | -0.715995 |
| C | 2.597726 | -0.633263 | -0.310660 |
| C | 3.260461 | 0.022378 | 0.745088 |
| C | 3.145893 | -0.443374 | 2.045285 |
| C | 2.363698 | -1.575507 | 2.280260 |
| C | 1.700973 | -2.252754 | 1.273779 |
| C | 1.819282 | -1.774308 | -0.039845 |
| H | 3.638660 | 0.048099 | 2.877386 |
| H | 1.117738 | -3.137465 | 1.506470 |
| H | 1.377259 | -2.324233 | -0.865280 |
| H | 2.786843 | -0.342490 | -1.339960 |
| P | -1.617828 | 1.234839 | -1.305034 |
| C | -2.911371 | 1.443286 | -0.020499 |
| H | -3.791456 | 1.925679 | -0.459380 |
| H | -3.199525 | 0.468327 | 0.381335 |
| H | -2.530312 | 2.052315 | 0.801367 |
| C | -1.337149 | 2.932140 | -1.922583 |
| H | -2.283779 | 3.378405 | -2.246389 |
| H | -0.904116 | 3.544829 | -1.127825 |
| H | -0.640891 | 2.867217 | -2.761998 |
| C | -2.525507 | 0.401597 | -2.659177 |

| | | | |
|---|---|---|---|
| H | -3.475715 | 0.916132 | -2.839220 |
| H | -1.909887 | 0.435933 | -3.559343 |
| H | -2.720490 | -0.640238 | -2.393670 |
| C | 0.674753 | -0.243064 | -3.661037 |
| O | 0.436923 | 0.962006 | -3.829486 |
| O | 0.589131 | -0.871198 | -2.532422 |
| C | 1.102307 | -1.118785 | -4.829480 |
| H | 1.049515 | -0.560129 | -5.765155 |
| H | 2.129767 | -1.464144 | -4.672507 |
| H | 0.469807 | -2.009913 | -4.886802 |
| C | 0.111463 | 1.084682 | 1.048263 |
| C | -0.467276 | 0.439586 | 2.152568 |
| C | 0.643442 | 2.369716 | 1.242455 |
| C | -0.494013 | 1.047385 | 3.411642 |
| H | -0.905025 | -0.549699 | 2.038143 |
| C | 0.617715 | 2.980103 | 2.500562 |
| H | 1.098551 | 2.901663 | 0.409050 |
| C | 0.047859 | 2.320973 | 3.591078 |
| H | -0.941513 | 0.522427 | 4.252784 |
| H | 1.043902 | 3.973264 | 2.625870 |
| H | 0.024151 | 2.795404 | 4.568633 |
| H | 3.871144 | 0.896169 | 0.538632 |
| F | 2.263912 | -2.030847 | 3.546671 |

TS-CMD

| | | | |
|---|---|---|---|
| Pd | 0.114278 | 0.379941 | -0.827567 |
| C | 1.859599 | -0.709575 | -0.064126 |
| C | 2.873966 | -0.076920 | 0.684591 |
| C | 3.511994 | -0.702471 | 1.752844 |
| C | 3.112892 | -1.989722 | 2.090285 |
| C | 2.126146 | -2.673476 | 1.392164 |
| C | 1.520557 | -2.026917 | 0.315152 |
| H | 4.294438 | -0.213177 | 2.324589 |
| H | 1.858814 | -3.684155 | 1.685204 |
| H | 0.768657 | -2.571250 | -0.253788 |
| H | 2.056905 | -0.578307 | -1.443088 |
| P | -1.853200 | 1.442910 | -1.342696 |
| C | -3.248195 | 1.073822 | -0.209552 |
| H | -4.155055 | 1.603676 | -0.519728 |
| H | -3.442902 | -0.002288 | -0.209553 |
| H | -2.977107 | 1.373669 | 0.805788 |
| C | -1.823465 | 3.277581 | -1.377086 |
| H | -2.808778 | 3.675596 | -1.641965 |
| H | -1.530197 | 3.653789 | -0.394154 |
| H | -1.088861 | 3.619289 | -2.111594 |
| C | -2.532045 | 1.010360 | -2.992473 |
| H | -3.486705 | 1.518600 | -3.164947 |
| H | -1.816978 | 1.297323 | -3.766953 |
| H | -2.671885 | -0.071176 | -3.057338 |
| C | 1.253826 | -0.860981 | -3.273808 |
| O | 2.353367 | -0.750102 | -2.634118 |

| | | | |
|---|---|---|---|
| O | 0.128127 | -0.582479 | -2.779034 |
| C | 1.335725 | -1.362361 | -4.692907 |
| H | 2.008065 | -0.719307 | -5.268161 |
| H | 1.769225 | -2.366885 | -4.695961 |
| H | 0.348856 | -1.382826 | -5.155892 |
| C | 0.075500 | 1.331107 | 0.924110 |
| C | -0.485349 | 0.738704 | 2.066440 |
| C | 0.640891 | 2.609334 | 1.059100 |
| C | -0.482692 | 1.400507 | 3.297942 |
| H | -0.913345 | -0.259414 | 2.006591 |
| C | 0.646385 | 3.272308 | 2.290811 |
| H | 1.095802 | 3.096569 | 0.198547 |
| C | 0.081053 | 2.671937 | 3.416398 |
| H | -0.916435 | 0.914283 | 4.169219 |
| H | 1.097348 | 4.259540 | 2.367849 |
| H | 0.085883 | 3.184712 | 4.374650 |
| H | 3.175626 | 0.935084 | 0.425738 |
| F | 3.716768 | -2.606096 | 3.133292 |

**3**

| | | | |
|---|---|---|---|
| Pd | 0.041039 | 0.340980 | -0.549005 |
| C | 1.628460 | -0.674098 | 0.279024 |
| C | 2.769519 | -0.071978 | 0.844592 |
| C | 3.808342 | -0.817882 | 1.412088 |
| C | 3.691967 | -2.198983 | 1.434252 |
| C | 2.587239 | -2.853363 | 0.907130 |
| C | 1.572462 | -2.083512 | 0.332115 |
| H | 4.685229 | -0.341884 | 1.840956 |
| H | 2.531000 | -3.937298 | 0.947758 |
| H | 0.713914 | -2.606302 | -0.086372 |
| H | 2.369405 | -0.440242 | -1.578302 |
| P | -1.849774 | 1.503871 | -1.361201 |
| C | -3.128500 | 2.000275 | -0.140811 |
| H | -3.946660 | 2.543944 | -0.625194 |
| H | -3.526799 | 1.109650 | 0.352738 |
| H | -2.671923 | 2.628449 | 0.628267 |
| C | -1.470953 | 3.098182 | -2.201909 |
| H | -2.381971 | 3.584384 | -2.567828 |
| H | -0.967781 | 3.766484 | -1.497570 |
| H | -0.796969 | 2.919006 | -3.044322 |
| C | -2.836106 | 0.609044 | -2.632536 |
| H | -3.656163 | 1.227055 | -3.013962 |
| H | -2.181793 | 0.316179 | -3.457129 |
| H | -3.250423 | -0.302989 | -2.193247 |
| C | 1.378341 | -0.748308 | -3.151790 |
| O | 2.537880 | -0.601838 | -2.546131 |
| O | 0.290607 | -0.563907 | -2.599247 |
| C | 1.497013 | -1.165475 | -4.586762 |
| H | 2.147334 | -0.468301 | -5.122765 |
| H | 1.967060 | -2.152291 | -4.638612 |
| H | 0.512577 | -1.199295 | -5.051677 |

| | | | |
|---|---|---|---|
| C | -0.156490 | 1.208324 | 1.223832 |
| C | -0.806812 | 0.566912 | 2.290010 |
| C | 0.316837 | 2.513735 | 1.435213 |
| C | -0.992220 | 1.212816 | 3.515535 |
| H | -1.163188 | -0.453436 | 2.172425 |
| C | 0.133931 | 3.160752 | 2.662348 |
| H | 0.839358 | 3.039336 | 0.637952 |
| C | -0.525331 | 2.514384 | 3.708394 |
| H | -1.496460 | 0.690440 | 4.325933 |
| H | 0.511898 | 4.172077 | 2.798479 |
| H | -0.666013 | 3.014263 | 4.663222 |
| F | 4.688497 | -2.936041 | 1.988618 |
| H | 2.852774 | 1.012343 | 0.859671 |

**4**

| | | | |
|---|---|---|---|
| C | 3.557321 | -0.943525 | -0.111064 |
| Pd | 1.620757 | -0.450708 | 0.082596 |
| C | 4.522892 | 0.076299 | -0.022175 |
| C | 4.018884 | -2.270593 | -0.139771 |
| H | 3.311394 | -3.089671 | -0.245776 |
| C | 5.888580 | -0.208223 | 0.080288 |
| H | 6.633213 | 0.578731 | 0.155417 |
| C | 5.377633 | -2.580281 | -0.038674 |
| H | 5.733344 | -3.606296 | -0.053026 |
| C | 6.286115 | -1.536958 | 0.072262 |
| P | -0.653537 | 0.168365 | 0.402592 |
| C | -1.143463 | 0.805992 | 2.063281 |
| H | -0.558676 | 1.698563 | 2.304344 |
| H | -2.208463 | 1.060420 | 2.095329 |
| H | -0.937669 | 0.048711 | 2.825536 |
| C | -1.873535 | -1.179078 | 0.123586 |
| H | -2.901777 | -0.816590 | 0.228644 |
| H | -1.732959 | -1.583965 | -0.882412 |
| H | -1.701167 | -1.985261 | 0.842347 |
| C | -1.258217 | 1.490234 | -0.723371 |
| H | -1.092049 | 1.178900 | -1.758338 |
| H | -2.323511 | 1.693613 | -0.570263 |
| H | -0.688417 | 2.407680 | -0.550333 |
| C | 1.406738 | -0.926463 | -1.827843 |
| C | 1.588591 | 0.033880 | -2.831611 |
| C | 0.989741 | -2.214721 | -2.187292 |
| C | 1.325694 | -0.283268 | -4.168044 |
| H | 1.945535 | 1.028870 | -2.581204 |
| C | 0.729007 | -2.525922 | -3.526062 |
| H | 0.868942 | -2.985882 | -1.430494 |
| C | 0.891532 | -1.561673 | -4.521155 |
| H | 1.473573 | 0.473775 | -4.935084 |
| H | 0.404903 | -3.530906 | -3.787581 |
| H | 0.693873 | -1.806975 | -5.561181 |
| F | 7.609888 | -1.826453 | 0.165906 |
| H | 4.218038 | 1.121217 | -0.031518 |

TS-RE

| | | | |
|---|---|---|---|
| C | 3.305261 | -1.099032 | -0.480610 |
| Pd | 1.408473 | -0.586554 | -0.011489 |
| C | 4.293031 | -0.099655 | -0.452979 |
| C | 3.698210 | -2.426019 | -0.233832 |
| H | 2.967501 | -3.229166 | -0.282068 |
| C | 5.620928 | -0.400272 | -0.146241 |
| H | 6.386776 | 0.368608 | -0.114163 |
| C | 5.021040 | -2.745734 | 0.075199 |
| H | 5.328488 | -3.767245 | 0.277048 |
| C | 5.957431 | -1.721621 | 0.114303 |
| P | -0.783558 | 0.005282 | 0.588596 |
| C | -1.010171 | 1.304793 | 1.880122 |
| H | -0.508866 | 2.224370 | 1.565157 |
| H | -2.071004 | 1.517294 | 2.054355 |
| H | -0.554262 | 0.976388 | 2.818722 |
| C | -1.867847 | -1.343240 | 1.227979 |
| H | -2.879490 | -0.979770 | 1.440715 |
| H | -1.924070 | -2.145647 | 0.487196 |
| H | -1.437450 | -1.758514 | 2.143751 |
| C | -1.787816 | 0.673372 | -0.801917 |
| H | -1.831385 | -0.068691 | -1.603557 |
| H | -2.804702 | 0.924557 | -0.480190 |
| H | -1.301845 | 1.567170 | -1.202250 |
| C | 1.831211 | -0.852934 | -1.979974 |
| C | 2.015124 | 0.283662 | -2.784518 |
| C | 1.460418 | -2.055945 | -2.602694 |
| C | 1.796661 | 0.226205 | -4.162216 |
| H | 2.327211 | 1.223787 | -2.337814 |
| C | 1.242676 | -2.109138 | -3.980713 |
| H | 1.339118 | -2.960876 | -2.013542 |
| C | 1.408176 | -0.969259 | -4.769371 |
| H | 1.937414 | 1.122118 | -4.762817 |
| H | 0.948796 | -3.051016 | -4.438604 |
| H | 1.247157 | -1.014499 | -5.842992 |
| F | 7.246813 | -2.024004 | 0.404779 |
| H | 4.031927 | 0.931634 | -0.675060 |

Ph*-Ph

| | | | |
|---|---|---|---|
| C | 3.369991 | -1.142716 | -1.542500 |
| C | 4.159223 | -0.014385 | -1.268290 |
| C | 3.234310 | -2.114751 | -0.538747 |
| C | 4.793272 | 0.145371 | -0.037846 |
| C | 3.862165 | -1.974120 | 0.697291 |
| C | 4.631913 | -0.841919 | 0.924435 |
| C | 2.699225 | -1.304402 | -2.854634 |
| C | 2.081770 | -0.214417 | -3.488112 |
| C | 2.663989 | -2.552838 | -3.495696 |
| C | 1.451730 | -0.367185 | -4.722063 |

| | | | |
|---|---|---|---|
| H | 2.073221 | 0.755000 | -2.996486 |
| C | 2.031204 | -2.707122 | -4.727964 |
| H | 3.159135 | -3.404066 | -3.035462 |
| C | 1.422701 | -1.614503 | -5.347258 |
| H | 0.972930 | 0.488453 | -5.190936 |
| H | 2.022815 | -3.681105 | -5.210097 |
| H | 0.930330 | -1.733840 | -6.308416 |
| F | 5.244879 | -0.695848 | 2.121555 |
| H | 4.301178 | 0.739440 | -2.037827 |
| H | 5.412344 | 1.011022 | 0.174734 |
| H | 3.751905 | -2.718855 | 1.478920 |
| H | 2.607454 | -2.984262 | -0.716428 |

0Fo-2Fm

**2**

| | | | |
|---|---|---|---|
| Pd | 0.438479 | 0.404331 | -0.757736 |
| C | 2.094375 | -1.327979 | -0.187555 |
| C | 2.913105 | -0.187911 | -0.301711 |
| C | 3.515711 | 0.379581 | 0.828229 |
| C | 3.289882 | -0.215660 | 2.057374 |
| C | 2.498791 | -1.352572 | 2.223057 |
| C | 1.920879 | -1.884923 | 1.087704 |
| H | 2.340042 | -1.790731 | 3.201072 |
| H | 1.739368 | -1.858586 | -1.065363 |
| P | -1.327274 | 1.676083 | -1.375291 |
| C | -1.816461 | 3.055574 | -0.269328 |
| H | -2.640561 | 3.616484 | -0.723458 |
| H | -2.128345 | 2.666886 | 0.701868 |
| H | -0.968876 | 3.727840 | -0.112677 |
| C | -1.076005 | 2.515299 | -2.982426 |
| H | -1.925362 | 3.173827 | -3.194371 |
| H | -0.156122 | 3.104483 | -2.955536 |
| H | -0.995414 | 1.752483 | -3.758255 |
| C | -2.869523 | 0.718471 | -1.588919 |
| H | -3.678991 | 1.376754 | -1.922628 |
| H | -2.678076 | -0.056480 | -2.334555 |
| H | -3.149750 | 0.256985 | -0.638613 |
| C | 0.521203 | -0.450787 | -3.635634 |
| O | -0.707891 | -0.602675 | -3.591578 |
| O | 1.244777 | 0.048278 | -2.684966 |
| C | 1.308384 | -0.850998 | -4.874254 |
| H | 2.018986 | -1.644668 | -4.620669 |
| H | 0.635330 | -1.203825 | -5.656985 |
| H | 1.893847 | -0.001321 | -5.239176 |
| C | -0.194715 | 0.646724 | 1.117178 |
| C | -1.120193 | -0.251748 | 1.671687 |
| C | 0.331226 | 1.648607 | 1.948041 |
| C | -1.489538 | -0.166752 | 3.018090 |
| H | -1.548773 | -1.041349 | 1.057378 |

| | | | |
|---|---|---|---|
| C | -0.038388 | 1.736469 | 3.293654 |
| H | 1.037991 | 2.372852 | 1.548590 |
| C | -0.950884 | 0.828977 | 3.834292 |
| H | -2.199915 | -0.882056 | 3.426750 |
| H | 0.388257 | 2.518028 | 3.918578 |
| H | -1.240369 | 0.898657 | 4.879553 |
| H | 3.123094 | 0.200911 | -1.293273 |
| F | 3.865646 | 0.312407 | 3.153708 |
| F | 1.173510 | -2.995472 | 1.205498 |
| H | 4.153957 | 1.252975 | 0.755494 |

TS-CMD

| | | | |
|---|---|---|---|
| Pd | 0.117788 | 0.385586 | -0.849194 |
| C | 1.924944 | -0.652890 | -0.088352 |
| C | 2.929400 | 0.026214 | 0.627206 |
| C | 3.540831 | -0.587713 | 1.708317 |
| C | 3.199756 | -1.864021 | 2.141436 |
| C | 2.211817 | -2.523107 | 1.421550 |
| C | 1.585206 | -1.959347 | 0.320205 |
| H | 3.687636 | -2.324894 | 2.992463 |
| H | 0.845178 | -2.545971 | -0.217264 |
| H | 2.066977 | -0.510516 | -1.457492 |
| P | -1.888995 | 1.371220 | -1.325780 |
| C | -3.252285 | 0.953380 | -0.172676 |
| H | -4.183773 | 1.439515 | -0.481462 |
| H | -3.399520 | -0.130047 | -0.157605 |
| H | -2.985783 | 1.278460 | 0.835926 |
| C | -1.923363 | 3.204692 | -1.365706 |
| H | -2.926463 | 3.564624 | -1.617615 |
| H | -1.630635 | 3.594538 | -0.388025 |
| H | -1.212797 | 3.570491 | -2.112017 |
| C | -2.566611 | 0.903821 | -2.965306 |
| H | -3.543386 | 1.371793 | -3.127480 |
| H | -1.872836 | 1.216818 | -3.748864 |
| H | -2.662053 | -0.182793 | -3.024316 |
| C | 1.271027 | -0.825633 | -3.296580 |
| O | 2.368561 | -0.681826 | -2.662962 |
| O | 0.139848 | -0.571032 | -2.797534 |
| C | 1.355383 | -1.339043 | -4.711006 |
| H | 0.370180 | -1.359472 | -5.177475 |
| H | 2.034731 | -0.706808 | -5.289583 |
| H | 1.781560 | -2.346820 | -4.701582 |
| C | 0.056309 | 1.329914 | 0.906890 |
| C | -0.470112 | 0.709342 | 2.049987 |
| C | 0.582862 | 2.623843 | 1.042895 |
| C | -0.468597 | 1.360144 | 3.287473 |
| H | -0.869773 | -0.300220 | 1.986453 |
| C | 0.586969 | 3.275155 | 2.280657 |
| H | 1.010170 | 3.131922 | 0.180339 |
| C | 0.057721 | 2.647121 | 3.408571 |
| H | -0.874020 | 0.853340 | 4.160548 |

| | | | |
|---|---|---|---|
| H | 1.009999 | 4.274240 | 2.360778 |
| H | 0.062637 | 3.150938 | 4.371470 |
| H | 3.237599 | 1.029675 | 0.351109 |
| F | 4.511374 | 0.070848 | 2.384369 |
| F | 1.862611 | -3.771866 | 1.816252 |

**3**

| | | | |
|---|---|---|---|
| Pd | 0.058185 | 0.391921 | -0.538991 |
| C | 1.625437 | -0.646623 | 0.290022 |
| C | 2.782781 | -0.045880 | 0.821910 |
| C | 3.795282 | -0.835423 | 1.356624 |
| C | 3.728020 | -2.220311 | 1.411639 |
| C | 2.576146 | -2.795535 | 0.889015 |
| C | 1.542733 | -2.054540 | 0.332180 |
| H | 0.680268 | -2.587282 | -0.058993 |
| H | 2.435000 | -0.342946 | -1.576211 |
| P | -1.836198 | 1.529209 | -1.375906 |
| C | -2.937667 | 2.380454 | -0.181677 |
| H | -3.783736 | 2.850563 | -0.693577 |
| H | -3.307066 | 1.659337 | 0.551988 |
| H | -2.367708 | 3.137325 | 0.363202 |
| C | -1.482460 | 2.854949 | -2.605674 |
| H | -2.406365 | 3.306554 | -2.983720 |
| H | -0.871716 | 3.632509 | -2.138263 |
| H | -0.919839 | 2.435298 | -3.443979 |
| C | -2.996937 | 0.437298 | -2.297023 |
| H | -3.830657 | 1.005887 | -2.723276 |
| H | -2.453685 | -0.070331 | -3.098322 |
| H | -3.393249 | -0.324184 | -1.619304 |
| C | 1.448832 | -0.605864 | -3.164097 |
| O | 2.604285 | -0.492979 | -2.541340 |
| O | 0.357867 | -0.417328 | -2.620477 |
| C | 1.580515 | -0.992849 | -4.605714 |
| H | 2.276454 | -0.317233 | -5.110680 |
| H | 2.002227 | -2.000765 | -4.669895 |
| H | 0.606250 | -0.969504 | -5.092131 |
| C | -0.191203 | 1.169964 | 1.268796 |
| C | -0.907956 | 0.496178 | 2.269517 |
| C | 0.321848 | 2.441568 | 1.569547 |
| C | -1.116887 | 1.080485 | 3.522413 |
| H | -1.297642 | -0.501412 | 2.081310 |
| C | 0.114927 | 3.026109 | 2.823446 |
| H | 0.894346 | 2.988985 | 0.823030 |
| C | -0.608743 | 2.349260 | 3.805828 |
| H | -1.671868 | 0.534429 | 4.282428 |
| H | 0.525784 | 4.011980 | 3.031167 |
| H | -0.767329 | 2.800325 | 4.781866 |
| H | 2.899063 | 1.033438 | 0.852190 |
| H | 4.524882 | -2.817552 | 1.838481 |
| F | 4.902620 | -0.233439 | 1.855173 |
| F | 2.470580 | -4.147593 | 0.925323 |

**4**

| | | | |
|---|---|---|---|
| C | 3.559732 | -0.938729 | -0.110187 |
| Pd | 1.620350 | -0.441579 | 0.084719 |
| C | 4.515431 | 0.088906 | -0.003373 |
| C | 4.008006 | -2.269184 | -0.158377 |
| H | 3.320454 | -3.101641 | -0.271002 |
| C | 5.863552 | -0.236648 | 0.084300 |
| C | 5.367141 | -2.536561 | -0.066822 |
| C | 6.330989 | -1.543446 | 0.056513 |
| H | 7.387493 | -1.775268 | 0.119229 |
| P | -0.652583 | 0.179700 | 0.396503 |
| C | -1.135143 | 0.804238 | 2.063495 |
| H | -0.546219 | 1.692142 | 2.311479 |
| H | -2.198880 | 1.063066 | 2.099227 |
| H | -0.931907 | 0.039086 | 2.818489 |
| C | -1.874271 | -1.162434 | 0.105183 |
| H | -2.901436 | -0.798233 | 0.213852 |
| H | -1.734874 | -1.558524 | -0.904443 |
| H | -1.703719 | -1.975350 | 0.816696 |
| C | -1.247620 | 1.513567 | -0.719254 |
| H | -1.084558 | 1.208882 | -1.756669 |
| H | -2.311443 | 1.722375 | -0.563843 |
| H | -0.671996 | 2.426001 | -0.539419 |
| C | 1.395924 | -0.932935 | -1.819734 |
| C | 1.574457 | 0.021629 | -2.828722 |
| C | 0.983795 | -2.225593 | -2.165852 |
| C | 1.312787 | -0.307846 | -4.162481 |
| H | 1.928074 | 1.019571 | -2.585758 |
| C | 0.724633 | -2.548036 | -3.502289 |
| H | 0.866305 | -2.990884 | -1.402706 |
| C | 0.883661 | -1.590825 | -4.504638 |
| H | 1.458116 | 0.443337 | -4.935604 |
| H | 0.405057 | -3.556371 | -3.755822 |
| H | 0.687435 | -1.845412 | -5.542630 |
| F | 6.774232 | 0.762853 | 0.195094 |
| F | 5.787257 | -3.825701 | -0.101496 |
| H | 4.235563 | 1.138627 | 0.009480 |

TS-RE

| | | | |
|---|---|---|---|
| C | 3.298420 | -1.098011 | -0.494647 |
| Pd | 1.404070 | -0.585697 | -0.017627 |
| C | 4.276148 | -0.088696 | -0.459209 |
| C | 3.678951 | -2.428183 | -0.244262 |
| H | 2.968622 | -3.247169 | -0.287104 |
| C | 5.584514 | -0.427755 | -0.146220 |
| C | 5.003140 | -2.704605 | 0.063322 |
| C | 5.990873 | -1.729265 | 0.120310 |
| H | 7.021723 | -1.971489 | 0.348682 |
| P | -0.789273 | 0.005486 | 0.591593 |
| C | -1.006642 | 1.304176 | 1.884495 |

| | | | |
|---|---|---|---|
| H | -0.506055 | 2.223405 | 1.567522 |
| H | -2.066395 | 1.517375 | 2.063978 |
| H | -0.546604 | 0.974708 | 2.820665 |
| C | -1.868208 | -1.344815 | 1.234319 |
| H | -2.878991 | -0.982177 | 1.452101 |
| H | -1.927314 | -2.146608 | 0.493141 |
| H | -1.433249 | -1.760479 | 2.147718 |
| C | -1.796164 | 0.673959 | -0.796185 |
| H | -1.842885 | -0.067921 | -1.597785 |
| H | -2.811848 | 0.925186 | -0.470972 |
| H | -1.311372 | 1.567977 | -1.197371 |
| C | 1.841828 | -0.855011 | -1.984756 |
| C | 2.029379 | 0.281904 | -2.787147 |
| C | 1.470373 | -2.058367 | -2.605336 |
| C | 1.810420 | 0.224707 | -4.164625 |
| H | 2.344952 | 1.220581 | -2.340131 |
| C | 1.252358 | -2.110723 | -3.983216 |
| H | 1.349163 | -2.963070 | -2.016032 |
| C | 1.419595 | -0.970441 | -4.770843 |
| H | 1.953691 | 1.119841 | -4.765493 |
| H | 0.957965 | -3.052049 | -4.441527 |
| H | 1.259063 | -1.015477 | -5.844499 |
| F | 6.518767 | 0.551511 | -0.099668 |
| F | 5.359787 | -3.985889 | 0.318542 |
| H | 4.040111 | 0.948188 | -0.673880 |

Ph*-Ph

| | | | |
|---|---|---|---|
| C | 3.370633 | -1.142454 | -1.542223 |
| C | 4.148456 | -0.005147 | -1.275855 |
| C | 3.235087 | -2.126018 | -0.550345 |
| C | 4.762426 | 0.117916 | -0.038420 |
| C | 3.874460 | -1.949465 | 0.667511 |
| C | 4.649857 | -0.836515 | 0.963826 |
| C | 2.700285 | -1.304589 | -2.854755 |
| C | 2.093082 | -0.211251 | -3.491357 |
| C | 2.657447 | -2.556120 | -3.488131 |
| C | 1.461449 | -0.365354 | -4.724085 |
| H | 2.092714 | 0.760191 | -3.004119 |
| C | 2.026507 | -2.709826 | -4.721147 |
| H | 3.144827 | -3.408955 | -3.023034 |
| C | 1.425582 | -1.615073 | -5.343975 |
| H | 0.988359 | 0.491248 | -5.196603 |
| H | 2.012212 | -3.685148 | -5.200046 |
| H | 0.933132 | -1.734841 | -6.304977 |
| F | 5.516782 | 1.211107 | 0.204079 |
| F | 3.728990 | -2.896807 | 1.618471 |
| H | 4.303643 | 0.761875 | -2.026582 |
| H | 5.139495 | -0.719152 | 1.923051 |
| H | 2.617297 | -3.003599 | -0.705542 |

**set1Fo**

1Fo

**2**

| | | | |
|---|---|---|---|
| Pd | 0.349322 | 0.257217 | -0.781490 |
| C | 1.987859 | -1.570288 | -0.374170 |
| C | 2.741559 | -0.385363 | -0.262871 |
| C | 3.217759 | 0.035266 | 0.989311 |
| C | 2.952728 | -0.724608 | 2.121435 |
| C | 2.214076 | -1.911774 | 2.031099 |
| C | 1.751010 | -2.307508 | 0.791378 |
| H | 3.801032 | 0.947599 | 1.065207 |
| H | 3.316063 | -0.401006 | 3.092392 |
| H | 1.997352 | -2.514982 | 2.906256 |
| H | 1.708983 | -1.967905 | -1.345498 |
| P | -1.475411 | 1.458934 | -1.369688 |
| C | -1.188546 | 3.263620 | -1.325274 |
| H | -2.080369 | 3.797798 | -1.670577 |
| H | -0.957080 | 3.572050 | -0.302760 |
| H | -0.339959 | 3.478472 | -1.978893 |
| C | -2.047195 | 1.126161 | -3.076874 |
| H | -2.977352 | 1.672567 | -3.267054 |
| H | -1.274209 | 1.458097 | -3.771569 |
| H | -2.219729 | 0.055555 | -3.210951 |
| C | -3.005925 | 1.230837 | -0.383664 |
| H | -3.811513 | 1.838253 | -0.810395 |
| H | -3.304924 | 0.179397 | -0.396253 |
| H | -2.834012 | 1.524354 | 0.653492 |
| C | 1.299740 | 0.839016 | -3.561843 |
| O | 1.017934 | 2.030475 | -3.363368 |
| O | 1.058833 | -0.130333 | -2.739411 |
| C | 1.980524 | 0.408459 | -4.852459 |
| H | 1.445086 | -0.433000 | -5.302232 |
| H | 2.030781 | 1.242179 | -5.554465 |
| H | 2.996281 | 0.061985 | -4.633241 |
| C | -0.238942 | 0.515039 | 1.106990 |
| C | -0.991127 | -0.465881 | 1.772920 |
| C | 0.149828 | 1.651300 | 1.833846 |
| C | -1.325397 | -0.325906 | 3.123184 |
| H | -1.321156 | -1.354947 | 1.239527 |
| C | -0.184700 | 1.794622 | 3.184664 |
| H | 0.730511 | 2.434356 | 1.350167 |
| C | -0.924945 | 0.806397 | 3.834949 |
| H | -1.903873 | -1.103726 | 3.617193 |
| H | 0.133722 | 2.682694 | 3.726573 |
| H | -1.189908 | 0.918666 | 4.883090 |
| H | 3.024254 | 0.144198 | -1.167345 |
| F | 1.050127 | -3.457046 | 0.690263 |

TS-CMD

| | | | |
|---|---|---|---|
| Pd | 0.129703 | 0.420979 | -0.812303 |
| C | 1.909333 | -0.702432 | -0.114912 |
| C | 2.981969 | 0.056745 | 0.362828 |
| C | 3.775794 | -0.291288 | 1.446640 |
| C | 3.488277 | -1.482198 | 2.113130 |
| C | 2.438976 | -2.298140 | 1.679994 |
| C | 1.675460 | -1.909282 | 0.582850 |
| H | 4.588816 | 0.357324 | 1.757428 |
| H | 4.091160 | -1.775224 | 2.968678 |
| H | 2.226154 | -3.230757 | 2.195377 |
| H | 0.875025 | -2.561722 | 0.239342 |
| H | 1.923623 | -0.877153 | -1.462803 |
| P | -1.731475 | 1.617136 | -1.386816 |
| C | -2.716851 | 2.492601 | -0.117512 |
| H | -3.563638 | 3.009827 | -0.580552 |
| H | -3.081142 | 1.776907 | 0.623461 |
| H | -2.083870 | 3.213657 | 0.405325 |
| C | -1.338989 | 2.926489 | -2.611894 |
| H | -2.249182 | 3.421364 | -2.967923 |
| H | -0.680693 | 3.669945 | -2.154254 |
| H | -0.813102 | 2.468946 | -3.453445 |
| C | -2.967912 | 0.578551 | -2.259769 |
| H | -3.791622 | 1.186179 | -2.650070 |
| H | -2.466318 | 0.062281 | -3.081831 |
| H | -3.368939 | -0.170617 | -1.571599 |
| C | 1.196891 | -0.732763 | -3.388205 |
| O | 2.129162 | -1.207031 | -2.664631 |
| O | 0.231532 | -0.053948 | -2.938739 |
| C | 1.275361 | -1.003397 | -4.870362 |
| H | 2.152898 | -0.492501 | -5.278876 |
| H | 1.414403 | -2.073976 | -5.042603 |
| H | 0.377526 | -0.651441 | -5.379327 |
| C | -0.117435 | 0.956062 | 1.089226 |
| C | -0.886896 | 0.175223 | 1.964815 |
| C | 0.457600 | 2.134484 | 1.588812 |
| C | -1.078452 | 0.560638 | 3.295355 |
| H | -1.337746 | -0.751542 | 1.616074 |
| C | 0.267711 | 2.519969 | 2.919879 |
| H | 1.072623 | 2.756951 | 0.942615 |
| C | -0.504442 | 1.737083 | 3.779223 |
| H | -1.675614 | -0.065622 | 3.955038 |
| H | 0.730365 | 3.434880 | 3.284285 |
| H | -0.652119 | 2.036552 | 4.813586 |
| F | 3.284013 | 1.217607 | -0.275234 |

**3**

| | | | |
|---|---|---|---|
| Pd | 0.137841 | 0.504797 | -0.599257 |
| C | 1.783811 | -0.447492 | 0.210240 |
| C | 3.053531 | 0.125522 | 0.104438 |
| C | 4.211906 | -0.393625 | 0.669780 |

| | | | |
|---|---|---|---|
| C | 4.118435 | -1.577207 | 1.402979 |
| C | 2.879955 | -2.202777 | 1.548805 |
| C | 1.740990 | -1.636373 | 0.967994 |
| H | 5.157413 | 0.123871 | 0.536365 |
| H | 5.009500 | -2.003134 | 1.856276 |
| H | 2.796772 | -3.122281 | 2.122604 |
| H | 1.804316 | -1.478491 | -1.472023 |
| P | -1.712808 | 1.712930 | -1.399383 |
| C | -2.788285 | 2.594001 | -0.203780 |
| H | -3.591138 | 3.131803 | -0.718706 |
| H | -3.217776 | 1.876354 | 0.499896 |
| H | -2.185152 | 3.297443 | 0.375941 |
| C | -1.219601 | 3.043728 | -2.570301 |
| H | -2.091597 | 3.552460 | -2.995628 |
| H | -0.598124 | 3.774691 | -2.045547 |
| H | -0.622723 | 2.605748 | -3.374724 |
| C | -2.921356 | 0.738972 | -2.391494 |
| H | -3.712647 | 1.377491 | -2.799843 |
| H | -2.396688 | 0.245494 | -3.213805 |
| H | -3.374624 | -0.031750 | -1.761612 |
| C | 1.217210 | -0.941309 | -3.187701 |
| O | 1.880619 | -1.777802 | -2.419223 |
| O | 0.540653 | -0.004592 | -2.756664 |
| C | 1.362083 | -1.226065 | -4.652530 |
| H | 2.404998 | -1.071585 | -4.946386 |
| H | 1.118454 | -2.272601 | -4.855040 |
| H | 0.715668 | -0.566209 | -5.229767 |
| C | -0.288538 | 0.978299 | 1.277637 |
| C | -1.175483 | 0.196932 | 2.034153 |
| C | 0.255589 | 2.124927 | 1.877067 |
| C | -1.521305 | 0.558293 | 3.340307 |
| H | -1.604294 | -0.708226 | 1.608490 |
| C | -0.091563 | 2.487575 | 3.182018 |
| H | 0.967404 | 2.737973 | 1.329490 |
| C | -0.984156 | 1.708412 | 3.920032 |
| H | -2.210597 | -0.065816 | 3.905589 |
| H | 0.347081 | 3.379410 | 3.624941 |
| H | -1.250295 | 1.988641 | 4.935957 |
| F | 3.192099 | 1.278985 | -0.616595 |
| H | 0.782490 | -2.129475 | 1.116669 |

**4**

| | | | |
|---|---|---|---|
| C | 3.620467 | -0.910472 | -0.233316 |
| Pd | 1.679453 | -0.364718 | -0.069808 |
| C | 4.288987 | -0.539313 | 0.926563 |
| C | 4.409186 | -1.546439 | -1.201252 |
| H | 3.955098 | -1.866009 | -2.135877 |
| C | 5.632360 | -0.743009 | 1.190741 |
| H | 6.069619 | -0.417045 | 2.129870 |
| C | 5.773178 | -1.779698 | -0.989743 |
| H | 6.360822 | -2.275665 | -1.758496 |
| C | 6.385116 | -1.380628 | 0.200240 |

| | | | |
|---|---|---|---|
| H | 7.444058 | -1.562343 | 0.362596 |
| P | -0.549300 | 0.343146 | 0.276431 |
| C | -0.870066 | 1.149554 | 1.902416 |
| H | -0.230824 | 2.030695 | 2.009840 |
| H | -1.917514 | 1.455905 | 1.996342 |
| H | -0.628251 | 0.455370 | 2.712463 |
| C | -1.832020 | -0.971132 | 0.214249 |
| H | -2.835103 | -0.556828 | 0.361212 |
| H | -1.784257 | -1.470788 | -0.757107 |
| H | -1.632247 | -1.715513 | 0.990175 |
| C | -1.185488 | 1.581403 | -0.923722 |
| H | -1.114147 | 1.167872 | -1.933433 |
| H | -2.226890 | 1.846168 | -0.711641 |
| H | -0.568592 | 2.483434 | -0.880879 |
| C | 1.270822 | -1.074377 | -1.858037 |
| C | 1.385018 | -0.256129 | -2.990030 |
| C | 0.844679 | -2.400300 | -2.014603 |
| C | 1.059353 | -0.754813 | -4.255769 |
| H | 1.740527 | 0.766048 | -2.894492 |
| C | 0.521328 | -2.891635 | -3.283782 |
| H | 0.775587 | -3.059945 | -1.154046 |
| C | 0.623598 | -2.071785 | -4.408526 |
| H | 1.156813 | -0.108112 | -5.125036 |
| H | 0.195742 | -3.924239 | -3.388917 |
| H | 0.375873 | -2.457578 | -5.393755 |
| F | 3.519186 | 0.091928 | 1.895560 |

TS-RE

| | | | |
|---|---|---|---|
| C | 3.298379 | -1.077182 | -0.483138 |
| Pd | 1.396604 | -0.567259 | 0.001640 |
| C | 4.307687 | -0.110731 | -0.399444 |
| C | 3.712415 | -2.408778 | -0.284869 |
| H | 2.979062 | -3.206806 | -0.365750 |
| C | 5.637951 | -0.404908 | -0.133299 |
| H | 6.360896 | 0.403643 | -0.081176 |
| C | 5.037036 | -2.737760 | 0.000417 |
| H | 5.313461 | -3.776896 | 0.157576 |
| C | 6.005781 | -1.734750 | 0.070481 |
| H | 7.042729 | -1.982090 | 0.279425 |
| P | -0.803476 | 0.008226 | 0.583714 |
| C | -1.033802 | 1.308288 | 1.873451 |
| H | -0.525604 | 2.225090 | 1.561676 |
| H | -2.095041 | 1.525074 | 2.039904 |
| H | -0.585935 | 0.977933 | 2.815210 |
| C | -1.894807 | -1.338038 | 1.215914 |
| H | -2.906902 | -0.972331 | 1.422867 |
| H | -1.948502 | -2.140121 | 0.474548 |
| H | -1.470592 | -1.754680 | 2.133935 |
| C | -1.796451 | 0.678459 | -0.813741 |
| H | -1.836948 | -0.063283 | -1.615848 |
| H | -2.814795 | 0.932062 | -0.498471 |

| | | | |
|---|---|---|---|
| H | -1.305140 | 1.571047 | -1.210131 |
| C | 1.868802 | -0.843429 | -1.956508 |
| C | 2.046096 | 0.284468 | -2.776096 |
| C | 1.480274 | -2.053978 | -2.556407 |
| C | 1.806049 | 0.204988 | -4.149681 |
| H | 2.373026 | 1.223008 | -2.342973 |
| C | 1.238939 | -2.123678 | -3.928529 |
| H | 1.360110 | -2.949331 | -1.952935 |
| C | 1.400249 | -0.994892 | -4.734886 |
| H | 1.943735 | 1.091750 | -4.764354 |
| H | 0.928558 | -3.068965 | -4.368082 |
| H | 1.221007 | -1.053197 | -5.805026 |
| F | 3.991507 | 1.201107 | -0.571212 |

Ph*-Ph

| | | | |
|---|---|---|---|
| C | 3.368504 | -1.113604 | -1.555941 |
| C | 4.196293 | -0.029026 | -1.243470 |
| C | 3.199880 | -2.074381 | -0.544476 |
| C | 4.829136 | 0.116846 | -0.016826 |
| C | 3.821105 | -1.954970 | 0.696535 |
| C | 4.638140 | -0.855677 | 0.963137 |
| C | 2.707504 | -1.272475 | -2.873710 |
| C | 2.036273 | -0.208242 | -3.495229 |
| C | 2.718618 | -2.521733 | -3.513367 |
| C | 1.390846 | -0.392681 | -4.716428 |
| H | 2.010376 | 0.764439 | -3.014367 |
| C | 2.074029 | -2.704853 | -4.735636 |
| H | 3.255023 | -3.349980 | -3.057502 |
| C | 1.406334 | -1.640362 | -5.341698 |
| H | 0.870856 | 0.441813 | -5.179307 |
| H | 2.100831 | -3.678363 | -5.217937 |
| H | 0.904170 | -1.780805 | -6.294987 |
| F | 4.422209 | 0.923838 | -2.178733 |
| H | 5.464605 | 0.980872 | 0.148888 |
| H | 5.125585 | -0.751238 | 1.928119 |
| H | 3.659731 | -2.714153 | 1.456222 |
| H | 2.546596 | -2.920129 | -0.741235 |

1Fo-1Fp

**2**

| | | | |
|---|---|---|---|
| Pd | 0.551121 | 0.597279 | -0.752223 |
| C | 2.057701 | -1.450478 | -0.331224 |
| C | 2.787429 | -0.251460 | -0.209639 |
| C | 3.228857 | 0.114382 | 1.069838 |
| C | 2.964310 | -0.635165 | 2.198871 |
| C | 2.229631 | -1.808022 | 2.023743 |
| C | 1.770737 | -2.237893 | 0.790859 |
| H | 3.303705 | -0.325065 | 3.179850 |
| H | 1.214426 | -3.164626 | 0.708463 |

| | | | |
|---|---|---|---|
| H | 1.780211 | -1.800587 | -1.319826 |
| P | -1.350866 | 1.648818 | -1.372921 |
| C | -1.943398 | 3.044762 | -0.341914 |
| H | -2.847933 | 3.474355 | -0.785745 |
| H | -2.159400 | 2.696762 | 0.669977 |
| H | -1.172742 | 3.817775 | -0.280399 |
| C | -1.255300 | 2.383293 | -3.047229 |
| H | -2.168997 | 2.950110 | -3.256415 |
| H | -0.389565 | 3.046006 | -3.117482 |
| H | -1.149025 | 1.575698 | -3.773565 |
| C | -2.783085 | 0.516581 | -1.461095 |
| H | -3.667290 | 1.050393 | -1.826235 |
| H | -2.519802 | -0.293822 | -2.145169 |
| H | -2.991332 | 0.108620 | -0.468929 |
| C | 0.688332 | -0.346687 | -3.579391 |
| O | -0.463446 | -0.781135 | -3.428705 |
| O | 1.346264 | 0.333941 | -2.696875 |
| C | 1.441851 | -0.578254 | -4.880338 |
| H | 2.404714 | -1.058150 | -4.679097 |
| H | 0.853101 | -1.198463 | -5.557785 |
| H | 1.658771 | 0.383385 | -5.357128 |
| C | -0.042130 | 0.870546 | 1.132130 |
| C | -0.861722 | -0.063268 | 1.784543 |
| C | 0.422667 | 1.970140 | 1.872163 |
| C | -1.190512 | 0.085188 | 3.136617 |
| H | -1.243311 | -0.925481 | 1.241512 |
| C | 0.099563 | 2.117901 | 3.223975 |
| H | 1.051970 | 2.720206 | 1.397000 |
| C | -0.711043 | 1.176324 | 3.861606 |
| H | -1.821414 | -0.656529 | 3.621460 |
| H | 0.481533 | 2.972741 | 3.777935 |
| H | -0.966748 | 1.293077 | 4.911454 |
| F | 3.955180 | 1.238910 | 1.199960 |
| H | 3.131255 | 0.288883 | -1.086704 |
| F | 1.972229 | -2.554344 | 3.113352 |

TS-CMD

| | | | |
|---|---|---|---|
| Pd | 0.129895 | 0.420957 | -0.812496 |
| C | 1.912564 | -0.702319 | -0.127127 |
| C | 2.981011 | 0.061189 | 0.355989 |
| C | 3.767129 | -0.270581 | 1.450509 |
| C | 3.451720 | -1.454859 | 2.102312 |
| C | 2.420015 | -2.291650 | 1.690070 |
| C | 1.675207 | -1.902688 | 0.581378 |
| H | 4.581355 | 0.361332 | 1.786054 |
| H | 2.224164 | -3.213626 | 2.227133 |
| H | 0.879458 | -2.560200 | 0.238435 |
| H | 1.936730 | -0.889094 | -1.475249 |
| P | -1.730908 | 1.617240 | -1.387830 |
| C | -2.715981 | 2.492869 | -0.118585 |
| H | -3.562715 | 3.009982 | -0.581790 |

| | | | |
|---|---|---|---|
| H | -3.080543 | 1.777419 | 0.622484 |
| H | -2.083149 | 3.214263 | 0.403950 |
| C | -1.336796 | 2.925890 | -2.612907 |
| H | -2.246622 | 3.420715 | -2.969850 |
| H | -0.678919 | 3.669559 | -2.155027 |
| H | -0.810362 | 2.468081 | -3.453965 |
| C | -2.966641 | 0.578093 | -2.260804 |
| H | -3.790225 | 1.185648 | -2.651407 |
| H | -2.465002 | 0.061750 | -3.082787 |
| H | -3.367985 | -0.170913 | -1.572658 |
| C | 1.197575 | -0.736379 | -3.393084 |
| O | 2.131797 | -1.215652 | -2.673983 |
| O | 0.236083 | -0.056193 | -2.938463 |
| C | 1.270607 | -1.003787 | -4.875873 |
| H | 2.148772 | -0.495187 | -5.285907 |
| H | 1.405363 | -2.074441 | -5.051065 |
| H | 0.372521 | -0.647454 | -5.381258 |
| C | -0.116640 | 0.954281 | 1.089217 |
| C | -0.883371 | 0.170801 | 1.964951 |
| C | 0.461293 | 2.130456 | 1.590901 |
| C | -1.067732 | 0.550460 | 3.298214 |
| H | -1.338375 | -0.753223 | 1.614164 |
| C | 0.278489 | 2.510149 | 2.924680 |
| H | 1.072320 | 2.756448 | 0.944208 |
| C | -0.489528 | 1.723804 | 3.784475 |
| H | -1.662339 | -0.077924 | 3.958086 |
| H | 0.743536 | 3.423083 | 3.290823 |
| H | -0.630786 | 2.018214 | 4.821098 |
| F | 3.292747 | 1.214125 | -0.283972 |
| F | 4.190286 | -1.809902 | 3.174406 |

**3**

| | | | |
|---|---|---|---|
| Pd | 0.130414 | 0.506181 | -0.609402 |
| C | 1.776188 | -0.454820 | 0.204415 |
| C | 3.048488 | 0.112523 | 0.097503 |
| C | 4.204419 | -0.387554 | 0.687467 |
| C | 4.070434 | -1.543543 | 1.443392 |
| C | 2.849855 | -2.180921 | 1.611149 |
| C | 1.725908 | -1.619817 | 0.997552 |
| H | 5.164174 | 0.102378 | 0.566444 |
| H | 2.784763 | -3.080042 | 2.215209 |
| H | 0.766510 | -2.107479 | 1.153559 |
| H | 1.769266 | -1.467764 | -1.471721 |
| P | -1.712543 | 1.721942 | -1.405675 |
| C | -2.782517 | 2.609127 | -0.210173 |
| H | -3.583967 | 3.148607 | -0.725450 |
| H | -3.213856 | 1.894694 | 0.495588 |
| H | -2.176187 | 3.311943 | 0.366923 |
| C | -1.212454 | 3.047425 | -2.579017 |
| H | -2.082284 | 3.558792 | -3.005467 |
| H | -0.588086 | 3.777019 | -2.055827 |

| | | | |
|---|---|---|---|
| H | -0.617640 | 2.604851 | -3.382395 |
| C | -2.924411 | 0.749563 | -2.394536 |
| H | -3.714430 | 1.389978 | -2.802246 |
| H | -2.402236 | 0.254136 | -3.217212 |
| H | -3.378912 | -0.019219 | -1.763220 |
| C | 1.199051 | -0.940111 | -3.193656 |
| O | 1.848225 | -1.779187 | -2.416269 |
| O | 0.532669 | 0.007400 | -2.769206 |
| C | 1.345843 | -1.234401 | -4.656063 |
| H | 2.391777 | -1.094968 | -4.946687 |
| H | 1.089784 | -2.278894 | -4.853728 |
| H | 0.710122 | -0.569605 | -5.239453 |
| C | -0.304557 | 0.970313 | 1.267278 |
| C | -1.200613 | 0.188800 | 2.012704 |
| C | 0.247853 | 2.105943 | 1.879523 |
| C | -1.546045 | 0.539126 | 3.322041 |
| H | -1.637312 | -0.707438 | 1.576148 |
| C | -0.099033 | 2.457408 | 3.187577 |
| H | 0.965624 | 2.719234 | 1.340012 |
| C | -0.999805 | 1.677948 | 3.915221 |
| H | -2.242338 | -0.084642 | 3.878949 |
| H | 0.346214 | 3.340570 | 3.641004 |
| H | -1.265474 | 1.949404 | 4.933580 |
| F | 3.202722 | 1.242282 | -0.650447 |
| F | 5.174826 | -2.060343 | 2.032603 |

**4**

| | | | |
|---|---|---|---|
| C | 3.617469 | -0.886869 | -0.221532 |
| Pd | 1.668834 | -0.354882 | -0.059391 |
| C | 4.302501 | -0.512422 | 0.927722 |
| C | 4.397852 | -1.522585 | -1.196914 |
| H | 3.934299 | -1.845971 | -2.125015 |
| C | 5.651672 | -0.710888 | 1.177308 |
| H | 6.126953 | -0.393236 | 2.098615 |
| C | 5.765855 | -1.758291 | -1.017220 |
| H | 6.363874 | -2.251326 | -1.777103 |
| C | 6.362448 | -1.346813 | 0.166398 |
| P | -0.564197 | 0.335221 | 0.275264 |
| C | -0.888709 | 1.143335 | 1.899388 |
| H | -0.254752 | 2.028501 | 2.004990 |
| H | -1.937845 | 1.444091 | 1.992216 |
| H | -0.643784 | 0.452349 | 2.711223 |
| C | -1.838199 | -0.987135 | 0.215523 |
| H | -2.843592 | -0.578243 | 0.361563 |
| H | -1.787891 | -1.488681 | -0.754688 |
| H | -1.634303 | -1.728513 | 0.993216 |
| C | -1.204897 | 1.567193 | -0.928447 |
| H | -1.130944 | 1.152049 | -1.937282 |
| H | -2.247767 | 1.827046 | -0.717726 |
| H | -0.592735 | 2.472476 | -0.886891 |
| C | 1.269232 | -1.076552 | -1.844130 |

| | | | |
|---|---|---|---|
| C | 1.380196 | -0.262704 | -2.979224 |
| C | 0.857475 | -2.407523 | -1.993385 |
| C | 1.065668 | -0.772466 | -4.243437 |
| H | 1.724233 | 0.763709 | -2.887792 |
| C | 0.545390 | -2.909332 | -3.261352 |
| H | 0.790983 | -3.062487 | -1.129124 |
| C | 0.644676 | -2.094860 | -4.390234 |
| H | 1.160206 | -0.129853 | -5.115967 |
| H | 0.230867 | -3.945742 | -3.361935 |
| H | 0.405802 | -2.488985 | -5.374291 |
| F | 3.559565 | 0.117150 | 1.910018 |
| F | 7.686941 | -1.568751 | 0.353156 |

TS-RE

| | | | |
|---|---|---|---|
| C | 3.298816 | -1.074154 | -0.484167 |
| Pd | 1.397342 | -0.564320 | 0.004730 |
| C | 4.310225 | -0.108963 | -0.401229 |
| C | 3.715494 | -2.404803 | -0.284603 |
| H | 2.983949 | -3.203905 | -0.363467 |
| C | 5.642985 | -0.397403 | -0.137339 |
| H | 6.386707 | 0.389303 | -0.078671 |
| C | 5.036868 | -2.747128 | -0.001379 |
| H | 5.338105 | -3.777116 | 0.157845 |
| C | 5.978580 | -1.728923 | 0.061418 |
| P | -0.804629 | 0.009620 | 0.581376 |
| C | -1.036829 | 1.307224 | 1.872870 |
| H | -0.529320 | 2.225108 | 1.563205 |
| H | -2.098419 | 1.522686 | 2.038516 |
| H | -0.589743 | 0.975657 | 2.814552 |
| C | -1.894177 | -1.339478 | 1.209870 |
| H | -2.906974 | -0.975471 | 1.416158 |
| H | -1.946060 | -2.140438 | 0.467174 |
| H | -1.470572 | -1.756880 | 2.127805 |
| C | -1.795635 | 0.680743 | -0.816813 |
| H | -1.834630 | -0.060004 | -1.619908 |
| H | -2.814573 | 0.933017 | -0.502557 |
| H | -1.304779 | 1.574410 | -1.211320 |
| C | 1.873747 | -0.843744 | -1.952207 |
| C | 2.047792 | 0.284280 | -2.772391 |
| C | 1.482768 | -2.054456 | -2.550411 |
| C | 1.802931 | 0.204426 | -4.145051 |
| H | 2.374429 | 1.223669 | -2.340881 |
| C | 1.236840 | -2.124134 | -3.921654 |
| H | 1.362711 | -2.949589 | -1.946550 |
| C | 1.395649 | -0.995595 | -4.728802 |
| H | 1.937810 | 1.091321 | -4.760058 |
| H | 0.924412 | -3.069345 | -4.359779 |
| H | 1.212955 | -1.054109 | -5.798271 |
| F | 4.001132 | 1.200770 | -0.572476 |
| F | 7.269161 | -2.037332 | 0.322323 |

Ph*-Ph

| | | | |
|---|---|---|---|
| C | 3.370195 | -1.113692 | -1.557030 |
| C | 4.203453 | -0.031904 | -1.247425 |
| C | 3.201008 | -2.070657 | -0.542918 |
| C | 4.841673 | 0.119109 | -0.023726 |
| C | 3.820210 | -1.963046 | 0.699890 |
| C | 4.632026 | -0.862044 | 0.934179 |
| C | 2.707330 | -1.272530 | -2.873681 |
| C | 2.031239 | -0.209140 | -3.491049 |
| C | 2.722365 | -2.520254 | -3.516063 |
| C | 1.385364 | -0.392820 | -4.712141 |
| H | 2.001151 | 0.762204 | -3.007484 |
| C | 2.075578 | -2.702936 | -4.737215 |
| H | 3.263359 | -3.347583 | -3.063796 |
| C | 1.403771 | -1.639141 | -5.339913 |
| H | 0.861965 | 0.440956 | -5.172342 |
| H | 2.104603 | -3.675303 | -5.221560 |
| H | 0.900509 | -1.779109 | -6.292627 |
| F | 4.434188 | 0.917430 | -2.179622 |
| F | 5.240252 | -0.733392 | 2.131894 |
| H | 5.486512 | 0.969168 | 0.166484 |
| H | 3.672799 | -2.705763 | 1.476205 |
| H | 2.545237 | -2.914996 | -0.734798 |

1Fo-1Fm

**2**

| | | | |
|---|---|---|---|
| Pd | 0.366531 | 0.298282 | -0.785964 |
| C | 1.992598 | -1.581979 | -0.390853 |
| C | 2.715329 | -0.383475 | -0.232551 |
| C | 3.140481 | -0.022988 | 1.050264 |
| C | 2.876432 | -0.799221 | 2.163180 |
| C | 2.159631 | -1.990910 | 2.005502 |
| C | 1.734901 | -2.358272 | 0.742009 |
| H | 3.218998 | -0.477234 | 3.140486 |
| H | 1.930214 | -2.621512 | 2.857603 |
| H | 1.739707 | -1.942622 | -1.383125 |
| P | -1.484941 | 1.459570 | -1.374483 |
| C | -1.222636 | 3.267931 | -1.363311 |
| H | -2.128161 | 3.783449 | -1.701236 |
| H | -0.978297 | 3.595614 | -0.349741 |
| H | -0.388867 | 3.484781 | -2.034903 |
| C | -2.074974 | 1.082293 | -3.065848 |
| H | -3.012244 | 1.616501 | -3.255813 |
| H | -1.312969 | 1.404481 | -3.777042 |
| H | -2.241648 | 0.007539 | -3.172146 |
| C | -2.998264 | 1.226157 | -0.363576 |
| H | -3.819661 | 1.808129 | -0.795588 |
| H | -3.278204 | 0.169587 | -0.347623 |

| | | | |
|---|---|---|---|
| H | -2.820899 | 1.548090 | 0.664101 |
| C | 1.299960 | 0.867239 | -3.585080 |
| O | 0.930258 | 2.041177 | -3.438250 |
| O | 1.116425 | -0.084828 | -2.726873 |
| C | 2.032224 | 0.437474 | -4.846968 |
| H | 1.581529 | -0.469864 | -5.259758 |
| H | 2.016934 | 1.237983 | -5.588105 |
| H | 3.072610 | 0.197515 | -4.601924 |
| C | -0.219398 | 0.556411 | 1.102517 |
| C | -0.953526 | -0.429942 | 1.779987 |
| C | 0.170049 | 1.698549 | 1.819747 |
| C | -1.270700 | -0.288740 | 3.134333 |
| H | -1.284339 | -1.322123 | 1.252347 |
| C | -0.145565 | 1.841287 | 3.175192 |
| H | 0.738784 | 2.484692 | 1.326756 |
| C | -0.868849 | 0.848432 | 3.837551 |
| H | -1.837148 | -1.069148 | 3.638115 |
| H | 0.175238 | 2.732099 | 3.710831 |
| H | -1.119910 | 0.961011 | 4.889053 |
| H | 3.039061 | 0.186360 | -1.097234 |
| F | 1.054415 | -3.514548 | 0.589311 |
| F | 3.848220 | 1.115234 | 1.196274 |

TS-CMD

| | | | |
|---|---|---|---|
| Pd | 0.131484 | 0.422579 | -0.822195 |
| C | 1.921052 | -0.709916 | -0.126520 |
| C | 2.977328 | 0.050771 | 0.382928 |
| C | 3.736847 | -0.299991 | 1.490953 |
| C | 3.436473 | -1.490424 | 2.151009 |
| C | 2.400672 | -2.280163 | 1.663645 |
| C | 1.659211 | -1.920543 | 0.551946 |
| H | 4.539771 | 0.346158 | 1.830899 |
| H | 3.996000 | -1.809826 | 3.024197 |
| H | 0.877788 | -2.590735 | 0.204039 |
| H | 1.938991 | -0.850736 | -1.472276 |
| P | -1.734642 | 1.608684 | -1.385231 |
| C | -2.719926 | 2.477153 | -0.111887 |
| H | -3.570820 | 2.989343 | -0.572950 |
| H | -3.078449 | 1.758995 | 0.629462 |
| H | -2.089863 | 3.201888 | 0.409234 |
| C | -1.351503 | 2.919239 | -2.611288 |
| H | -2.265486 | 3.409566 | -2.963789 |
| H | -0.695373 | 3.665979 | -2.155963 |
| H | -0.826841 | 2.464129 | -3.454875 |
| C | -2.964275 | 0.558725 | -2.252574 |
| H | -3.793696 | 1.159670 | -2.640949 |
| H | -2.460895 | 0.045372 | -3.075313 |
| H | -3.357262 | -0.192318 | -1.561890 |
| C | 1.204129 | -0.715433 | -3.400375 |
| O | 2.152583 | -1.164930 | -2.682822 |
| O | 0.224436 | -0.060346 | -2.944608 |

| | | | |
|---|---|---|---|
| C | 1.277311 | -0.986987 | -4.882440 |
| H | 2.152844 | -0.476471 | -5.295393 |
| H | 1.416817 | -2.057883 | -5.053008 |
| H | 0.376527 | -0.638248 | -5.388284 |
| C | -0.105959 | 0.967716 | 1.078485 |
| C | -0.852830 | 0.179491 | 1.966640 |
| C | 0.462338 | 2.154490 | 1.565386 |
| C | -1.027507 | 0.565486 | 3.299422 |
| H | -1.297861 | -0.753532 | 1.627484 |
| C | 0.288727 | 2.540534 | 2.898573 |
| H | 1.059735 | 2.782831 | 0.908367 |
| C | -0.460047 | 1.749845 | 3.771368 |
| H | -1.605496 | -0.067103 | 3.969823 |
| H | 0.745619 | 3.461855 | 3.253848 |
| H | -0.594700 | 2.049527 | 4.807390 |
| F | 3.296714 | 1.212694 | -0.242849 |
| F | 2.118762 | -3.444023 | 2.302300 |

**3**

| | | | |
|---|---|---|---|
| Pd | 0.138399 | 0.501789 | -0.603539 |
| C | 1.783662 | -0.451293 | 0.210531 |
| C | 3.055079 | 0.119504 | 0.107294 |
| C | 4.207441 | -0.399007 | 0.685171 |
| C | 4.116577 | -1.577179 | 1.427137 |
| C | 2.869649 | -2.173413 | 1.548896 |
| C | 1.725162 | -1.636796 | 0.970805 |
| H | 5.156389 | 0.112926 | 0.557098 |
| H | 4.986074 | -2.022587 | 1.898784 |
| H | 1.800171 | -1.479113 | -1.489074 |
| P | -1.712367 | 1.710040 | -1.398004 |
| C | -2.786068 | 2.589416 | -0.200267 |
| H | -3.590349 | 3.125717 | -0.714420 |
| H | -3.213601 | 1.871362 | 0.504132 |
| H | -2.183127 | 3.294059 | 0.378126 |
| C | -1.221225 | 3.039876 | -2.570256 |
| H | -2.094496 | 3.547191 | -2.994510 |
| H | -0.599976 | 3.772052 | -2.046966 |
| H | -0.625315 | 2.601873 | -3.375332 |
| C | -2.919262 | 0.731219 | -2.386402 |
| H | -3.712841 | 1.367433 | -2.793762 |
| H | -2.394988 | 0.238384 | -3.209297 |
| H | -3.369423 | -0.039878 | -1.754805 |
| C | 1.214676 | -0.934090 | -3.200435 |
| O | 1.881093 | -1.772567 | -2.435745 |
| O | 0.535573 | -0.002407 | -2.762830 |
| C | 1.360203 | -1.210896 | -4.666219 |
| H | 2.403113 | -1.054362 | -4.958976 |
| H | 1.117307 | -2.256551 | -4.874097 |
| H | 0.713436 | -0.548529 | -5.240086 |
| C | -0.288269 | 0.979291 | 1.272583 |
| C | -1.169023 | 0.195493 | 2.033126 |

| | | | |
|---|---|---|---|
| C | 0.255056 | 2.128758 | 1.866643 |
| C | -1.509541 | 0.557483 | 3.340510 |
| H | -1.596816 | -0.711707 | 1.610869 |
| C | -0.087332 | 2.491854 | 3.172763 |
| H | 0.961817 | 2.743649 | 1.314583 |
| C | -0.973479 | 1.710235 | 3.915819 |
| H | -2.193079 | -0.068736 | 3.910173 |
| H | 0.350128 | 3.385798 | 3.612454 |
| H | -1.235315 | 1.990498 | 4.932780 |
| F | 3.200265 | 1.267528 | -0.620303 |
| H | 0.779928 | -2.147175 | 1.134377 |
| F | 2.764636 | -3.321636 | 2.267136 |

**4**

| | | | |
|---|---|---|---|
| C | 3.618451 | -0.905872 | -0.225220 |
| Pd | 1.675021 | -0.360620 | -0.064863 |
| C | 4.293379 | -0.537678 | 0.933321 |
| C | 4.391290 | -1.542695 | -1.203832 |
| H | 3.956160 | -1.868741 | -2.143859 |
| C | 5.637747 | -0.747494 | 1.186221 |
| H | 6.085865 | -0.426484 | 2.121621 |
| C | 5.745220 | -1.765922 | -0.974209 |
| C | 6.389840 | -1.384929 | 0.195504 |
| H | 7.448590 | -1.582693 | 0.324159 |
| P | -0.553680 | 0.343285 | 0.273487 |
| C | -0.872713 | 1.149539 | 1.899421 |
| H | -0.233931 | 2.031050 | 2.006377 |
| H | -1.920202 | 1.455526 | 1.993574 |
| H | -0.630649 | 0.455535 | 2.709522 |
| C | -1.833454 | -0.973114 | 0.211204 |
| H | -2.836847 | -0.559901 | 0.358719 |
| H | -1.785740 | -1.472359 | -0.760320 |
| H | -1.632595 | -1.717325 | 0.986972 |
| C | -1.187693 | 1.580582 | -0.927989 |
| H | -1.115886 | 1.166637 | -1.937457 |
| H | -2.229195 | 1.845279 | -0.716591 |
| H | -0.571027 | 2.482729 | -0.884937 |
| C | 1.267414 | -1.070649 | -1.852926 |
| C | 1.385028 | -0.252342 | -2.983995 |
| C | 0.845987 | -2.397807 | -2.008034 |
| C | 1.066625 | -0.753860 | -4.250514 |
| H | 1.737312 | 0.770870 | -2.887931 |
| C | 0.530080 | -2.891276 | -3.278308 |
| H | 0.774920 | -3.056509 | -1.146953 |
| C | 0.635459 | -2.072233 | -4.403223 |
| H | 1.167152 | -0.108373 | -5.120199 |
| H | 0.208819 | -3.925075 | -3.383905 |
| H | 0.394622 | -2.460255 | -5.389185 |
| F | 3.532936 | 0.093397 | 1.907072 |
| F | 6.476356 | -2.386115 | -1.937637 |

TS-RE

| | | | |
|---|---|---|---|
| C | 3.295093 | -1.073845 | -0.491165 |
| Pd | 1.395095 | -0.563255 | -0.002124 |
| C | 4.307967 | -0.109397 | -0.408460 |
| C | 3.696178 | -2.407823 | -0.284314 |
| H | 2.982935 | -3.223011 | -0.352919 |
| C | 5.636034 | -0.409445 | -0.139506 |
| H | 6.364258 | 0.394032 | -0.088693 |
| C | 5.019490 | -2.708335 | -0.001476 |
| C | 6.009065 | -1.736899 | 0.070128 |
| H | 7.036203 | -2.014193 | 0.280577 |
| P | -0.806946 | 0.009572 | 0.584535 |
| C | -1.034306 | 1.307982 | 1.875776 |
| H | -0.528766 | 2.225961 | 1.563205 |
| H | -2.095365 | 1.522703 | 2.045666 |
| H | -0.583124 | 0.977469 | 2.815868 |
| C | -1.891557 | -1.340649 | 1.218148 |
| H | -2.904002 | -0.977948 | 1.428296 |
| H | -1.945125 | -2.142206 | 0.476246 |
| H | -1.463596 | -1.756881 | 2.134580 |
| C | -1.802968 | 0.678594 | -0.810881 |
| H | -1.844118 | -0.062858 | -1.613201 |
| H | -2.821042 | 0.930036 | -0.493229 |
| H | -1.314385 | 1.572498 | -1.207644 |
| C | 1.876424 | -0.842794 | -1.959119 |
| C | 2.049957 | 0.286853 | -2.776842 |
| C | 1.491285 | -2.054445 | -2.558525 |
| C | 1.808038 | 0.207658 | -4.150069 |
| H | 2.374547 | 1.225835 | -2.343127 |
| C | 1.248273 | -2.123394 | -3.930242 |
| H | 1.374901 | -2.950966 | -1.956130 |
| C | 1.405103 | -0.993084 | -4.735306 |
| H | 1.942117 | 1.095223 | -4.764225 |
| H | 0.940886 | -3.069258 | -4.370318 |
| H | 1.224940 | -1.051100 | -5.805250 |
| F | 3.997385 | 1.202589 | -0.585970 |
| F | 5.362857 | -4.004692 | 0.206292 |

Ph*-Ph

| | | | |
|---|---|---|---|
| C | 3.359729 | -1.172881 | -1.544415 |
| C | 4.168521 | -0.052195 | -1.295769 |
| C | 3.227144 | -2.093738 | -0.497018 |
| C | 4.789001 | 0.104414 | -0.066295 |
| C | 3.848553 | -1.935220 | 0.733746 |
| C | 4.649056 | -0.817603 | 0.961509 |
| C | 2.682572 | -1.336529 | -2.853105 |
| C | 2.050168 | -0.238024 | -3.455531 |
| C | 2.679047 | -2.566668 | -3.528134 |
| C | 1.434153 | -0.363923 | -4.699449 |
| H | 2.022577 | 0.715559 | -2.934618 |

| | | | |
|---|---|---|---|
| C | 2.064890 | -2.690250 | -4.772712 |
| H | 3.168474 | -3.426376 | -3.082043 |
| C | 1.440128 | -1.590919 | -5.363327 |
| H | 0.942702 | 0.496288 | -5.145921 |
| H | 2.077575 | -3.649172 | -5.283685 |
| H | 0.959400 | -1.690572 | -6.332592 |
| F | 2.441857 | -3.183191 | -0.664741 |
| H | 3.693811 | -2.683225 | 1.504110 |
| H | 4.332732 | 0.686572 | -2.073356 |
| H | 5.152889 | -0.662689 | 1.909322 |
| F | 5.568422 | 1.192203 | 0.132574 |

**set2Fo**

2Fo

**2**

| | | | |
|---|---|---|---|
| Pd | 0.278260 | 0.433905 | -0.845389 |
| C | 2.561702 | -0.478840 | -0.344733 |
| C | 2.986959 | 0.188423 | 0.812545 |
| C | 2.955762 | -0.377341 | 2.075994 |
| C | 2.484302 | -1.685694 | 2.196448 |
| C | 2.075497 | -2.416091 | 1.081945 |
| C | 2.142332 | -1.804809 | -0.164875 |
| H | 3.281774 | 0.196711 | 2.935507 |
| H | 2.441127 | -2.145910 | 3.179224 |
| H | 1.733620 | -3.442094 | 1.161025 |
| H | 2.739043 | -0.041616 | -1.337589 |
| P | -1.670327 | 1.409507 | -1.360466 |
| C | -1.876337 | 3.158466 | -0.857861 |
| H | -2.833789 | 3.543955 | -1.224362 |
| H | -1.839205 | 3.239195 | 0.230515 |
| H | -1.063668 | 3.756501 | -1.278857 |
| C | -1.975919 | 1.441667 | -3.163104 |
| H | -2.974488 | 1.841589 | -3.369738 |
| H | -1.221560 | 2.066585 | -3.647038 |
| H | -1.874783 | 0.430830 | -3.562570 |
| C | -3.152686 | 0.577307 | -0.677189 |
| H | -4.063503 | 1.091350 | -1.002268 |
| H | -3.180410 | -0.458588 | -1.025754 |
| H | -3.100783 | 0.578269 | 0.413965 |
| C | 1.541224 | 0.093695 | -3.533207 |
| O | 2.495712 | 0.770557 | -3.120339 |
| O | 0.498862 | -0.223834 | -2.835513 |
| C | 1.555904 | -0.472187 | -4.944061 |
| H | 0.550458 | -0.509422 | -5.371034 |
| H | 2.221821 | 0.115070 | -5.579139 |
| H | 1.935763 | -1.499259 | -4.903002 |
| C | -0.105502 | 0.937874 | 1.050887 |
| C | -0.756182 | 0.031058 | 1.903462 |

| | | | |
|---|---|---|---|
| C | 0.338003 | 2.152575 | 1.598049 |
| C | -0.938167 | 0.318131 | 3.260455 |
| H | -1.118951 | -0.918474 | 1.514005 |
| C | 0.159882 | 2.440611 | 2.954369 |
| H | 0.849405 | 2.877409 | 0.968084 |
| C | -0.481731 | 1.525153 | 3.791128 |
| H | -1.440390 | -0.403908 | 3.900981 |
| H | 0.524559 | 3.383511 | 3.356164 |
| H | -0.625852 | 1.751493 | 4.844431 |
| F | 3.464160 | 1.436764 | 0.677925 |
| F | 1.837192 | -2.538803 | -1.247426 |

TS-CMD

| | | | |
|---|---|---|---|
| Pd | 0.201674 | 0.490825 | -0.915063 |
| C | 2.051381 | -0.554386 | -0.177624 |
| C | 2.999239 | 0.246545 | 0.473247 |
| C | 3.672820 | -0.103195 | 1.633562 |
| C | 3.392177 | -1.348405 | 2.198241 |
| C | 2.472244 | -2.214838 | 1.605621 |
| C | 1.841628 | -1.791886 | 0.445491 |
| H | 4.388810 | 0.579586 | 2.078012 |
| H | 3.899553 | -1.649022 | 3.110516 |
| H | 2.246190 | -3.187892 | 2.028073 |
| H | 2.184713 | -0.610387 | -1.474564 |
| P | -1.739810 | 1.573119 | -1.409913 |
| C | -1.901849 | 3.282798 | -0.768366 |
| H | -2.854319 | 3.722943 | -1.082347 |
| H | -1.846757 | 3.268099 | 0.322654 |
| H | -1.079736 | 3.895979 | -1.147560 |
| C | -2.030066 | 1.768154 | -3.209406 |
| H | -2.983911 | 2.274405 | -3.391668 |
| H | -1.213359 | 2.344618 | -3.649631 |
| H | -2.031134 | 0.785011 | -3.684559 |
| C | -3.272319 | 0.754559 | -0.823522 |
| H | -4.155159 | 1.326178 | -1.129113 |
| H | -3.331859 | -0.252766 | -1.244704 |
| H | -3.247633 | 0.673436 | 0.265744 |
| C | 1.609202 | -0.322304 | -3.463915 |
| O | 2.527040 | -0.796925 | -2.729629 |
| O | 0.566049 | 0.245341 | -3.025256 |
| C | 1.779864 | -0.457269 | -4.958567 |
| H | 0.982656 | 0.061319 | -5.492165 |
| H | 2.754104 | -0.057691 | -5.253006 |
| H | 1.770528 | -1.518912 | -5.224310 |
| C | -0.250658 | 0.785818 | 1.007412 |
| C | -0.994791 | -0.159706 | 1.729986 |
| C | 0.197590 | 1.929648 | 1.686342 |
| C | -1.283180 | 0.032530 | 3.085084 |
| H | -1.345120 | -1.065356 | 1.239365 |
| C | -0.090197 | 2.123046 | 3.041087 |
| H | 0.790314 | 2.675423 | 1.161094 |

| | | | |
|---|---|---|---|
| C | -0.835446 | 1.176930 | 3.746209 |
| H | -1.856489 | -0.719054 | 3.623758 |
| H | 0.274509 | 3.015545 | 3.545221 |
| H | -1.059301 | 1.326714 | 4.799207 |
| F | 3.287564 | 1.450648 | -0.074822 |
| F | 0.962231 | -2.645568 | -0.130894 |

**3**

| | | | |
|---|---|---|---|
| Pd | 0.135872 | 0.479027 | -0.641189 |
| C | 1.770463 | -0.520601 | 0.170843 |
| C | 3.003980 | 0.090860 | 0.408903 |
| C | 4.065902 | -0.480711 | 1.101093 |
| C | 3.897147 | -1.766427 | 1.615119 |
| C | 2.695379 | -2.447940 | 1.422929 |
| C | 1.684650 | -1.803043 | 0.718800 |
| H | 4.989509 | 0.073293 | 1.233242 |
| H | 4.706145 | -2.240288 | 2.163474 |
| H | 2.535430 | -3.449259 | 1.809224 |
| F | 0.524344 | -2.496750 | 0.540620 |
| H | 2.140581 | -1.085687 | -1.631897 |
| P | -1.744615 | 1.652238 | -1.383451 |
| C | -2.785447 | 2.549491 | -0.171165 |
| H | -3.622610 | 3.048422 | -0.670179 |
| H | -3.166154 | 1.846668 | 0.574197 |
| H | -2.176436 | 3.287397 | 0.357068 |
| C | -1.349186 | 2.946039 | -2.630138 |
| H | -2.256861 | 3.415216 | -3.025477 |
| H | -0.720102 | 3.713379 | -2.170290 |
| H | -0.787662 | 2.489255 | -3.449180 |
| C | -2.961967 | 0.595471 | -2.270528 |
| H | -3.790767 | 1.189353 | -2.671375 |
| H | -2.456247 | 0.077720 | -3.089581 |
| H | -3.359389 | -0.156738 | -1.583329 |
| C | 1.302237 | -0.782012 | -3.298066 |
| O | 2.261498 | -1.335166 | -2.591704 |
| O | 0.416435 | -0.073726 | -2.811052 |
| C | 1.375067 | -1.090916 | -4.763328 |
| H | 2.344481 | -0.773385 | -5.158061 |
| H | 1.302159 | -2.172522 | -4.911316 |
| H | 0.569265 | -0.586482 | -5.294937 |
| C | -0.215992 | 1.035984 | 1.229056 |
| C | -1.029063 | 0.262193 | 2.070295 |
| C | 0.310654 | 2.235481 | 1.731185 |
| C | -1.324476 | 0.687555 | 3.369403 |
| H | -1.427992 | -0.686264 | 1.719704 |
| C | 0.014105 | 2.659009 | 3.030611 |
| H | 0.967060 | 2.842888 | 1.113066 |
| C | -0.808503 | 1.889937 | 3.855053 |
| H | -1.955613 | 0.069491 | 4.004685 |
| H | 0.436098 | 3.591787 | 3.399115 |
| H | -1.036374 | 2.218466 | 4.865808 |

| | | | |
|---|---|---|---|
| F | 3.201343 | 1.345296 | -0.086822 |

**4**

| | | | |
|---|---|---|---|
| C | 3.544871 | -0.944921 | -0.008293 |
| Pd | 1.583632 | -0.450363 | 0.144043 |
| C | 4.544072 | -0.023903 | -0.319640 |
| C | 4.030617 | -2.223138 | 0.263275 |
| C | 5.905705 | -0.303628 | -0.349071 |
| H | 6.615548 | 0.479285 | -0.595810 |
| C | 5.373112 | -2.584793 | 0.255700 |
| H | 5.661926 | -3.605002 | 0.486899 |
| C | 6.315483 | -1.604900 | -0.057394 |
| H | 7.372167 | -1.855792 | -0.073362 |
| P | -0.685216 | 0.139250 | 0.367503 |
| C | -1.200675 | 0.695378 | 2.048091 |
| H | -0.619529 | 1.574618 | 2.341094 |
| H | -2.265863 | 0.949559 | 2.073943 |
| H | -1.008534 | -0.098947 | 2.775302 |
| C | -1.889804 | -1.196274 | -0.005303 |
| H | -2.921591 | -0.841156 | 0.087556 |
| H | -1.718965 | -1.555068 | -1.023974 |
| H | -1.732840 | -2.033154 | 0.680976 |
| C | -1.254051 | 1.515357 | -0.707908 |
| H | -1.070874 | 1.250495 | -1.752764 |
| H | -2.320616 | 1.719035 | -0.565501 |
| H | -0.680779 | 2.418614 | -0.480985 |
| C | 1.383160 | -0.882432 | -1.770023 |
| C | 1.571990 | 0.113410 | -2.734403 |
| C | 1.009120 | -2.171643 | -2.164391 |
| C | 1.348142 | -0.174459 | -4.084942 |
| H | 1.907119 | 1.104535 | -2.443928 |
| C | 0.788321 | -2.448096 | -3.517957 |
| H | 0.903915 | -2.964852 | -1.430152 |
| C | 0.950608 | -1.451908 | -4.481393 |
| H | 1.498688 | 0.606111 | -4.827317 |
| H | 0.498992 | -3.453589 | -3.815194 |
| H | 0.783403 | -1.672799 | -5.532173 |
| F | 4.175073 | 1.257280 | -0.611822 |
| F | 3.132869 | -3.204062 | 0.570967 |

TS-RE

| | | | |
|---|---|---|---|
| C | 3.285565 | -1.089162 | -0.487720 |
| Pd | 1.381227 | -0.569278 | 0.014867 |
| C | 4.313656 | -0.133170 | -0.436048 |
| C | 3.735937 | -2.396714 | -0.239161 |
| C | 5.650913 | -0.418662 | -0.201739 |
| H | 6.372101 | 0.391690 | -0.180007 |
| C | 5.055984 | -2.748948 | 0.001007 |
| H | 5.304804 | -3.789057 | 0.184124 |
| C | 6.023359 | -1.744863 | 0.013243 |

| | | | |
|---|---|---|---|
| H | 7.063245 | -1.993968 | 0.201080 |
| P | -0.820677 | 0.014673 | 0.578253 |
| C | -1.067606 | 1.316389 | 1.862752 |
| H | -0.564789 | 2.236260 | 1.551337 |
| H | -2.131404 | 1.525211 | 2.022888 |
| H | -0.622373 | 0.991739 | 2.807693 |
| C | -1.905657 | -1.338179 | 1.205369 |
| H | -2.922366 | -0.980116 | 1.402930 |
| H | -1.945579 | -2.143159 | 0.466379 |
| H | -1.485023 | -1.748708 | 2.127709 |
| C | -1.806670 | 0.675049 | -0.828776 |
| H | -1.837942 | -0.069850 | -1.628348 |
| H | -2.828602 | 0.923566 | -0.521108 |
| H | -1.318307 | 1.569383 | -1.224832 |
| C | 1.913260 | -0.865637 | -1.932047 |
| C | 2.081860 | 0.277678 | -2.735775 |
| C | 1.501954 | -2.064548 | -2.544513 |
| C | 1.816391 | 0.223951 | -4.104595 |
| H | 2.416473 | 1.208050 | -2.293174 |
| C | 1.240080 | -2.103974 | -3.914493 |
| H | 1.384331 | -2.963973 | -1.952361 |
| C | 1.394828 | -0.963686 | -4.704251 |
| H | 1.944530 | 1.122451 | -4.703957 |
| H | 0.914605 | -3.039331 | -4.364112 |
| H | 1.195441 | -1.001540 | -5.771736 |
| F | 3.995796 | 1.173486 | -0.622603 |
| F | 2.826115 | -3.404779 | -0.224952 |

Ph*-Ph

| | | | |
|---|---|---|---|
| C | 3.359165 | -1.142295 | -1.555450 |
| C | 4.240803 | -0.089271 | -1.277522 |
| C | 3.160801 | -2.032632 | -0.491627 |
| C | 4.881001 | 0.083676 | -0.058388 |
| C | 3.771908 | -1.907009 | 0.747941 |
| C | 4.639260 | -0.837034 | 0.959310 |
| C | 2.690926 | -1.304466 | -2.870388 |
| C | 1.966928 | -0.247220 | -3.439607 |
| C | 2.771881 | -2.519927 | -3.564588 |
| C | 1.337996 | -0.403634 | -4.673460 |
| H | 1.891204 | 0.698071 | -2.910627 |
| C | 2.144470 | -2.673592 | -4.799318 |
| H | 3.333784 | -3.345215 | -3.137719 |
| C | 1.424894 | -1.616517 | -5.357586 |
| H | 0.777540 | 0.424148 | -5.099382 |
| H | 2.219478 | -3.621120 | -5.325895 |
| H | 0.934512 | -1.737272 | -6.319685 |
| F | 4.501830 | 0.804335 | -2.255578 |
| F | 2.312573 | -3.067917 | -0.671017 |
| H | 5.556256 | 0.922191 | 0.072315 |
| H | 5.128844 | -0.720158 | 1.921181 |
| H | 3.557616 | -2.635849 | 1.521911 |

2Fo-1Fp

**2**

| | | | |
|---|---|---|---|
| Pd | 0.282806 | 0.457074 | -0.860675 |
| C | 2.526867 | -0.486433 | -0.327107 |
| C | 2.970823 | 0.177091 | 0.826282 |
| C | 2.953328 | -0.379582 | 2.093322 |
| C | 2.473708 | -1.680522 | 2.193295 |
| C | 2.047774 | -2.428456 | 1.103679 |
| C | 2.106821 | -1.811379 | -0.139538 |
| H | 3.282293 | 0.173235 | 2.964093 |
| H | 1.708696 | -3.451083 | 1.214254 |
| H | 2.715096 | -0.058987 | -1.325064 |
| P | -1.679470 | 1.414096 | -1.366902 |
| C | -1.907599 | 3.157311 | -0.854119 |
| H | -2.871788 | 3.531082 | -1.214966 |
| H | -1.867687 | 3.232802 | 0.234525 |
| H | -1.105320 | 3.769398 | -1.274838 |
| C | -1.990681 | 1.450905 | -3.168429 |
| H | -2.995761 | 1.836607 | -3.370291 |
| H | -1.247176 | 2.089530 | -3.651187 |
| H | -1.874996 | 0.443972 | -3.573700 |
| C | -3.147355 | 0.558041 | -0.682201 |
| H | -4.066330 | 1.061939 | -1.000023 |
| H | -3.163375 | -0.476011 | -1.036907 |
| H | -3.090739 | 0.553231 | 0.408716 |
| C | 1.575129 | 0.083227 | -3.537768 |
| O | 2.565919 | 0.690360 | -3.101254 |
| O | 0.506631 | -0.181623 | -2.858389 |
| C | 1.573557 | -0.453193 | -4.959873 |
| H | 0.569829 | -0.441386 | -5.391940 |
| H | 2.265824 | 0.120172 | -5.579335 |
| H | 1.913873 | -1.494653 | -4.939178 |
| C | -0.097199 | 0.953115 | 1.038126 |
| C | -0.727654 | 0.035706 | 1.894753 |
| C | 0.336690 | 2.171994 | 1.583770 |
| C | -0.897350 | 0.315919 | 3.254808 |
| H | -1.084440 | -0.916439 | 1.506042 |
| C | 0.169843 | 2.453442 | 2.942971 |
| H | 0.831351 | 2.905650 | 0.950563 |
| C | -0.449732 | 1.526825 | 3.783956 |
| H | -1.380142 | -0.415496 | 3.899252 |
| H | 0.526692 | 3.399706 | 3.343833 |
| H | -0.582648 | 1.746772 | 4.839974 |
| F | 3.455055 | 1.418923 | 0.690383 |
| F | 1.782838 | -2.545576 | -1.212960 |
| F | 2.434712 | -2.251639 | 3.408799 |

TS-CMD

| | | | |
|---|---|---|---|
| Pd | 0.204554 | 0.491964 | -0.915608 |
| C | 2.057015 | -0.555968 | -0.192173 |
| C | 2.991471 | 0.244375 | 0.479842 |
| C | 3.643893 | -0.096687 | 1.654341 |
| C | 3.334656 | -1.341128 | 2.189907 |
| C | 2.438202 | -2.224117 | 1.600111 |
| C | 1.837300 | -1.794343 | 0.427179 |
| H | 4.352444 | 0.567365 | 2.134266 |
| H | 2.221989 | -3.190888 | 2.038258 |
| H | 2.210157 | -0.608074 | -1.487973 |
| P | -1.740028 | 1.568909 | -1.410197 |
| C | -1.900489 | 3.282361 | -0.778678 |
| H | -2.854181 | 3.720136 | -1.092201 |
| H | -1.842179 | 3.274572 | 0.312250 |
| H | -1.080056 | 3.893717 | -1.164385 |
| C | -2.036368 | 1.751362 | -3.209827 |
| H | -2.991470 | 2.255160 | -3.392123 |
| H | -1.221972 | 2.325933 | -3.656708 |
| H | -2.038076 | 0.765063 | -3.678419 |
| C | -3.268700 | 0.752005 | -0.812108 |
| H | -4.153515 | 1.320702 | -1.117338 |
| H | -3.329058 | -0.257914 | -1.226912 |
| H | -3.239278 | 0.677516 | 0.277500 |
| C | 1.617903 | -0.312805 | -3.470371 |
| O | 2.545165 | -0.780162 | -2.742201 |
| O | 0.571751 | 0.243474 | -3.025016 |
| C | 1.781810 | -0.443767 | -4.965952 |
| H | 0.979890 | 0.072663 | -5.494511 |
| H | 2.753126 | -0.040237 | -5.264518 |
| H | 1.774911 | -1.504928 | -5.233823 |
| C | -0.244090 | 0.788303 | 1.007245 |
| C | -0.978690 | -0.160784 | 1.735067 |
| C | 0.202886 | 1.934615 | 1.683033 |
| C | -1.257304 | 0.029471 | 3.092539 |
| H | -1.330344 | -1.067116 | 1.246525 |
| C | -0.075232 | 2.126005 | 3.040148 |
| H | 0.786591 | 2.684481 | 1.153413 |
| C | -0.809528 | 1.175507 | 3.750728 |
| H | -1.822830 | -0.724921 | 3.635382 |
| H | 0.288608 | 3.020177 | 3.541820 |
| H | -1.024854 | 1.323132 | 4.805714 |
| F | 3.293450 | 1.446086 | -0.057313 |
| F | 0.974740 | -2.650383 | -0.163090 |
| F | 3.938872 | -1.712819 | 3.333299 |

**3**

| | | | |
|---|---|---|---|
| Pd | 0.135034 | 0.476950 | -0.652592 |
| C | 1.776339 | -0.527829 | 0.154199 |
| C | 3.003736 | 0.089384 | 0.407338 |
| C | 4.060901 | -0.463182 | 1.123198 |

| | | | |
|---|---|---|---|
| C | 3.860857 | -1.736850 | 1.636506 |
| C | 2.681523 | -2.443533 | 1.448317 |
| C | 1.685884 | -1.802836 | 0.717994 |
| H | 4.989652 | 0.072981 | 1.278230 |
| H | 2.543721 | -3.438554 | 1.854547 |
| F | 0.535151 | -2.503718 | 0.533465 |
| H | 2.124845 | -1.075612 | -1.642416 |
| P | -1.744515 | 1.652082 | -1.384446 |
| C | -2.781516 | 2.548022 | -0.168424 |
| H | -3.619372 | 3.047771 | -0.665374 |
| H | -3.161213 | 1.844592 | 0.576839 |
| H | -2.171209 | 3.285297 | 0.359137 |
| C | -1.348578 | 2.946452 | -2.629822 |
| H | -2.256400 | 3.417297 | -3.022710 |
| H | -0.717754 | 3.712432 | -2.170137 |
| H | -0.789440 | 2.489752 | -3.450492 |
| C | -2.962612 | 0.595611 | -2.270008 |
| H | -3.791449 | 1.190106 | -2.669745 |
| H | -2.457769 | 0.078062 | -3.089676 |
| H | -3.359832 | -0.156450 | -1.582565 |
| C | 1.292160 | -0.777937 | -3.311498 |
| O | 2.250643 | -1.328247 | -2.602429 |
| O | 0.404769 | -0.070502 | -2.825056 |
| C | 1.366692 | -1.087359 | -4.776311 |
| H | 2.335501 | -0.767232 | -5.170465 |
| H | 1.297281 | -2.169256 | -4.923786 |
| H | 0.559870 | -0.585582 | -5.308868 |
| C | -0.212912 | 1.031556 | 1.218864 |
| C | -1.022953 | 0.255633 | 2.060894 |
| C | 0.317682 | 2.228595 | 1.722367 |
| C | -1.310006 | 0.675819 | 3.363586 |
| H | -1.426734 | -0.690115 | 1.708415 |
| C | 0.029460 | 2.646825 | 3.025417 |
| H | 0.970146 | 2.838781 | 1.102740 |
| C | -0.789050 | 1.875119 | 3.851379 |
| H | -1.938675 | 0.056214 | 3.999718 |
| H | 0.454547 | 3.577581 | 3.395303 |
| H | -1.010273 | 2.199433 | 4.864899 |
| F | 3.209626 | 1.335640 | -0.095700 |
| F | 4.857692 | -2.315505 | 2.341039 |

**4**

| | | | |
|---|---|---|---|
| C | 3.544649 | -0.942967 | 0.001705 |
| Pd | 1.580124 | -0.449938 | 0.146801 |
| C | 4.544054 | -0.022861 | -0.310548 |
| C | 4.032387 | -2.221970 | 0.264496 |
| C | 5.907938 | -0.294966 | -0.350324 |
| H | 6.636820 | 0.469158 | -0.593394 |
| C | 5.373202 | -2.593351 | 0.250594 |
| H | 5.688561 | -3.606171 | 0.471911 |
| C | 6.287907 | -1.598538 | -0.064284 |

| | | | |
|---|---|---|---|
| P | -0.686779 | 0.138469 | 0.364074 |
| C | -1.198238 | 0.696393 | 2.044916 |
| H | -0.616110 | 1.575579 | 2.336048 |
| H | -2.263178 | 0.951328 | 2.072026 |
| H | -1.005675 | -0.097362 | 2.772607 |
| C | -1.891148 | -1.197555 | -0.006114 |
| H | -2.922646 | -0.842013 | 0.087813 |
| H | -1.721974 | -1.557195 | -1.024734 |
| H | -1.733674 | -2.033733 | 0.680876 |
| C | -1.254675 | 1.513626 | -0.712527 |
| H | -1.073244 | 1.247431 | -1.757319 |
| H | -2.320853 | 1.718259 | -0.568935 |
| H | -0.680597 | 2.416750 | -0.487184 |
| C | 1.376022 | -0.880718 | -1.766568 |
| C | 1.568619 | 0.114601 | -2.730491 |
| C | 1.002807 | -2.170085 | -2.160582 |
| C | 1.350913 | -0.174789 | -4.081733 |
| H | 1.901274 | 1.106494 | -2.439693 |
| C | 0.788200 | -2.447832 | -3.514906 |
| H | 0.892943 | -2.962432 | -1.426065 |
| C | 0.955331 | -1.452687 | -4.478515 |
| H | 1.504510 | 0.605053 | -4.824169 |
| H | 0.499666 | -3.453435 | -3.812351 |
| H | 0.793050 | -1.674684 | -5.529777 |
| F | 4.180924 | 1.257622 | -0.596443 |
| F | 3.142135 | -3.205025 | 0.571082 |
| F | 7.603187 | -1.911134 | -0.090195 |

TS-RE

| | | | |
|---|---|---|---|
| C | 3.285119 | -1.088808 | -0.489934 |
| Pd | 1.380761 | -0.568356 | 0.015503 |
| C | 4.314433 | -0.133901 | -0.437457 |
| C | 3.736766 | -2.395678 | -0.239065 |
| C | 5.654450 | -0.410985 | -0.204701 |
| H | 6.394530 | 0.379883 | -0.176225 |
| C | 5.055124 | -2.756862 | 0.001167 |
| H | 5.329640 | -3.787891 | 0.189971 |
| C | 5.996862 | -1.738362 | 0.006662 |
| P | -0.821726 | 0.015452 | 0.576568 |
| C | -1.068020 | 1.315404 | 1.862618 |
| H | -0.565283 | 2.235730 | 1.552462 |
| H | -2.131803 | 1.524008 | 2.022911 |
| H | -0.622922 | 0.989438 | 2.807145 |
| C | -1.905756 | -1.338817 | 1.201643 |
| H | -2.922567 | -0.981273 | 1.399407 |
| H | -1.945470 | -2.142914 | 0.461692 |
| H | -1.485257 | -1.750182 | 2.123651 |
| C | -1.806762 | 0.677283 | -0.830260 |
| H | -1.838081 | -0.066776 | -1.630606 |
| H | -2.828707 | 0.925504 | -0.522541 |
| H | -1.318450 | 1.572139 | -1.225190 |

| | | | |
|---|---|---|---|
| C | 1.919034 | -0.867156 | -1.930347 |
| C | 2.084588 | 0.276777 | -2.734053 |
| C | 1.505058 | -2.065664 | -2.542091 |
| C | 1.814459 | 0.223638 | -4.101923 |
| H | 2.418630 | 1.207844 | -2.292531 |
| C | 1.238630 | -2.104121 | -3.911162 |
| H | 1.386974 | -2.965340 | -1.950439 |
| C | 1.391236 | -0.963648 | -4.700973 |
| H | 1.939956 | 1.122705 | -4.700904 |
| H | 0.910826 | -3.039042 | -4.359874 |
| H | 1.188473 | -1.000959 | -5.767765 |
| F | 4.002599 | 1.170408 | -0.624146 |
| F | 2.833052 | -3.404307 | -0.223513 |
| F | 7.288663 | -2.047787 | 0.241137 |

Ph*-Ph

| | | | |
|---|---|---|---|
| C | 3.361232 | -1.143119 | -1.556033 |
| C | 4.252672 | -0.097370 | -1.282892 |
| C | 3.156322 | -2.026031 | -0.487520 |
| C | 4.899509 | 0.082475 | -0.067723 |
| C | 3.766893 | -1.907978 | 0.753645 |
| C | 4.635155 | -0.841353 | 0.932405 |
| C | 2.690521 | -1.305220 | -2.869855 |
| C | 1.961626 | -0.249382 | -3.435008 |
| C | 2.775399 | -2.518961 | -3.566356 |
| C | 1.331963 | -0.405326 | -4.668529 |
| H | 1.882632 | 0.694284 | -2.903377 |
| C | 2.145468 | -2.672710 | -4.799839 |
| H | 3.342147 | -3.342799 | -3.142808 |
| C | 1.421698 | -1.616799 | -5.354780 |
| H | 0.768189 | 0.421322 | -5.092131 |
| H | 2.222630 | -3.618918 | -5.328372 |
| H | 0.930215 | -1.737322 | -6.316291 |
| F | 5.245684 | -0.697164 | 2.123804 |
| F | 4.522049 | 0.789569 | -2.259904 |
| F | 2.301165 | -3.052686 | -0.656732 |
| H | 5.586699 | 0.905993 | 0.083680 |
| H | 3.563715 | -2.616972 | 1.546961 |

<u>2Fo-2Fm</u>

**2**

| | | | |
|---|---|---|---|
| Pd | 0.339638 | 0.566486 | -0.760295 |
| C | 2.186681 | -1.678631 | -0.360851 |
| C | 2.624532 | -0.355074 | -0.234272 |
| C | 2.942954 | 0.107364 | 1.047139 |
| C | 2.801476 | -0.708288 | 2.161927 |
| C | 2.334868 | -2.010116 | 2.026763 |
| C | 2.029199 | -2.488957 | 0.762994 |

| | | | |
|---|---|---|---|
| H | 2.208041 | -2.640436 | 2.899660 |
| P | -1.562650 | 1.565822 | -1.383323 |
| C | -1.208555 | 3.148756 | -2.231124 |
| H | -2.128759 | 3.579346 | -2.640729 |
| H | -0.760028 | 3.854956 | -1.527854 |
| H | -0.496978 | 2.958779 | -3.036944 |
| C | -2.423128 | 0.554827 | -2.641397 |
| H | -3.253397 | 1.115779 | -3.083768 |
| H | -1.695732 | 0.282909 | -3.410283 |
| H | -2.808966 | -0.358241 | -2.180668 |
| C | -2.856181 | 1.989643 | -0.162756 |
| H | -3.703699 | 2.466086 | -0.666918 |
| H | -3.193766 | 1.085940 | 0.349524 |
| H | -2.447906 | 2.667384 | 0.590483 |
| C | 1.892625 | 0.917469 | -3.339436 |
| O | 2.856692 | 1.329743 | -2.676685 |
| O | 0.762487 | 0.524152 | -2.844560 |
| C | 1.994575 | 0.806231 | -4.851506 |
| H | 1.056210 | 1.091031 | -5.334930 |
| H | 2.817166 | 1.420477 | -5.221431 |
| H | 2.193994 | -0.238956 | -5.113089 |
| C | -0.279944 | 0.562141 | 1.131947 |
| C | -0.975308 | -0.541827 | 1.650690 |
| C | 0.013677 | 1.627448 | 1.997799 |
| C | -1.343899 | -0.589922 | 2.999645 |
| H | -1.231589 | -1.379788 | 1.004986 |
| C | -0.352761 | 1.579055 | 3.346125 |
| H | 0.552260 | 2.497916 | 1.628509 |
| C | -1.034987 | 0.470933 | 3.851744 |
| H | -1.876558 | -1.458503 | 3.381050 |
| H | -0.099293 | 2.408819 | 4.001994 |
| H | -1.322516 | 0.435251 | 4.899189 |
| H | 2.869057 | 0.262333 | -1.117162 |
| F | 1.594446 | -3.750139 | 0.612942 |
| F | 3.408182 | 1.349844 | 1.205417 |
| F | 1.972085 | -2.208894 | -1.569735 |
| F | 3.121589 | -0.240243 | 3.375892 |

TS-CMD

| | | | |
|---|---|---|---|
| Pd | -0.052453 | 0.669776 | -0.014596 |
| C | 1.823701 | -0.614486 | -0.026698 |
| C | 2.992522 | 0.094029 | 0.264784 |
| C | 3.940421 | -0.371327 | 1.167231 |
| C | 3.754550 | -1.586845 | 1.812574 |
| C | 2.611470 | -2.323108 | 1.530706 |
| C | 1.674170 | -1.841370 | 0.625879 |
| H | 4.487893 | -1.953907 | 2.521721 |
| H | 1.451032 | -0.594138 | -1.274591 |
| P | -1.909558 | 1.964850 | 0.114637 |
| C | -2.481818 | 2.639675 | 1.715326 |
| H | -3.382890 | 3.244724 | 1.569512 |

| | | | |
|---|---|---|---|
| H | -2.694994 | 1.820973 | 2.406785 |
| H | -1.694382 | 3.252130 | 2.161034 |
| C | -1.750622 | 3.439863 | -0.961921 |
| H | -2.692643 | 3.997039 | -1.005697 |
| H | -0.962757 | 4.092602 | -0.576827 |
| H | -1.468582 | 3.106094 | -1.963285 |
| C | -3.379393 | 1.095200 | -0.551819 |
| H | -4.241154 | 1.769411 | -0.602153 |
| H | -3.141455 | 0.723488 | -1.551221 |
| H | -3.624946 | 0.243711 | 0.088219 |
| C | 0.264054 | -0.055344 | -2.934129 |
| O | 1.283634 | -0.717570 | -2.577998 |
| O | -0.471133 | 0.603902 | -2.138942 |
| C | -0.082729 | -0.054032 | -4.403478 |
| H | 0.733869 | 0.412238 | -4.963109 |
| H | -0.170831 | -1.084746 | -4.757869 |
| H | -1.011261 | 0.487331 | -4.587471 |
| C | 0.188743 | 0.845864 | 1.954493 |
| C | -0.376959 | -0.087066 | 2.836231 |
| C | 0.949721 | 1.893596 | 2.493997 |
| C | -0.184049 | 0.022671 | 4.217326 |
| H | -0.964062 | -0.917896 | 2.450535 |
| C | 1.143057 | 2.002667 | 3.875051 |
| H | 1.408922 | 2.629985 | 1.837615 |
| C | 0.574518 | 1.069439 | 4.743069 |
| H | -0.625816 | -0.717542 | 4.880907 |
| H | 1.744147 | 2.819098 | 4.269467 |
| H | 0.724854 | 1.154258 | 5.816068 |
| F | 3.223232 | 1.271625 | -0.344743 |
| F | 2.414478 | -3.504325 | 2.143195 |
| F | 5.043056 | 0.355080 | 1.423696 |
| F | 0.586875 | -2.595361 | 0.379702 |

**3**

| | | | |
|---|---|---|---|
| Pd | 0.138213 | 0.477513 | -0.644400 |
| C | 1.777628 | -0.518989 | 0.176354 |
| C | 2.998981 | 0.115303 | 0.401678 |
| C | 4.039118 | -0.476111 | 1.113211 |
| C | 3.895429 | -1.750307 | 1.644639 |
| C | 2.692050 | -2.409536 | 1.435513 |
| C | 1.666001 | -1.798206 | 0.720656 |
| H | 4.700218 | -2.218555 | 2.199173 |
| H | 2.140916 | -1.089343 | -1.653804 |
| P | -1.743777 | 1.645837 | -1.379772 |
| C | -2.782035 | 2.544261 | -0.167467 |
| H | -3.620461 | 3.040058 | -0.667312 |
| H | -3.161003 | 1.843125 | 0.580262 |
| H | -2.173576 | 3.285103 | 0.357138 |
| C | -1.347287 | 2.933899 | -2.630795 |
| H | -2.255309 | 3.401362 | -3.027100 |
| H | -0.718214 | 3.703136 | -2.174228 |

| | | | |
|---|---|---|---|
| H | -0.786685 | 2.473937 | -3.448596 |
| C | -2.956620 | 0.579188 | -2.259159 |
| H | -3.787677 | 1.168307 | -2.662044 |
| H | -2.449904 | 0.059101 | -3.076004 |
| H | -3.350906 | -0.170463 | -1.567457 |
| C | 1.288747 | -0.788483 | -3.309917 |
| O | 2.255944 | -1.339450 | -2.610226 |
| O | 0.407119 | -0.081714 | -2.813684 |
| C | 1.350070 | -1.099192 | -4.774381 |
| H | 2.315974 | -0.781142 | -5.177208 |
| H | 1.277505 | -2.181152 | -4.919976 |
| H | 0.539385 | -0.596615 | -5.300108 |
| C | -0.213731 | 1.045110 | 1.223518 |
| C | -1.021320 | 0.271438 | 2.069301 |
| C | 0.318561 | 2.244224 | 1.719120 |
| C | -1.305335 | 0.697405 | 3.370823 |
| H | -1.424981 | -0.676258 | 1.722130 |
| C | 0.033034 | 2.667666 | 3.021119 |
| H | 0.970157 | 2.851389 | 1.095740 |
| C | -0.783429 | 1.898970 | 3.851835 |
| H | -1.931651 | 0.079995 | 4.011218 |
| H | 0.459375 | 3.599600 | 3.386253 |
| H | -1.002147 | 2.227371 | 4.864532 |
| F | 3.211847 | 1.357890 | -0.093471 |
| F | 2.520472 | -3.650610 | 1.931810 |
| F | 5.196653 | 0.190268 | 1.291956 |
| F | 0.521650 | -2.502754 | 0.548959 |

**4**

| | | | |
|---|---|---|---|
| C | 3.684951 | -0.935003 | -0.239398 |
| Pd | 1.706446 | -0.407833 | -0.141353 |
| C | 4.268227 | -0.522984 | 0.950967 |
| C | 4.542624 | -1.562764 | -1.133086 |
| C | 5.604650 | -0.700255 | 1.272959 |
| C | 5.893520 | -1.756823 | -0.839149 |
| C | 6.443143 | -1.330577 | 0.362342 |
| H | 7.493037 | -1.485773 | 0.581139 |
| P | -0.496971 | 0.294795 | 0.216070 |
| C | -0.731933 | 1.117564 | 1.846484 |
| H | -0.081860 | 1.994430 | 1.915586 |
| H | -1.771734 | 1.433091 | 1.983518 |
| H | -0.459815 | 0.428805 | 2.651376 |
| C | -1.780983 | -1.016197 | 0.218920 |
| H | -2.775430 | -0.594522 | 0.398330 |
| H | -1.772241 | -1.528003 | -0.747045 |
| H | -1.554524 | -1.749923 | 0.997502 |
| C | -1.160385 | 1.524471 | -0.974028 |
| H | -1.129646 | 1.100019 | -1.981055 |
| H | -2.190601 | 1.799552 | -0.724996 |
| H | -0.534881 | 2.421362 | -0.961535 |
| C | 1.200340 | -1.076517 | -1.919983 |

| | | | |
|---|---|---|---|
| C | 1.293541 | -0.237100 | -3.034602 |
| C | 0.727119 | -2.383916 | -2.070248 |
| C | 0.902295 | -0.705560 | -4.292840 |
| H | 1.686256 | 0.770911 | -2.936002 |
| C | 0.338591 | -2.842247 | -3.333148 |
| H | 0.676529 | -3.055760 | -1.217973 |
| C | 0.420710 | -2.005933 | -4.446792 |
| H | 0.986972 | -0.048629 | -5.155425 |
| H | -0.019340 | -3.863438 | -3.441914 |
| H | 0.123641 | -2.367936 | -5.427205 |
| F | 3.444490 | 0.102102 | 1.861490 |
| F | 6.685481 | -2.371947 | -1.739894 |
| F | 6.091274 | -0.269030 | 2.453842 |
| F | 4.103281 | -2.012138 | -2.325351 |

TS-RE

| | | | |
|---|---|---|---|
| C | 3.283016 | -1.087707 | -0.510450 |
| Pd | 1.380110 | -0.565772 | -0.000030 |
| C | 4.295829 | -0.116659 | -0.450406 |
| C | 3.708151 | -2.400740 | -0.248990 |
| C | 5.624490 | -0.434173 | -0.196928 |
| C | 5.035345 | -2.722909 | 0.005044 |
| C | 6.018758 | -1.744533 | 0.031460 |
| H | 7.053215 | -1.992529 | 0.236631 |
| P | -0.823688 | 0.014829 | 0.579226 |
| C | -1.058787 | 1.312603 | 1.868634 |
| H | -0.559296 | 2.233672 | 1.555572 |
| H | -2.121372 | 1.520047 | 2.037800 |
| H | -0.605894 | 0.985589 | 2.809046 |
| C | -1.897698 | -1.343653 | 1.210583 |
| H | -2.913652 | -0.988972 | 1.417263 |
| H | -1.941425 | -2.146768 | 0.469836 |
| H | -1.468562 | -1.755188 | 2.128495 |
| C | -1.818226 | 0.676543 | -0.820465 |
| H | -1.854281 | -0.066606 | -1.621427 |
| H | -2.838318 | 0.922529 | -0.505142 |
| H | -1.334381 | 1.572991 | -1.217212 |
| C | 1.930981 | -0.867601 | -1.944832 |
| C | 2.096897 | 0.277453 | -2.746552 |
| C | 1.515608 | -2.066161 | -2.555156 |
| C | 1.824521 | 0.225154 | -4.113862 |
| H | 2.433092 | 1.207684 | -2.305322 |
| C | 1.247145 | -2.103222 | -3.923690 |
| H | 1.398374 | -2.966242 | -1.964275 |
| C | 1.399425 | -0.961798 | -4.712066 |
| H | 1.950450 | 1.124027 | -4.712750 |
| H | 0.918868 | -3.037568 | -4.372872 |
| H | 1.195458 | -0.998387 | -5.778617 |
| F | 4.002063 | 1.186259 | -0.640920 |
| F | 5.367751 | -4.004543 | 0.246694 |
| F | 6.540659 | 0.550859 | -0.155518 |

| | | | |
|---|---|---|---|
| F | 2.817074 | -3.414132 | -0.235978 |

Ph*-Ph

| | | | |
|---|---|---|---|
| C | 3.363048 | -1.143074 | -1.553594 |
| C | 4.239581 | -0.081314 | -1.297162 |
| C | 3.154909 | -2.046254 | -0.503405 |
| C | 4.869175 | 0.066501 | -0.065352 |
| C | 3.785358 | -1.895002 | 0.727468 |
| C | 4.650671 | -0.837538 | 0.963031 |
| C | 2.692007 | -1.304934 | -2.867528 |
| C | 1.969105 | -0.245631 | -3.433621 |
| C | 2.772563 | -2.521595 | -3.559209 |
| C | 1.338171 | -0.402736 | -4.666081 |
| H | 1.894485 | 0.699688 | -2.904614 |
| C | 2.143606 | -2.674104 | -4.793072 |
| H | 3.334786 | -3.347129 | -3.133390 |
| C | 1.424052 | -1.616099 | -5.349448 |
| H | 0.777520 | 0.424925 | -5.091495 |
| H | 2.217273 | -3.621351 | -5.319959 |
| H | 0.932380 | -1.736565 | -6.310795 |
| F | 5.706564 | 1.098130 | 0.120002 |
| F | 3.540489 | -2.785846 | 1.700228 |
| H | 5.141404 | -0.720975 | 1.922213 |
| F | 4.509465 | 0.814580 | -2.258710 |
| F | 2.312793 | -3.078772 | -0.661623 |

C6F5H

**2**

| | | | |
|---|---|---|---|
| Pd | 0.206668 | 0.347091 | -0.775160 |
| C | 2.046964 | -1.247977 | -0.232621 |
| C | 3.040560 | -0.263000 | -0.202542 |
| C | 3.633495 | 0.139560 | 0.990964 |
| C | 3.251833 | -0.476116 | 2.179594 |
| C | 2.289885 | -1.486555 | 2.180557 |
| C | 1.704683 | -1.858629 | 0.978965 |
| H | 1.681512 | -1.675445 | -1.188652 |
| P | -1.481254 | 1.680578 | -1.398683 |
| C | -2.478185 | 2.587801 | -0.163589 |
| H | -3.243585 | 3.186775 | -0.668449 |
| H | -2.955725 | 1.882012 | 0.519857 |
| H | -1.830980 | 3.239756 | 0.427525 |
| C | -0.865554 | 2.969972 | -2.540370 |
| H | -1.699908 | 3.515411 | -2.994253 |
| H | -0.228297 | 3.671534 | -1.995799 |
| H | -0.269927 | 2.476657 | -3.312288 |
| C | -2.715059 | 0.751373 | -2.381008 |
| H | -3.478754 | 1.429864 | -2.776454 |
| H | -2.199331 | 0.252949 | -3.204377 |
| H | -3.193445 | -0.006834 | -1.755868 |

| | | | |
|---|---|---|---|
| C | 0.811320 | -0.998077 | -3.428781 |
| O | 0.946178 | -2.079387 | -2.834649 |
| O | 0.543493 | 0.134836 | -2.862996 |
| C | 1.002520 | -0.929179 | -4.934277 |
| H | 2.033685 | -0.620849 | -5.140306 |
| H | 0.843053 | -1.912555 | -5.380057 |
| H | 0.339173 | -0.188916 | -5.388621 |
| C | -0.180270 | 0.754286 | 1.134777 |
| C | -1.074704 | -0.029581 | 1.880948 |
| C | 0.489610 | 1.800380 | 1.789789 |
| C | -1.270527 | 0.206117 | 3.245134 |
| H | -1.613170 | -0.847092 | 1.405470 |
| C | 0.293211 | 2.037040 | 3.154956 |
| H | 1.176732 | 2.440430 | 1.239024 |
| C | -0.587835 | 1.240752 | 3.887215 |
| H | -1.955194 | -0.425474 | 3.806592 |
| H | 0.831450 | 2.846346 | 3.643375 |
| H | -0.740185 | 1.423270 | 4.947540 |
| F | 4.569492 | 1.092402 | 1.007779 |
| F | 1.953765 | -2.076722 | 3.327909 |
| F | 3.814200 | -0.101848 | 3.324870 |
| F | 3.486028 | 0.284012 | -1.337102 |
| F | 0.801836 | -2.840842 | 0.992290 |

TS-CMD

| | | | |
|---|---|---|---|
| Pd | 0.148329 | 0.433754 | -0.840673 |
| C | 1.986912 | -0.736526 | -0.199761 |
| C | 3.018184 | 0.075615 | 0.279894 |
| C | 3.688548 | -0.171041 | 1.469581 |
| C | 3.327427 | -1.287382 | 2.222430 |
| C | 2.320058 | -2.142673 | 1.778467 |
| C | 1.679075 | -1.853195 | 0.582282 |
| H | 1.968433 | -0.925552 | -1.491238 |
| P | -1.703591 | 1.622442 | -1.389186 |
| C | -2.678446 | 2.496177 | -0.113083 |
| H | -3.529333 | 3.008738 | -0.573720 |
| H | -3.036924 | 1.781162 | 0.631167 |
| H | -2.045206 | 3.222014 | 0.402441 |
| C | -1.312503 | 2.921708 | -2.621962 |
| H | -2.225433 | 3.410401 | -2.979203 |
| H | -0.656176 | 3.670755 | -2.170933 |
| H | -0.787572 | 2.457389 | -3.460221 |
| C | -2.929591 | 0.561008 | -2.243423 |
| H | -3.763760 | 1.156719 | -2.629477 |
| H | -2.426853 | 0.047677 | -3.066492 |
| H | -3.314185 | -0.189221 | -1.547412 |
| C | 1.191974 | -0.724213 | -3.441284 |
| O | 2.126800 | -1.237172 | -2.755752 |
| O | 0.261203 | -0.011811 | -2.958973 |
| C | 1.198006 | -0.992515 | -4.926807 |
| H | 2.159665 | -0.685859 | -5.347646 |

| | | | |
|---|---|---|---|
| H | 1.098885 | -2.068857 | -5.096863 |
| H | 0.384835 | -0.463742 | -5.424995 |
| C | -0.108687 | 0.929507 | 1.070829 |
| C | -0.864198 | 0.114969 | 1.927629 |
| C | 0.483756 | 2.084375 | 1.603594 |
| C | -1.016245 | 0.441543 | 3.279301 |
| H | -1.333235 | -0.790840 | 1.548888 |
| C | 0.331817 | 2.410345 | 2.955483 |
| H | 1.080147 | 2.736687 | 0.968927 |
| C | -0.420201 | 1.591432 | 3.798805 |
| H | -1.599185 | -0.210421 | 3.926160 |
| H | 0.808530 | 3.305921 | 3.347906 |
| H | -0.536573 | 1.843878 | 4.849357 |
| F | 3.396710 | 1.153260 | -0.428423 |
| F | 3.953675 | -1.542433 | 3.369424 |
| F | 4.662099 | 0.634824 | 1.908843 |
| F | 1.991805 | -3.212592 | 2.511907 |
| F | 0.719302 | -2.702345 | 0.176494 |

**3**

| | | | |
|---|---|---|---|
| Pd | 0.127114 | 0.473968 | -0.652292 |
| C | 1.769649 | -0.530223 | 0.168485 |
| C | 2.985339 | 0.108017 | 0.407393 |
| C | 4.022100 | -0.457161 | 1.144034 |
| C | 3.848996 | -1.727350 | 1.687190 |
| C | 2.655062 | -2.411493 | 1.475948 |
| C | 1.650910 | -1.799629 | 0.731565 |
| H | 2.112886 | -1.094124 | -1.650853 |
| P | -1.747664 | 1.649450 | -1.384848 |
| C | -2.784827 | 2.548729 | -0.172664 |
| H | -3.620721 | 3.047587 | -0.673637 |
| H | -3.167509 | 1.847700 | 0.573232 |
| H | -2.175274 | 3.287220 | 0.353930 |
| C | -1.341087 | 2.938077 | -2.631446 |
| H | -2.245970 | 3.410396 | -3.029011 |
| H | -0.710053 | 3.703487 | -2.171221 |
| H | -0.780421 | 2.477431 | -3.448784 |
| C | -2.960826 | 0.587906 | -2.269308 |
| H | -3.788433 | 1.180688 | -2.673845 |
| H | -2.453098 | 0.067584 | -3.085323 |
| H | -3.360131 | -0.161298 | -1.580026 |
| C | 1.272947 | -0.796974 | -3.313173 |
| O | 2.233640 | -1.349865 | -2.606676 |
| O | 0.392190 | -0.084894 | -2.822000 |
| C | 1.339208 | -1.111004 | -4.776536 |
| H | 2.307622 | -0.796343 | -5.176020 |
| H | 1.264634 | -2.193087 | -4.920126 |
| H | 0.532085 | -0.607443 | -5.306774 |
| C | -0.224494 | 1.043407 | 1.214905 |
| C | -1.033632 | 0.271382 | 2.060568 |
| C | 0.314093 | 2.239199 | 1.711458 |

| | | | |
|---|---|---|---|
| C | -1.311335 | 0.694982 | 3.364258 |
| H | -1.444014 | -0.672914 | 1.711897 |
| C | 0.034822 | 2.660179 | 3.015657 |
| H | 0.965304 | 2.846134 | 1.087379 |
| C | -0.782019 | 1.892586 | 3.846946 |
| H | -1.938698 | 0.078892 | 4.004820 |
| H | 0.466192 | 3.589323 | 3.381852 |
| H | -0.995679 | 2.218949 | 4.861320 |
| F | 3.207034 | 1.342006 | -0.100344 |
| F | 4.830217 | -2.293047 | 2.396504 |
| F | 5.176339 | 0.194765 | 1.342149 |
| F | 2.495301 | -3.638017 | 1.992435 |
| F | 0.512658 | -2.508808 | 0.552974 |

**4**

| | | | |
|---|---|---|---|
| C | 3.687185 | -0.917615 | -0.233653 |
| Pd | 1.700056 | -0.405090 | -0.136273 |
| C | 4.281178 | -0.494562 | 0.946224 |
| C | 4.540643 | -1.546955 | -1.129512 |
| C | 5.620311 | -0.655264 | 1.268951 |
| C | 5.897352 | -1.738828 | -0.863150 |
| C | 6.438825 | -1.291650 | 0.338734 |
| P | -0.505474 | 0.283232 | 0.215983 |
| C | -0.739639 | 1.108896 | 1.844835 |
| H | -0.093719 | 1.989095 | 1.910330 |
| H | -1.780585 | 1.420037 | 1.983052 |
| H | -0.463228 | 0.423408 | 2.651049 |
| C | -1.782420 | -1.034149 | 0.224579 |
| H | -2.778193 | -0.616652 | 0.406250 |
| H | -1.774514 | -1.547404 | -0.740575 |
| H | -1.550393 | -1.765440 | 1.003781 |
| C | -1.174963 | 1.506876 | -0.976400 |
| H | -1.145124 | 1.079851 | -1.982331 |
| H | -2.205572 | 1.778934 | -0.725804 |
| H | -0.552637 | 2.405990 | -0.967570 |
| C | 1.194802 | -1.081710 | -1.912038 |
| C | 1.286860 | -0.245826 | -3.029062 |
| C | 0.728516 | -2.391934 | -2.056655 |
| C | 0.901553 | -0.722032 | -4.286292 |
| H | 1.673624 | 0.764747 | -2.933535 |
| C | 0.346110 | -2.857592 | -3.318805 |
| H | 0.678474 | -3.060009 | -1.201418 |
| C | 0.427386 | -2.025620 | -4.435740 |
| H | 0.985027 | -0.068386 | -5.151427 |
| H | -0.006472 | -3.880954 | -3.424107 |
| H | 0.134971 | -2.393394 | -5.415358 |
| F | 3.471550 | 0.131819 | 1.863649 |
| F | 7.738589 | -1.472290 | 0.599863 |
| F | 4.094593 | -2.008464 | -2.312996 |
| F | 6.694063 | -2.351036 | -1.750914 |
| F | 6.130877 | -0.221325 | 2.430500 |

TS-RE

| | | | |
|---|---|---|---|
| C | 3.283439 | -1.088733 | -0.512917 |
| Pd | 1.380334 | -0.566477 | 0.001107 |
| C | 4.296540 | -0.118897 | -0.450861 |
| C | 3.711635 | -2.399666 | -0.248857 |
| C | 5.629496 | -0.419561 | -0.199158 |
| C | 5.035142 | -2.736486 | 0.006061 |
| C | 6.006015 | -1.739781 | 0.027380 |
| P | -0.823382 | 0.016120 | 0.577529 |
| C | -1.056959 | 1.312456 | 1.868385 |
| H | -0.556108 | 2.233294 | 1.556851 |
| H | -2.119354 | 1.521120 | 2.037101 |
| H | -0.605161 | 0.983535 | 2.808637 |
| C | -1.898837 | -1.342209 | 1.206260 |
| H | -2.914519 | -0.986612 | 1.412558 |
| H | -1.943043 | -2.144362 | 0.464508 |
| H | -1.470940 | -1.755206 | 2.124077 |
| C | -1.815544 | 0.680746 | -0.822316 |
| H | -1.852336 | -0.061451 | -1.624121 |
| H | -2.835440 | 0.927862 | -0.507352 |
| H | -1.330293 | 1.577040 | -1.217688 |
| C | 1.936123 | -0.871214 | -1.942989 |
| C | 2.098639 | 0.274082 | -2.745292 |
| C | 1.516925 | -2.069432 | -2.551676 |
| C | 1.819951 | 0.221999 | -4.111285 |
| H | 2.435453 | 1.204891 | -2.305826 |
| C | 1.242203 | -2.105841 | -3.918942 |
| H | 1.399823 | -2.969499 | -1.960795 |
| C | 1.391888 | -0.964589 | -4.707981 |
| H | 1.943023 | 1.121172 | -4.710253 |
| H | 0.910648 | -3.039776 | -4.366485 |
| H | 1.183196 | -1.000895 | -5.773561 |
| F | 4.005975 | 1.182733 | -0.641356 |
| F | 2.825571 | -3.414813 | -0.234845 |
| F | 5.383701 | -4.005499 | 0.251638 |
| F | 7.280863 | -2.044194 | 0.279332 |
| F | 6.552429 | 0.548956 | -0.151960 |

Ph*-Ph

| | | | |
|---|---|---|---|
| C | 3.364520 | -1.145019 | -1.555215 |
| C | 4.245859 | -0.088445 | -1.297991 |
| C | 3.154746 | -2.044353 | -0.503107 |
| C | 4.883210 | 0.071333 | -0.071464 |
| C | 3.779602 | -1.907844 | 0.732537 |
| C | 4.649043 | -0.843651 | 0.950126 |
| C | 2.692607 | -1.305530 | -2.869244 |
| C | 1.958999 | -0.249327 | -3.426969 |
| C | 2.783448 | -2.517178 | -3.568027 |
| C | 1.328259 | -0.404334 | -4.659847 |

| | | | |
|---|---|---|---|
| H | 1.876036 | 0.691845 | -2.891671 |
| C | 2.152806 | -2.668159 | -4.801244 |
| H | 3.354802 | -3.339874 | -3.148625 |
| C | 1.423428 | -1.613007 | -5.350207 |
| H | 0.759961 | 0.420935 | -5.079631 |
| H | 2.233504 | -3.611627 | -5.333768 |
| H | 0.931196 | -1.732127 | -6.311389 |
| F | 4.522208 | 0.805134 | -2.256888 |
| F | 5.253496 | -0.701878 | 2.128886 |
| F | 5.724742 | 1.088456 | 0.126770 |
| F | 3.542569 | -2.783435 | 1.711872 |
| F | 2.309953 | -3.072706 | -0.656095 |