

## “Supporting Information for”

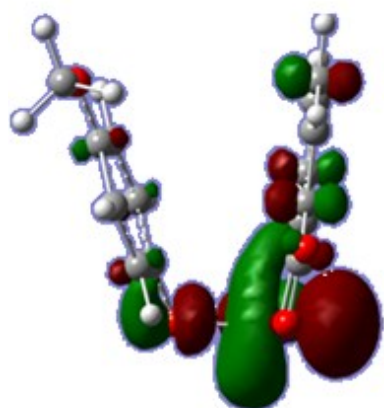
### Mechanistic Investigation into Phenol Oxidation by IBX Elucidated by DFT Calculations

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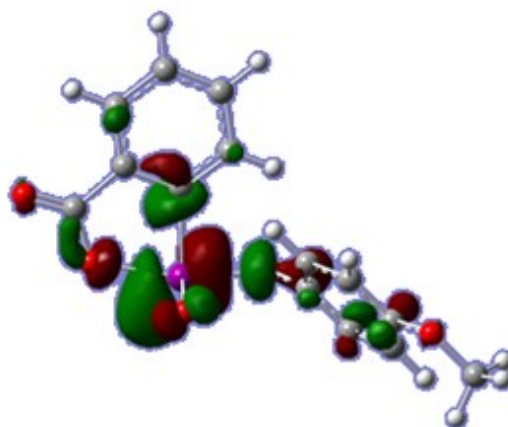
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#### Content

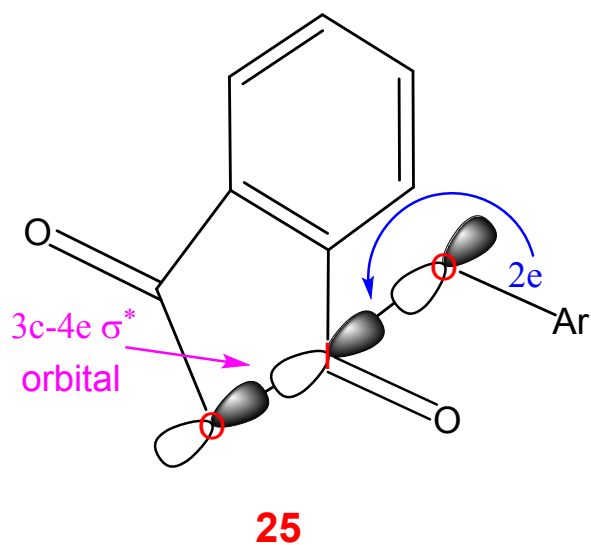
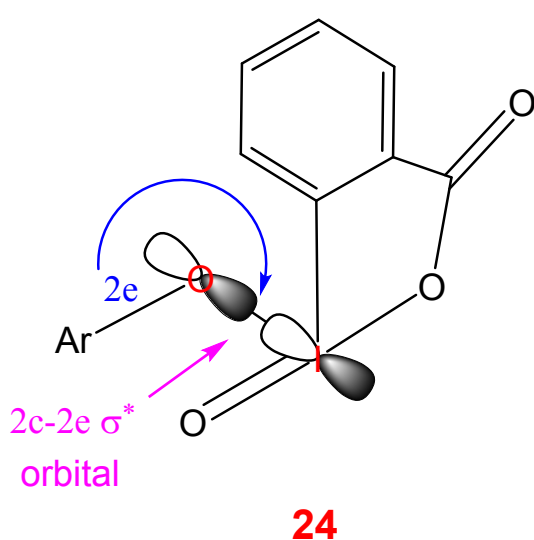
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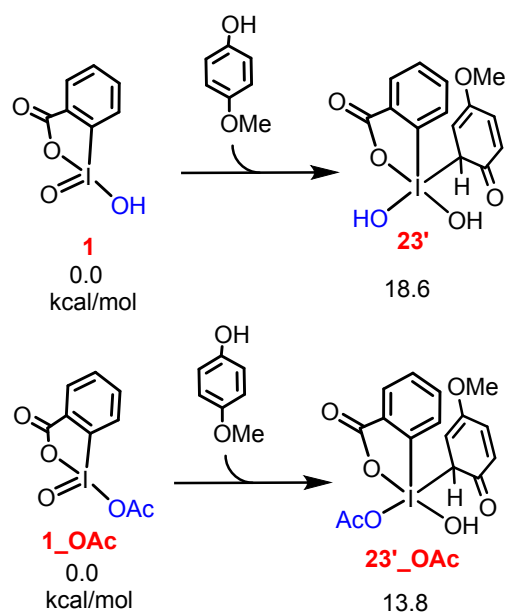
LUMO for **24**  
-1.964 eV



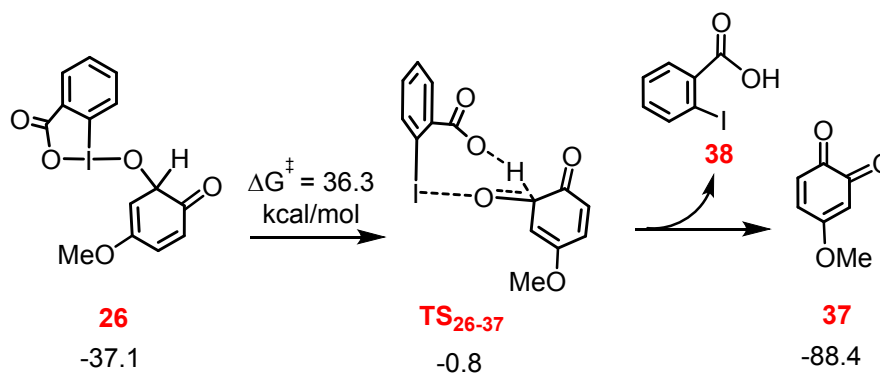
LUMO + 2 for **25**  
+0.229 eV



**Fig. S1** Spatial plots for LUMO of **24** and LUMO + 2 of **25**. For the redox process to take place from **24**, two electrons from the phenolate ligand are required to transfer to the LUMO of **24** which is a 2c-2e  $\sigma^*$  orbital. In contrast, the promotion of two electrons from the phenolate to the iodine(V) centre in **25** results in a 3c-4e  $\sigma^*$  orbital (LUMO +2) to be occupied. Since the 2c-2e  $\sigma^*$  orbital with an energy of -1.964 eV lies much lower in energy than the 3c-4e  $\sigma^*$  orbital ( $E = +0.229$  eV), **24** is more susceptible than **25** to drive the redox step.



**Fig. S2** Calculated relative free energies for dearomatized phenolate complexes **23'** and **23'\_OAc**.



**Fig. S3** Calculated mechanism for the second redox process via transition structure **TS<sub>26-37</sub>**.

**Table S1.** Cartesian coordinates and total energies for the calculated structures in N,N'-dimethylformamide (DMF):

**1**

E(SMD/M06-2X/BS1) = -581.621085 au

H(SMD/M06-2X/BS1) = -581.498110 au

G(SMD/M06-2X/BS1) = -581.547506 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -868.164172 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.93236000  | 0.24191800  | 0.10964200  |
| C | 1.10502400  | -1.90093900 | -0.06463200 |
| C | 1.56922400  | 0.49195000  | -0.00661200 |
| C | 3.37924600  | -1.07767600 | 0.13981800  |
| C | 2.47596300  | -2.13838200 | 0.05231800  |
| C | 0.69108700  | -0.57886300 | -0.08540000 |
| H | 4.44091000  | -1.28402100 | 0.22833600  |
| H | 2.83810800  | -3.16106000 | 0.07226300  |
| H | 0.39496500  | -2.71674400 | -0.14211300 |
| H | 3.62262000  | 1.07711800  | 0.17201400  |
| C | 0.99416700  | 1.87829200  | -0.06447600 |
| I | -1.31438900 | 0.02398500  | -0.19446900 |
| O | -0.31839000 | 1.88902700  | -0.20086600 |
| O | 1.68192600  | 2.87458600  | -0.00707600 |
| O | -1.88552100 | -1.85575700 | -0.19034200 |
| O | -1.80115300 | 0.27565000  | 1.49235300  |
| H | -1.93133400 | -2.15237400 | 0.73988100  |

**16-p-OMe**

E(SMD/M06-2X/BS1) = -421.8035633 au

H(SMD/M06-2X/BS1) = -421.658234 au

G(SMD/M06-2X/BS1) = -421.697834 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -421.9836904 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.81400200 | 0.00007600  | 0.08587700  |
| C | -1.12516000 | 1.20845700  | -0.01308900 |
| C | -1.12527700 | -1.20835400 | -0.01297300 |
| C | 0.25259500  | 1.20912100  | -0.21281000 |
| H | -1.67670000 | 2.14002500  | 0.06948200  |
| C | 0.25250600  | -1.20917500 | -0.21268900 |
| H | -1.67681700 | -2.13991600 | 0.06969900  |
| C | 0.93877800  | -0.00007200 | -0.31867100 |
| H | 0.80423900  | 2.14088600  | -0.29670700 |
| H | 0.80401100  | -2.14103200 | -0.29645100 |
| O | -3.17109000 | 0.00025300  | 0.33447000  |
| H | -3.64642800 | -0.00192300 | -0.51280200 |

|   |            |             |             |
|---|------------|-------------|-------------|
| O | 2.29314400 | -0.00011400 | -0.54803300 |
| C | 3.05665400 | 0.00004400  | 0.65237300  |
| H | 2.84529000 | -0.89311700 | 1.25323200  |
| H | 4.10845200 | 0.00023600  | 0.36074900  |
| H | 2.84496600 | 0.89314500  | 1.25320700  |

## 17

E(SMD/M06-2X/BS1) = -1003.452012 au

H(SMD/M06-2X/BS1) = -1003.179105 au

G(SMD/M06-2X/BS1) = -1003.249823 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1290.169715 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.13830700 | 0.94220000  | 2.12844100  |
| C | 0.96668700  | 2.15852000  | 0.69751100  |
| C | -0.21506200 | 0.16017800  | 1.44167100  |
| C | -1.00235200 | 2.32935000  | 2.10696000  |
| C | 0.04153700  | 2.93160500  | 1.40277500  |
| C | 0.80859500  | 0.78316500  | 0.74395900  |
| H | -1.71789300 | 2.94832300  | 2.63856200  |
| H | 0.13532200  | 4.01276900  | 1.39288400  |
| H | 1.76880200  | 2.61656500  | 0.12895400  |
| H | -1.94860500 | 0.45810300  | 2.66485100  |
| C | -0.28244700 | -1.34087000 | 1.40520300  |
| I | 2.06851800  | -0.57199100 | -0.24563900 |
| O | 0.69079900  | -1.88469200 | 0.70300000  |
| O | -1.14938500 | -1.96966900 | 1.97564300  |
| O | 3.09605500  | 0.93222300  | -0.98812700 |
| O | 3.31401400  | -0.95986600 | 0.95413300  |
| H | 3.79831200  | 1.15033400  | -0.34443100 |
| O | 0.52227000  | 0.71191600  | -2.38264900 |
| H | 0.72578100  | 1.66355400  | -2.40913800 |
| C | -0.75315800 | 0.52016400  | -1.91041900 |
| C | -1.17234900 | -0.79090700 | -1.72129700 |
| C | -1.58964600 | 1.58012400  | -1.55583900 |
| C | -2.41239400 | -1.05689800 | -1.13795200 |
| H | -0.52000400 | -1.60930400 | -2.01278900 |
| C | -2.82516900 | 1.31718500  | -0.98255700 |
| H | -1.26384800 | 2.60680500  | -1.70408400 |
| C | -3.23943000 | -0.00072400 | -0.75231400 |
| H | -2.70791400 | -2.08746700 | -0.98127200 |
| H | -3.47910900 | 2.13037700  | -0.68319700 |
| O | -4.44989200 | -0.15119400 | -0.15329000 |
| C | -4.82167100 | -1.46701500 | 0.21642600  |
| H | -4.07407200 | -1.91462700 | 0.88195700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.77196200 | -1.37778100 | 0.74400400  |
| H | -4.95615900 | -2.10834900 | -0.66251800 |

**TS<sub>17-18</sub>**

E(SMD/M06-2X/BS1) = -1079.824919 au

H(SMD/M06-2X/BS1) = -1079.528604 au

G(SMD/M06-2X/BS1) = -1079.601322 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1366.58471au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.17680900 | -0.76041600 | 2.20422000  |
| C | 0.90395800  | 1.12356200  | 1.92241000  |
| C | -0.19633200 | -0.92874500 | 1.23112800  |
| C | -1.11183900 | 0.35007800  | 3.04135800  |
| C | -0.07957700 | 1.27813200  | 2.90360000  |
| C | 0.81950500  | 0.00921600  | 1.10635800  |
| H | -1.87105100 | 0.49854000  | 3.80196800  |
| H | -0.03741300 | 2.14253900  | 3.55827700  |
| H | 1.68371100  | 1.86851800  | 1.81915300  |
| H | -1.97537500 | -1.49125300 | 2.28626900  |
| C | -0.21400400 | -2.07602900 | 0.27856900  |
| I | 2.10362000  | -0.49739400 | -0.47936000 |
| O | 0.77034000  | -2.01392800 | -0.63982900 |
| O | -1.00595000 | -2.98245700 | 0.30629400  |
| O | 3.15152200  | 1.43814400  | -0.16662000 |
| O | 3.32439800  | -1.34444400 | 0.47512800  |
| O | 0.46820000  | 0.99934100  | -1.52031800 |
| C | -0.83814400 | 0.88255900  | -1.23318600 |
| C | -1.58854800 | -0.19853800 | -1.71282700 |
| C | -1.49505700 | 1.81705600  | -0.40629200 |
| C | -2.92792200 | -0.37594400 | -1.35718900 |
| H | -1.10071900 | -0.92576500 | -2.35573500 |
| C | -2.82519800 | 1.65042100  | -0.05503300 |
| H | -0.93748000 | 2.66879200  | -0.02526100 |
| C | -3.55299500 | 0.54569000  | -0.51716000 |
| H | -3.46392500 | -1.23766100 | -1.73922200 |
| H | -3.32282400 | 2.36691900  | 0.59248200  |
| O | -4.84918000 | 0.46297500  | -0.10270200 |
| C | -5.58594700 | -0.66556500 | -0.52940300 |
| H | -5.12579800 | -1.59871600 | -0.18172800 |
| H | -6.57887800 | -0.56754100 | -0.08853200 |
| H | -5.67780400 | -0.69635400 | -1.62190700 |
| H | 3.63591400  | 1.50977200  | 0.67866000  |
| H | 0.97699700  | 2.34763300  | -1.19394600 |
| O | 1.53649800  | 3.13250600  | -0.78714500 |

|   |            |            |             |
|---|------------|------------|-------------|
| H | 2.53574100 | 2.31874800 | -0.38403000 |
| H | 1.81387400 | 3.71175400 | -1.51815400 |

## 18

E(SMD/M06-2X/BS1) = -1079.824958 au

H(SMD/M06-2X/BS1) = -1079.526419 au

G(SMD/M06-2X/BS1) = -1079.600965 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1366.584462 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.16367800 | -0.76723300 | 2.21892800  |
| C | 0.91490600  | 1.11835500  | 1.93032000  |
| C | -0.18854100 | -0.93217100 | 1.23983800  |
| C | -1.09444900 | 0.34101600  | 3.05859500  |
| C | -0.06349100 | 1.26996500  | 2.91721100  |
| C | 0.82697800  | 0.00598900  | 1.11227100  |
| H | -1.84945200 | 0.48726500  | 3.82378500  |
| H | -0.01841800 | 2.13294900  | 3.57358200  |
| H | 1.69320700  | 1.86441900  | 1.82409500  |
| H | -1.96196300 | -1.49815900 | 2.30298800  |
| C | -0.21457700 | -2.07359700 | 0.28164200  |
| I | 2.09514000  | -0.49914700 | -0.48718000 |
| O | 0.76052500  | -2.00465400 | -0.64971200 |
| O | -1.00208000 | -2.98307900 | 0.31034600  |
| O | 3.17175900  | 1.45963800  | -0.16509900 |
| O | 3.31486700  | -1.34846100 | 0.46710300  |
| O | 0.47449800  | 0.95895700  | -1.51527600 |
| C | -0.83238900 | 0.85483300  | -1.22741700 |
| C | -1.59684700 | -0.21604400 | -1.70894200 |
| C | -1.47920300 | 1.79618600  | -0.39958000 |
| C | -2.93882400 | -0.37688000 | -1.35522800 |
| H | -1.11805000 | -0.94815500 | -2.35303100 |
| C | -2.81137200 | 1.64557000  | -0.04910600 |
| H | -0.91186900 | 2.64112600  | -0.01789300 |
| C | -3.55281700 | 0.55090300  | -0.51383400 |
| H | -3.48552900 | -1.23069500 | -1.73983700 |
| H | -3.30064300 | 2.36740300  | 0.59886900  |
| O | -4.85024300 | 0.48400400  | -0.10070100 |
| C | -5.60285000 | -0.63132500 | -0.53460800 |
| H | -5.15773900 | -1.57297300 | -0.19036800 |
| H | -6.59526400 | -0.52050000 | -0.09562000 |
| H | -5.69241100 | -0.65534700 | -1.62747100 |
| H | 3.64557600  | 1.54259400  | 0.68491000  |
| H | 0.98722200  | 2.39130600  | -1.20238300 |
| O | 1.52272300  | 3.16879600  | -0.80482700 |

|   |            |            |             |
|---|------------|------------|-------------|
| H | 2.57903900 | 2.31511600 | -0.37388500 |
| H | 1.79043000 | 3.74340300 | -1.54240500 |

## 19

E(SMD/M06-2X/BS1) = -927.0170296 au

H(SMD/M06-2X/BS1) = -926.772039 au

G(SMD/M06-2X/BS1) = -926.837364 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1213.684236 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.16367800 | -0.76723300 | 2.21892800  |
| C | 0.91490600  | 1.11835500  | 1.93032000  |
| C | -0.18854100 | -0.93217100 | 1.23983800  |
| C | -1.09444900 | 0.34101600  | 3.05859500  |
| C | -0.06349100 | 1.26996500  | 2.91721100  |
| C | 0.82697800  | 0.00598900  | 1.11227100  |
| H | -1.84945200 | 0.48726500  | 3.82378500  |
| H | -0.01841800 | 2.13294900  | 3.57358200  |
| H | 1.69320700  | 1.86441900  | 1.82409500  |
| H | -1.96196300 | -1.49815900 | 2.30298800  |
| C | -0.21457700 | -2.07359700 | 0.28164200  |
| I | 2.09514000  | -0.49914700 | -0.48718000 |
| O | 0.76052500  | -2.00465400 | -0.64971200 |
| O | -1.00208000 | -2.98307900 | 0.31034600  |
| O | 3.17175900  | 1.45963800  | -0.16509900 |
| O | 3.31486700  | -1.34846100 | 0.46710300  |
| O | 0.47449800  | 0.95895700  | -1.51527600 |
| C | -0.83238900 | 0.85483300  | -1.22741700 |
| C | -1.59684700 | -0.21604400 | -1.70894200 |
| C | -1.47920300 | 1.79618600  | -0.39958000 |
| C | -2.93882400 | -0.37688000 | -1.35522800 |
| H | -1.11805000 | -0.94815500 | -2.35303100 |
| C | -2.81137200 | 1.64557000  | -0.04910600 |
| H | -0.91186900 | 2.64112600  | -0.01789300 |
| C | -3.55281700 | 0.55090300  | -0.51383400 |
| H | -3.48552900 | -1.23069500 | -1.73983700 |
| H | -3.30064300 | 2.36740300  | 0.59886900  |
| O | -4.85024300 | 0.48400400  | -0.10070100 |
| C | -5.60285000 | -0.63132500 | -0.53460800 |
| H | -5.15773900 | -1.57297300 | -0.19036800 |
| H | -6.59526400 | -0.52050000 | -0.09562000 |
| H | -5.69241100 | -0.65534700 | -1.62747100 |
| H | 3.64557600  | 1.54259400  | 0.68491000  |
| H | 0.98722200  | 2.39130600  | -1.20238300 |
| O | 1.52272300  | 3.16879600  | -0.80482700 |



|   |            |            |             |
|---|------------|------------|-------------|
| H | 2.57903900 | 2.31511600 | -0.37388500 |
| H | 1.79043000 | 3.74340300 | -1.54240500 |

**20**

E(SMD/M06-2X/BS1) = -1079.808216 au

H(SMD/M06-2X/BS1) = -1079.512225 au

G(SMD/M06-2X/BS1) = -1079.587641 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1366.568669 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.97592400  | 2.68030500  | -0.45581400 |
| C | 0.43570200  | 1.78854700  | 0.38576000  |
| C | 2.67366900  | 1.32121500  | -0.43463200 |
| C | 2.00486700  | 3.59330300  | -0.05604000 |
| C | 0.74877600  | 3.14999400  | 0.35946400  |
| C | 1.42018700  | 0.90060100  | -0.01178100 |
| H | 2.22485200  | 4.65551300  | -0.06703900 |
| H | -0.00330200 | 3.86871000  | 0.66854600  |
| H | -0.54653800 | 1.46115900  | 0.70317200  |
| H | 3.95966300  | 3.00194600  | -0.78300900 |
| C | 3.66278800  | 0.27914000  | -0.83616700 |
| I | 1.24816000  | -1.19190600 | -0.17331300 |
| O | 3.19064500  | -0.97653700 | -0.73274000 |
| O | 4.78434500  | 0.50837200  | -1.21227700 |
| O | -0.77880400 | -1.02520200 | 0.96329500  |
| C | -2.00533300 | -0.65592600 | 0.45284000  |
| C | -2.79697300 | 0.26180200  | 1.13502100  |
| C | -2.46100900 | -1.23240700 | -0.73461300 |
| C | -4.05265800 | 0.61399600  | 0.63861300  |
| H | -2.44055200 | 0.70098700  | 2.06314000  |
| C | -3.70346500 | -0.87281700 | -1.23382400 |
| H | -1.83716800 | -1.94615200 | -1.26042400 |
| C | -4.50945900 | 0.04932300  | -0.55380800 |
| H | -4.65477800 | 1.32566100  | 1.19086300  |
| H | -4.07510400 | -1.30727400 | -2.15644200 |
| O | -5.70931400 | 0.32666800  | -1.12401200 |
| C | -6.54659600 | 1.25264700  | -0.45423300 |
| H | -6.06894900 | 2.23594900  | -0.37318800 |
| H | -7.44900200 | 1.33850100  | -1.06024800 |
| H | -6.81489100 | 0.89612800  | 0.54703500  |
| O | 0.51315200  | -1.12797300 | -1.78344500 |
| O | 2.01544200  | -0.96162200 | 1.93500700  |
| H | 0.92251100  | -0.61601200 | 2.81280600  |
| O | -0.04672400 | -0.39290300 | 3.17812500  |
| H | -0.25898900 | -1.04966700 | 3.86354000  |

|   |             |             |            |
|---|-------------|-------------|------------|
| H | -0.60412700 | -0.73393100 | 2.01034500 |
| H | 2.66541000  | -0.24527500 | 2.03015100 |

## 21

E(SMD/M06-2X/BS1) = -1079.806102 au

H(SMD/M06-2X/BS1) = -1079.51121 au

G(SMD/M06-2X/BS1) = -1079.586362 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1366.566737 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.47461700 | 0.75698900  | 0.73039900  |
| C | -1.97099100 | 1.99323900  | 0.33801600  |
| C | -3.34671200 | -0.00433300 | 0.43310600  |
| C | -4.34928500 | 2.13951100  | 0.82558600  |
| C | -3.10853700 | 2.74914300  | 0.63282900  |
| C | -2.12379200 | 0.62026400  | 0.24223000  |
| H | -5.21855400 | 2.74672200  | 1.05544200  |
| H | -3.01831700 | 3.82760800  | 0.71648800  |
| H | -1.00773300 | 2.47080900  | 0.20359500  |
| H | -5.42738100 | 0.26030100  | 0.88432000  |
| C | -3.39575600 | -1.49238500 | 0.33021900  |
| I | -0.65067700 | -0.78613100 | -0.27969600 |
| O | -2.21332300 | -2.05482100 | 0.03753400  |
| O | -4.39297200 | -2.15220200 | 0.49506000  |
| O | 0.71825700  | 0.98798200  | -0.45072400 |
| C | 2.03092700  | 0.70942500  | -0.11043200 |
| C | 2.93294300  | 0.26350100  | -1.06735000 |
| C | 2.42239600  | 0.85901600  | 1.22100600  |
| C | 4.25349500  | -0.01033700 | -0.70931300 |
| H | 2.61243700  | 0.12933500  | -2.09690600 |
| C | 3.73048500  | 0.57808800  | 1.58073300  |
| H | 1.69302900  | 1.18720700  | 1.95341600  |
| C | 4.65610200  | 0.14717100  | 0.61936400  |
| H | 4.94647600  | -0.34831200 | -1.47046500 |
| H | 4.06120700  | 0.68903200  | 2.60838600  |
| O | 5.91013900  | -0.09348700 | 1.07168800  |
| C | 6.87108000  | -0.53168800 | 0.12582600  |
| H | 7.01967300  | 0.21335400  | -0.66419400 |
| H | 7.80138200  | -0.66325800 | 0.67890300  |
| H | 6.57823500  | -1.48657800 | -0.32539600 |
| O | -1.07002800 | -0.52705900 | -2.05122700 |
| O | -0.37115500 | -0.58000100 | 1.74320100  |
| H | 0.36129900  | -1.16297200 | 2.01282300  |
| H | 0.54369500  | 1.39167900  | -1.51778500 |
| O | 0.00583800  | 1.60917100  | -2.64596400 |

|   |             |            |             |
|---|-------------|------------|-------------|
| H | -0.56387700 | 0.71813700 | -2.58907600 |
| H | 0.64382200  | 1.50963400 | -3.37554700 |

**TS<sub>17-22</sub>**

E(SMD/M06-2X/BS1) = -1079.835715 au

H(SMD/M06-2X/BS1) = -1079.541068 au

G(SMD/M06-2X/BS1) = -1079.615162 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1366.598508 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.19296100 | 1.10408500  | 2.03536600  |
| C | 0.84595000  | 2.11153600  | 0.36729200  |
| C | -0.32389700 | 0.22874200  | 1.39191600  |
| C | -1.03705300 | 2.47802100  | 1.85144400  |
| C | -0.02458100 | 2.97900200  | 1.03117100  |
| C | 0.66456100  | 0.75510100  | 0.57672600  |
| H | -1.71281900 | 3.16669900  | 2.34859100  |
| H | 0.08492000  | 4.05052700  | 0.89787900  |
| H | 1.62867500  | 2.47606500  | -0.29081900 |
| H | -1.97777200 | 0.70087300  | 2.66797700  |
| C | -0.40434000 | -1.27147400 | 1.53004400  |
| I | 1.86952400  | -0.66854000 | -0.37121900 |
| O | 0.50750800  | -1.89766000 | 0.83763700  |
| O | -1.24772700 | -1.80065800 | 2.23122900  |
| O | 2.91429900  | 0.62640500  | -1.18150400 |
| O | 3.08021400  | -1.02005000 | 0.97597300  |
| H | 3.90583700  | 0.92752300  | -0.33137200 |
| O | 0.13469700  | 0.29284000  | -2.41959700 |
| H | 0.39208000  | 1.21569300  | -2.59561500 |
| C | -1.13237200 | 0.25299300  | -1.88474100 |
| C | -1.62814700 | -0.98875900 | -1.50893900 |
| C | -1.88041300 | 1.40752500  | -1.65291800 |
| C | -2.86424400 | -1.08703000 | -0.86838500 |
| H | -1.03911800 | -1.88186300 | -1.69735000 |
| C | -3.11278700 | 1.31055000  | -1.02321200 |
| H | -1.48994500 | 2.37930600  | -1.94488000 |
| C | -3.60873600 | 0.06653800  | -0.61418000 |
| H | -3.22263200 | -2.06433400 | -0.56771000 |
| H | -3.70202700 | 2.19981600  | -0.82234100 |
| O | 4.53945600  | 0.84356200  | 0.58271900  |
| H | 3.94362500  | -0.10328800 | 0.92590600  |
| H | 5.43920400  | 0.57895900  | 0.31561400  |
| O | -4.81261400 | 0.08223800  | 0.01599600  |
| C | -5.29391000 | -1.15279900 | 0.51420200  |
| H | -4.59411000 | -1.58838000 | 1.23734300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -6.23850300 | -0.93226700 | 1.01249300  |
| H | -5.47129500 | -1.87029300 | -0.29546200 |

## 22

E(SMD/M06-2X/BS1) = -1003.438695 au

H(SMD/M06-2X/BS1) = -1003.16555 au

G(SMD/M06-2X/BS1) = -1003.237884 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1290.154585 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.05620300 | 0.89109600  | 1.79633400  |
| C | 0.65164000  | 2.23894400  | -0.00126900 |
| C | 0.04464100  | 0.23234700  | 1.25881200  |
| C | -1.30480900 | 2.21416100  | 1.42907000  |
| C | -0.45808000 | 2.88612900  | 0.54452700  |
| C | 0.85647300  | 0.92223400  | 0.37353800  |
| H | -2.16927800 | 2.72927000  | 1.83612700  |
| H | -0.66411300 | 3.91655200  | 0.27381700  |
| H | 1.32910200  | 2.73282700  | -0.69111900 |
| H | -1.70704300 | 0.36210900  | 2.48567000  |
| C | 0.38383400  | -1.20823600 | 1.55460900  |
| I | 2.46004700  | -0.15006000 | -0.41331100 |
| O | 1.38877400  | -1.65230900 | 0.84690300  |
| O | -0.25219500 | -1.85734200 | 2.36472300  |
| O | 3.30334800  | 1.26820100  | -1.08174500 |
| O | 3.52437400  | -0.20860000 | 1.19650900  |
| H | 0.26562700  | -2.25088400 | -1.07229500 |
| H | 4.11707700  | 0.56914700  | 1.11441000  |
| O | 0.05418900  | -1.48006000 | -1.62992300 |
| C | -1.20532700 | -1.03847700 | -1.31080500 |
| C | -2.05880900 | -1.75842400 | -0.48549500 |
| C | -1.60885600 | 0.19637600  | -1.82561600 |
| C | -3.31479200 | -1.24547500 | -0.14959000 |
| H | -1.74309500 | -2.71598100 | -0.07890500 |
| C | -2.85285100 | 0.70699500  | -1.49454000 |
| H | -0.93183800 | 0.75328300  | -2.46653500 |
| C | -3.71444100 | -0.00584900 | -0.64833800 |
| H | -3.17627700 | 1.67050200  | -1.87614800 |
| O | -4.90668200 | 0.58719600  | -0.37655600 |
| C | -5.78738700 | -0.10492200 | 0.48905100  |
| H | -6.67302500 | 0.52366200  | 0.58788100  |
| H | -6.07749700 | -1.07608600 | 0.07106500  |
| H | -5.33753900 | -0.25651600 | 1.47756400  |
| H | -3.95923300 | -1.82275800 | 0.50295800  |

**TS<sub>22-23</sub>**

E(SMD/M06-2X/BS1) = -1079.830848 au

H(SMD/M06-2X/BS1) = -1079.536518 au

G(SMD/M06-2X/BS1) = -1079.611178 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1366.591104 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.34256200  | 1.72940400  | -1.61225100 |
| C | 2.86995900  | -0.99269800 | -1.06691200 |
| C | 2.41153800  | 1.36558900  | -0.64317200 |
| C | 4.02965900  | 0.73784100  | -2.30879600 |
| C | 3.79920600  | -0.61146300 | -2.03640100 |
| C | 2.19763300  | 0.01880700  | -0.40238400 |
| H | 4.75479000  | 1.01609200  | -3.06661000 |
| H | 4.34597400  | -1.37640700 | -2.57812400 |
| H | 2.69293100  | -2.03863900 | -0.84028700 |
| H | 3.51789500  | 2.78314700  | -1.80368200 |
| C | 1.65237900  | 2.37549600  | 0.17961500  |
| I | 0.78350200  | -0.42310400 | 1.07698300  |
| O | 0.86721600  | 1.82253100  | 1.06773000  |
| O | 1.79289800  | 3.57109100  | 0.00543300  |
| O | 1.19930000  | -2.20694500 | 1.13455400  |
| O | 2.04058300  | -0.13921600 | 2.51823100  |
| H | -0.17218000 | -2.14744700 | -1.04575900 |
| O | 0.30777400  | -3.16567000 | -0.89390600 |
| H | 0.74269300  | -2.88487900 | 0.09595100  |
| H | 2.03700300  | 0.82069600  | 2.70463700  |
| H | -0.37323500 | -3.85456400 | -0.77513600 |
| O | -0.43795200 | -0.89377000 | -0.83517300 |
| C | -1.76097400 | -0.57176600 | -0.71692000 |
| C | -2.76321500 | -1.53728500 | -0.87795400 |
| C | -2.12730700 | 0.74083100  | -0.42375700 |
| C | -4.09839700 | -1.18495100 | -0.75611900 |
| H | -2.50101700 | -2.56619200 | -1.10782100 |
| C | -3.47000900 | 1.09828100  | -0.29012300 |
| H | -1.35398900 | 1.49528800  | -0.30246000 |
| C | -4.46455800 | 0.13333000  | -0.45722000 |
| H | -4.88007600 | -1.92699600 | -0.88536700 |
| H | -3.71951200 | 2.12772400  | -0.06066400 |
| O | -5.79770500 | 0.37296700  | -0.35093000 |
| C | -6.19315600 | 1.69636800  | -0.03887000 |
| H | -5.87298600 | 2.40225900  | -0.81419400 |
| H | -7.28250400 | 1.68431400  | 0.00991700  |
| H | -5.79021500 | 2.01552100  | 0.92956900  |

**23**

E(SMD/M06-2X/BS1) = -1003.446916 au

H(SMD/M06-2X/BS1) = -1003.174401 au

G(SMD/M06-2X/BS1) = -1003.246142 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1290.159587 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.34353000  | 2.22070800  | -0.57071700 |
| C | 3.14631800  | -0.49355300 | -1.31125500 |
| C | 2.37320800  | 1.40525200  | 0.00461300  |
| C | 4.21331900  | 1.67873800  | -1.51415700 |
| C | 4.11733800  | 0.33512800  | -1.87897100 |
| C | 2.29686100  | 0.07875500  | -0.38209200 |
| H | 4.97460400  | 2.30515000  | -1.96744100 |
| H | 4.80364000  | -0.07749800 | -2.61142900 |
| H | 3.06605100  | -1.54010100 | -1.58232600 |
| H | 3.40819500  | 3.26181700  | -0.27130600 |
| C | 1.40480200  | 1.89474800  | 1.04164300  |
| I | 0.76910600  | -0.97106300 | 0.58738100  |
| O | 0.61062400  | 0.94501300  | 1.50085000  |
| O | 1.37346400  | 3.04787600  | 1.41482200  |
| O | 1.12436000  | -2.54639600 | -0.51667300 |
| O | 2.24986900  | -1.55636600 | 1.74216600  |
| H | 0.64447700  | -2.41363400 | -1.35756400 |
| H | 1.89013000  | -2.07797800 | 2.48560700  |
| O | -0.31775600 | -0.29898600 | -1.01862400 |
| C | -1.66249000 | -0.17978600 | -0.78747000 |
| C | -2.49396500 | -1.30578600 | -0.81359900 |
| C | -2.21483600 | 1.07284800  | -0.52811700 |
| C | -3.85795900 | -1.17096300 | -0.60119200 |
| H | -2.06188200 | -2.28337900 | -1.01226100 |
| C | -3.58642000 | 1.21659400  | -0.32211500 |
| H | -1.56172500 | 1.93997000  | -0.49736900 |
| C | -4.41476800 | 0.09085500  | -0.35736900 |
| H | -4.51433000 | -2.03527100 | -0.62275900 |
| H | -3.99215600 | 2.20341400  | -0.13166300 |
| O | -5.75853500 | 0.12187300  | -0.16785200 |
| C | -6.35006100 | 1.38480700  | 0.08082700  |
| H | -6.19352600 | 2.07108600  | -0.75957200 |
| H | -7.41798600 | 1.20063100  | 0.20231200  |
| H | -5.95360300 | 1.83796200  | 0.99691300  |

**TS<sub>23-24</sub>**

E(SMD/M06-2X/BS1) = -1079.832301 au

H(SMD/M06-2X/BS1) = -1079.537843 au

G(SMD/M06-2X/BS1) = -1079.611058 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1366.590581 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.97365400 | 2.06696500  | 1.41898400  |
| C | 0.79614500  | 1.95011600  | -0.76860300 |
| C | -0.16165400 | 0.95151900  | 1.23911900  |
| C | -0.89569300 | 3.12347900  | 0.51249100  |
| C | -0.01511000 | 3.06950500  | -0.56848300 |
| C | 0.69702000  | 0.92379900  | 0.15438100  |
| H | -1.52842900 | 3.99507100  | 0.64583000  |
| H | 0.03347300  | 3.89505600  | -1.27124300 |
| H | 1.45030400  | 1.87255400  | -1.63072600 |
| H | -1.65688500 | 2.09138800  | 2.26201300  |
| C | -0.18930900 | -0.24498800 | 2.15746900  |
| I | 1.77683000  | -0.85699900 | -0.08675800 |
| O | 0.61160200  | -1.19929400 | 1.77269100  |
| O | -0.89892800 | -0.26676000 | 3.14721100  |
| O | 2.58861900  | -0.26055000 | -1.62465400 |
| O | 3.22809700  | 0.30978900  | 1.07258100  |
| H | 3.88990900  | 0.95862700  | 0.19961500  |
| O | 4.25872900  | 1.31163500  | -0.83460400 |
| H | 3.55266800  | 0.65728300  | -1.37134900 |
| H | 4.00996000  | 2.24381000  | -0.97977000 |
| H | 3.81981700  | -0.28646100 | 1.56938500  |
| O | 0.26234200  | -1.69802400 | -1.10654900 |
| C | -1.01628100 | -1.21229200 | -1.00641500 |
| C | -1.88421700 | -1.71381200 | -0.04122100 |
| C | -1.45336000 | -0.20901400 | -1.87900900 |
| C | -3.18204100 | -1.21303200 | 0.07332400  |
| H | -1.53340000 | -2.48632700 | 0.63525700  |
| C | -2.73801100 | 0.29608100  | -1.76685900 |
| H | -0.76896500 | 0.17364500  | -2.63026800 |
| C | -3.61019500 | -0.19789600 | -0.78555900 |
| H | -3.83851700 | -1.61630100 | 0.83551800  |
| H | -3.08987400 | 1.07993400  | -2.43027200 |
| O | -4.84301200 | 0.36630200  | -0.75092400 |
| C | -5.74153600 | -0.09818400 | 0.24112200  |
| H | -5.34377000 | 0.07071000  | 1.24852100  |
| H | -6.65849900 | 0.47783500  | 0.11309500  |
| H | -5.96198800 | -1.16413000 | 0.11209100  |

**24**

E(SMD/M06-2X/BS1) = -927.0430905 au

H(SMD/M06-2X/BS1) = -926.79785 au

G(SMD/M06-2X/BS1) = -926.863469 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1213.709833 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.82416200 | 2.24892100  | 1.12242400  |
| C | 1.10303600  | 2.12215200  | -0.93529500 |
| C | 0.09792800  | 1.20840400  | 1.10197300  |
| C | -0.78255300 | 3.21851300  | 0.11974300  |
| C | 0.17386400  | 3.16201300  | -0.89682000 |
| C | 1.02909000  | 1.17790900  | 0.07545700  |
| H | -1.50466300 | 4.02886400  | 0.12809900  |
| H | 0.19126900  | 3.92488300  | -1.66833900 |
| H | 1.84327000  | 2.03315100  | -1.72466300 |
| H | -1.56564500 | 2.28332500  | 1.91434100  |
| C | 0.12270000  | 0.08906200  | 2.11645400  |
| I | 2.22887700  | -0.52048900 | -0.02284600 |
| O | 1.00730500  | -0.82307200 | 1.83544600  |
| O | -0.61858000 | 0.09832200  | 3.08336000  |
| O | 2.94261300  | -0.13288700 | -1.60226300 |
| O | 0.83497000  | -1.76189400 | -0.76154600 |
| C | -0.47506600 | -1.35509700 | -0.74860800 |
| C | -1.34031900 | -1.81123800 | 0.24080900  |
| C | -0.93748200 | -0.48478400 | -1.74465500 |
| C | -2.67416000 | -1.40728800 | 0.24565200  |
| H | -0.96008200 | -2.46865500 | 1.01508900  |
| C | -2.25797700 | -0.07436600 | -1.73931600 |
| H | -0.24705800 | -0.13892500 | -2.50845800 |
| C | -3.13485600 | -0.52911500 | -0.74052400 |
| H | -3.33391300 | -1.77348800 | 1.02307800  |
| H | -2.63791700 | 0.60023000  | -2.49973500 |
| O | -4.40304000 | -0.06765200 | -0.81737500 |
| C | -5.31902200 | -0.49966700 | 0.17627900  |
| H | -4.99293400 | -0.19285500 | 1.17645600  |
| H | -6.26815300 | -0.01794500 | -0.05936500 |
| H | -5.44690400 | -1.58771600 | 0.15191700  |

**TS<sub>22</sub>**

E(SMD/M06-2X/BS1) = -1079.832595 au

H(SMD/M06-2X/BS1) = -1079.537619 au

G(SMD/M06-2X/BS1) = -1079.611976 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1366.593075 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.22689700  | -2.79412500 | -1.04420000 |
| C | 0.17539000  | -0.16883300 | -2.02403900 |
| C | -0.64843900 | -1.86816000 | -0.47886400 |
| C | 1.06062300  | -2.41945500 | -2.09494300 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.04120300  | -1.11227700 | -2.57927600 |
| C | -0.65576500 | -0.57575400 | -0.99200900 |
| H | 1.74114300  | -3.14552800 | -2.52788900 |
| H | 1.70632800  | -0.81807000 | -3.38473700 |
| H | 0.16125600  | 0.86133800  | -2.36833100 |
| H | 0.25381100  | -3.79882000 | -0.63474900 |
| C | -1.43851700 | -2.21103800 | 0.75612700  |
| I | -1.90680200 | 0.91274100  | -0.18577400 |
| O | -2.26268600 | -1.26467900 | 1.12920200  |
| O | -1.24646900 | -3.25381400 | 1.35589500  |
| O | -1.19711200 | 2.28034600  | -1.05669900 |
| O | -3.27415900 | 0.45009400  | -1.50659200 |
| O | -0.36195300 | 1.03487700  | 1.42682700  |
| C | 0.96038900  | 0.94278700  | 1.08579000  |
| C | 1.58369800  | 2.01860700  | 0.44366700  |
| C | 1.68225700  | -0.22407500 | 1.32697500  |
| C | 2.90878400  | 1.91617900  | 0.04771400  |
| H | 1.00909800  | 2.91685200  | 0.24648300  |
| C | 3.01711900  | -0.32961900 | 0.93534600  |
| H | 1.20156600  | -1.07030900 | 1.81155900  |
| C | 3.63548300  | 0.74311500  | 0.28826100  |
| H | 3.40474700  | 2.74120700  | -0.45415900 |
| H | 3.55330800  | -1.25008700 | 1.13513900  |
| O | 4.92475500  | 0.74125100  | -0.13872800 |
| C | 5.67794500  | -0.43733500 | 0.08276400  |
| H | 5.23403200  | -1.29713900 | -0.43269800 |
| H | 6.67059100  | -0.24485100 | -0.32570100 |
| H | 5.76378500  | -0.66164200 | 1.15243000  |
| H | -2.88304800 | 0.42625100  | -2.40186800 |
| H | -0.79952300 | 0.34245400  | 2.47548400  |
| O | -1.40369500 | -0.29884200 | 3.16126700  |
| H | -1.92487100 | -0.88033500 | 2.38727800  |
| H | -0.82356200 | -0.89054600 | 3.67852700  |

## 28

E(SMD/M06-2X/BS1) = -1003.446461 au

H(SMD/M06-2X/BS1) = -1003.173146 au

G(SMD/M06-2X/BS1) = -1003.245195 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1290.161469 au

|   |             |            |             |
|---|-------------|------------|-------------|
| C | -0.02103200 | 2.87035900 | -0.73226800 |
| C | -0.13368300 | 0.25701000 | -1.73725600 |
| C | 0.82180700  | 1.88666800 | -0.21212200 |
| C | -0.92035700 | 2.54623900 | -1.74500400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.97574300 | 1.24827100  | -2.24651900 |
| C | 0.75036900  | 0.59304100  | -0.72671900 |
| H | -1.58063600 | 3.31052000  | -2.14090100 |
| H | -1.68106100 | 0.99711200  | -3.03227900 |
| H | -0.17987800 | -0.76537900 | -2.10178200 |
| H | 0.02610800  | 3.88060300  | -0.34035100 |
| I | 1.86244700  | -1.02384900 | 0.06391400  |
| O | 1.18125600  | -2.30179500 | -0.96150600 |
| O | 3.28886600  | -0.56244600 | -1.23257800 |
| O | 0.35334000  | -1.16343200 | 1.47062500  |
| C | -0.94587500 | -1.02017300 | 1.10316300  |
| C | -1.62075100 | -2.02706400 | 0.39784300  |
| C | -1.62642000 | 0.16034400  | 1.40780400  |
| C | -2.93605500 | -1.83914500 | -0.00354800 |
| H | -1.08902200 | -2.93976300 | 0.15204300  |
| C | -2.94777600 | 0.35596500  | 1.00640300  |
| H | -1.10074000 | 0.94055500  | 1.95176900  |
| C | -3.60733900 | -0.64568700 | 0.28874500  |
| H | -3.46518300 | -2.61025300 | -0.55558700 |
| H | -3.44400400 | 1.28788200  | 1.25255400  |
| O | -4.88852300 | -0.55322600 | -0.15993000 |
| C | -5.57159600 | 0.66106200  | 0.08741400  |
| H | -5.05645800 | 1.51050900  | -0.37721900 |
| H | -6.56046700 | 0.55100400  | -0.35924800 |
| H | -5.67972300 | 0.84921800  | 1.16219200  |
| H | 2.94886900  | -0.66795400 | -2.14036200 |
| C | 1.77222400  | 2.16300300  | 0.89091900  |
| O | 2.52142200  | 1.31606400  | 1.34306800  |
| O | 1.73502500  | 3.41063700  | 1.34145100  |
| H | 2.39479600  | 3.49417500  | 2.05953100  |

### TS<sub>28</sub>

E(SMD/M06-2X/BS1) = -1079.83201 au

H(SMD/M06-2X/BS1) = -1079.537025 au

G(SMD/M06-2X/BS1) = -1079.611436 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1366.59134 au

|   |             |            |            |
|---|-------------|------------|------------|
| C | -0.01822900 | 2.90847600 | 0.47113600 |
| C | 0.47067300  | 0.39939500 | 1.62007300 |
| C | -0.78499400 | 1.81285200 | 0.07726100 |
| C | 0.99973800  | 2.75046200 | 1.40863300 |
| C | 1.23753100  | 1.50515900 | 1.98931900 |
| C | -0.51733700 | 0.58046800 | 0.66388100 |
| H | 1.60454300  | 3.60464100 | 1.69574400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.02419000  | 1.38710100  | 2.72782200  |
| H | 0.64427600  | -0.58277300 | 2.04941600  |
| H | -0.23398600 | 3.87690300  | 0.03126900  |
| I | -1.45717400 | -1.17556400 | -0.01512800 |
| O | -0.75334200 | -2.26253700 | 1.19103400  |
| O | -3.10541900 | -0.64395200 | 1.24234300  |
| O | 0.01832600  | -1.36899200 | -1.38668900 |
| C | 1.30887100  | -1.08158200 | -1.03547200 |
| C | 2.05322900  | -1.96783900 | -0.24858300 |
| C | 1.88105700  | 0.12079600  | -1.44595000 |
| C | 3.34549900  | -1.63631000 | 0.13264200  |
| H | 1.59900800  | -2.89885500 | 0.07282200  |
| C | 3.17883700  | 0.45904300  | -1.06568400 |
| H | 1.29199800  | 0.80384800  | -2.05106000 |
| C | 3.91408400  | -0.41904800 | -0.26301600 |
| H | 3.93474400  | -2.30896800 | 0.74820500  |
| H | 3.59711000  | 1.40443100  | -1.39176800 |
| O | 5.17691600  | -0.18074500 | 0.17589100  |
| C | 5.75567900  | 1.06636700  | -0.16322100 |
| H | 5.16253400  | 1.90032300  | 0.23072500  |
| H | 6.74444100  | 1.07728700  | 0.29651700  |
| H | 5.86007100  | 1.17767000  | -1.24877000 |
| H | -2.83871700 | -0.24946800 | 2.09257700  |
| C | -1.93382600 | 1.97825200  | -0.88281700 |
| O | -2.32051300 | 3.08330000  | -1.21603500 |
| O | -4.62741600 | 0.53962900  | -0.23244600 |
| H | -4.05160600 | 0.03019600  | 0.56715300  |
| H | -5.02373100 | 1.36399700  | 0.11008900  |
| O | -2.47157900 | 0.84202600  | -1.24966600 |
| H | -3.76529300 | 0.78976100  | -0.87362800 |

### TS<sub>24-25</sub>

E(SMD/M06-2X/BS1) = -927.0258164 au

H(SMD/M06-2X/BS1) = -926.781644 au

G(SMD/M06-2X/BS1) = -926.846443 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1213.695704 au

|   |             |            |             |
|---|-------------|------------|-------------|
| C | -2.03414900 | 2.89282000 | 0.07346400  |
| C | 0.08018800  | 1.22428400 | 0.90010500  |
| C | -2.15994900 | 1.51215800 | -0.03492700 |
| C | -0.85273500 | 3.43783900 | 0.57435200  |
| C | 0.18927300  | 2.61198800 | 0.99717400  |
| C | -1.08963400 | 0.71786100 | 0.34732800  |
| H | -0.75197900 | 4.51485200 | 0.66212500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.09258600  | 3.04423900  | 1.41506400  |
| H | 0.87306000  | 0.57495700  | 1.25602000  |
| H | -2.87232300 | 3.51978500  | -0.21293600 |
| C | -3.45214500 | 0.84030000  | -0.44191000 |
| I | -1.36418700 | -1.35311600 | 0.17651100  |
| O | -3.41203700 | -0.45144600 | -0.31255600 |
| O | -4.40264100 | 1.49855800  | -0.82811100 |
| O | -0.49311500 | -1.70720800 | 1.68070900  |
| O | 0.15185100  | -1.60418100 | -1.14593200 |
| C | 1.34350300  | -0.97826400 | -0.90195500 |
| C | 1.67370800  | 0.17750400  | -1.62181600 |
| C | 2.22700600  | -1.48907200 | 0.04777000  |
| C | 2.88279400  | 0.80821400  | -1.39266700 |
| H | 0.96782500  | 0.56996900  | -2.34758000 |
| C | 3.44353500  | -0.85013500 | 0.28662100  |
| H | 1.95993700  | -2.38704300 | 0.59447900  |
| C | 3.77361400  | 0.30360900  | -0.43189200 |
| H | 3.15977800  | 1.70280500  | -1.94112600 |
| H | 4.12151000  | -1.26287200 | 1.02426300  |
| O | 4.92466800  | 0.99661600  | -0.27681500 |
| C | 5.85501100  | 0.51658700  | 0.68020400  |
| H | 6.70040700  | 1.20434700  | 0.64998600  |
| H | 5.42343600  | 0.51435700  | 1.68746100  |
| H | 6.19772400  | -0.49310600 | 0.42768000  |

## 25

E(SMD/M06-2X/BS1) = -927.0522485 au

H(SMD/M06-2X/BS1) = -926.806873 au

G(SMD/M06-2X/BS1) = -926.873471 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1213.721048 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.72353900 | 1.95798800  | 0.39249600  |
| C | -1.21930500 | 1.85145300  | -0.90486400 |
| C | -3.03765100 | 0.75211400  | 0.29152700  |
| C | -3.15644400 | 3.10750500  | -0.15334300 |
| C | -1.91904500 | 3.05476800  | -0.79721000 |
| C | -1.80333900 | 0.72734700  | -0.34137000 |
| H | -3.68399700 | 4.05302500  | -0.08251200 |
| H | -1.49198800 | 3.95588000  | -1.22494100 |
| H | -0.26092700 | 1.79937500  | -1.40940600 |
| H | -4.68820900 | 1.98076900  | 0.88909600  |
| C | -3.58231500 | -0.54003500 | 0.82455300  |
| I | -0.94806700 | -1.19112600 | -0.34577200 |
| O | -2.79123000 | -1.57452100 | 0.58744200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -4.64611700 | -0.62109700 | 1.39632600  |
| O | -0.11086600 | -1.36522000 | 1.20291000  |
| O | 0.63158600  | -0.40738100 | -1.31333300 |
| C | 1.81356100  | -0.12170800 | -0.67500800 |
| C | 2.98057500  | -0.70270100 | -1.16013000 |
| C | 1.88402100  | 0.77429500  | 0.39763900  |
| C | 4.22129000  | -0.38196800 | -0.60735800 |
| H | 2.91560500  | -1.40276800 | -1.98727800 |
| C | 3.11282300  | 1.08852100  | 0.95688100  |
| H | 0.97739500  | 1.21419800  | 0.80058300  |
| C | 4.29107200  | 0.51910300  | 0.45712600  |
| H | 5.11483800  | -0.84158000 | -1.01358700 |
| H | 3.18177900  | 1.78101000  | 1.78994300  |
| O | 5.44234600  | 0.89957300  | 1.06885700  |
| C | 6.64854400  | 0.33614800  | 0.58608200  |
| H | 7.44730100  | 0.76220200  | 1.19409400  |
| H | 6.65162400  | -0.75462200 | 0.69619100  |
| H | 6.81690000  | 0.59436400  | -0.46601400 |

### TS<sub>24-26</sub>-*p*-OMe

E(SMD/M06-2X/BS1) = -927.0351854 au

H(SMD/M06-2X/BS1) = -926.7909830 au

G(SMD/M06-2X/BS1) = -926.856586 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1213.701762 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.76460500  | 2.47593300  | 0.16790400  |
| C | 0.49136400  | 1.51466800  | -1.18632500 |
| C | 2.52387800  | 1.10719700  | 0.10968400  |
| C | 1.87755800  | 3.36033400  | -0.44774200 |
| C | 0.75063600  | 2.88556800  | -1.11993800 |
| C | 1.39494100  | 0.66646000  | -0.56474300 |
| H | 2.06562000  | 4.42843600  | -0.40335300 |
| H | 0.06716700  | 3.58256800  | -1.59458800 |
| H | -0.37891900 | 1.11181200  | -1.69550000 |
| H | 3.64277500  | 2.83162900  | 0.69767900  |
| C | 3.42209900  | 0.07675700  | 0.75679800  |
| I | 1.02879900  | -1.38009700 | -0.53137800 |
| O | 3.01304500  | -1.13690200 | 0.57763600  |
| O | 4.42264900  | 0.42434400  | 1.36927800  |
| O | -0.62146800 | -1.22419300 | -1.27643800 |
| O | -0.12230400 | -1.01786400 | 1.54164000  |
| C | -1.23979300 | -0.52431000 | 1.16465000  |
| C | -1.47287000 | 0.89742400  | 1.19837200  |
| C | -2.28003800 | -1.36613900 | 0.64816500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.68959900 | 1.40343700  | 0.85022100  |
| H | -0.67554000 | 1.53752700  | 1.56412200  |
| C | -3.51180700 | -0.85101200 | 0.29393600  |
| H | -2.09352800 | -2.43337100 | 0.60589800  |
| C | -3.72105400 | 0.53337800  | 0.39131200  |
| H | -2.90708800 | 2.46490400  | 0.90731100  |
| H | -4.29192100 | -1.50951500 | -0.06730400 |
| O | -4.86149300 | 1.13957800  | 0.07957400  |
| C | -5.95644300 | 0.34617500  | -0.37909600 |
| H | -6.76927000 | 1.04635000  | -0.56570600 |
| H | -5.69415600 | -0.17459800 | -1.30459200 |
| H | -6.25575300 | -0.37554800 | 0.38633000  |

## 26

E(SMD/M06-2X/BS1) = -927.1115547 au

H(SMD/M06-2X/BS1) = -926.865177 au

G(SMD/M06-2X/BS1) = -926.932314 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1213.776368 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.90703700 | 1.91441500  | 0.37719300  |
| C | -1.16616000 | 2.03165800  | -0.25476700 |
| C | -3.17723600 | 0.73915300  | 0.20701400  |
| C | -3.27104100 | 3.14298600  | 0.23293800  |
| C | -1.91120300 | 3.19861800  | -0.08082200 |
| C | -1.82854500 | 0.82357000  | -0.10231300 |
| H | -3.83220800 | 4.06256200  | 0.36316800  |
| H | -1.42066100 | 4.16027000  | -0.19445700 |
| H | -0.11256400 | 2.06369800  | -0.50644600 |
| H | -4.96276300 | 1.84403800  | 0.61977700  |
| C | -3.79485200 | -0.62108000 | 0.34762000  |
| I | -0.91278800 | -1.05403900 | -0.30993700 |
| O | -2.94349300 | -1.59892900 | 0.14755800  |
| O | -4.97054100 | -0.77697400 | 0.62000400  |
| O | 0.80535800  | -0.09097500 | -0.75052100 |
| O | 1.63576900  | -2.58259400 | -0.08955200 |
| C | 2.37523700  | -1.65548000 | 0.20056200  |
| C | 3.77926700  | -1.84363700 | 0.58445000  |
| C | 1.83490300  | -0.22500400 | 0.20297500  |
| C | 4.61349100  | -0.79043700 | 0.56544200  |
| H | 4.12786100  | -2.85448300 | 0.76846600  |
| C | 2.87149100  | 0.83832800  | -0.00313600 |
| H | 1.43460000  | -0.09746400 | 1.23109400  |
| C | 4.16825100  | 0.56444400  | 0.21977700  |
| H | 5.67308600  | -0.91126600 | 0.77465500  |

|   |            |            |             |
|---|------------|------------|-------------|
| H | 2.50917600 | 1.83210700 | -0.24122400 |
| O | 5.19943600 | 1.43655200 | 0.15596000  |
| C | 4.87085700 | 2.76974500 | -0.19663100 |
| H | 5.80864400 | 3.32497900 | -0.20579100 |
| H | 4.40851700 | 2.80802000 | -1.18979400 |
| H | 4.18728400 | 3.21128200 | 0.53779700  |

**TS<sub>26-27</sub>**

E(SMD/M06-2X/BS1) = -1156.272318 au

H(SMD/M06-2X/BS1) = -1155.949439 au

G(SMD/M06-2X/BS1) = -1156.031082 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1443.084109 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.63470200 | 1.59015100  | 0.08731300  |
| C | -2.08660600 | 1.54817200  | 1.28908500  |
| C | -3.77171600 | 0.51970700  | -0.14181400 |
| C | -4.22652700 | 2.63482100  | 0.91029300  |
| C | -2.96370800 | 2.61162800  | 1.50689500  |
| C | -2.52216200 | 0.52964800  | 0.45653900  |
| H | -4.89297300 | 3.47121100  | 1.09372500  |
| H | -2.65458500 | 3.42729500  | 2.15279500  |
| H | -1.10777500 | 1.51311500  | 1.75507100  |
| H | -5.61288200 | 1.58443700  | -0.38319600 |
| C | -4.14158700 | -0.64921900 | -1.00696400 |
| I | -1.38306900 | -1.16739600 | -0.00283600 |
| O | -3.19756100 | -1.55946000 | -1.08180200 |
| O | -5.21616700 | -0.72735700 | -1.57090000 |
| O | 0.10529900  | -0.44049200 | 1.15009000  |
| O | 2.63773300  | -1.05049400 | 2.00861300  |
| C | 2.50203400  | -0.14266800 | 1.14995100  |
| C | 1.20812900  | 0.12616500  | 0.51079900  |
| C | 3.60096500  | 0.61011500  | 0.61480800  |
| C | 1.05354900  | 1.30263000  | -0.29098100 |
| H | 1.57873900  | -0.71016900 | -0.53660500 |
| C | 3.42582100  | 1.64981800  | -0.27713300 |
| H | 4.59904900  | 0.40803500  | 0.99414500  |
| C | 2.12964700  | 2.01542800  | -0.74716800 |
| H | 0.05224100  | 1.57165300  | -0.62177100 |
| H | 1.98797600  | 2.84694800  | -1.42496800 |
| O | 1.84913000  | -1.60135100 | -1.39640600 |
| H | 1.67192800  | -1.23447900 | -2.28342400 |
| H | 2.87728800  | -1.77108800 | -1.32260100 |
| O | 4.34494100  | -1.92592700 | -1.16863400 |
| H | 4.56444900  | -2.13001400 | -0.20760200 |

|   |            |             |             |
|---|------------|-------------|-------------|
| H | 4.72439600 | -1.04265000 | -1.31380500 |
| O | 4.86376500 | -2.28596900 | 1.38774400  |
| H | 4.05938000 | -1.81859000 | 1.76307100  |
| O | 4.54674600 | 2.29097000  | -0.66878800 |
| C | 4.42194100 | 3.38262400  | -1.57023600 |
| H | 3.98190700 | 3.06453400  | -2.52119900 |
| H | 3.82161200 | 4.18963800  | -1.13782200 |
| H | 5.43665900 | 3.74116700  | -1.74409000 |
| H | 4.77369400 | -3.21252000 | 1.66091400  |

### 27-H,H,OMe,H

E(SMD/M06-2X/BS1) = -927.1454083 au

H(SMD/M06-2X/BS1) = -926.898567 au

G(SMD/M06-2X/BS1) = -926.965015 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1213.814354 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.50522000 | 1.96436500  | 0.63528000  |
| C | -1.02382700 | 1.07635500  | 1.63748500  |
| C | -2.88919400 | 0.84157200  | 0.08523300  |
| C | -2.88371200 | 2.64112400  | 1.67928000  |
| C | -1.65495800 | 2.19906800  | 2.17507300  |
| C | -1.66784000 | 0.43068100  | 0.59470700  |
| H | -3.35559900 | 3.51632800  | 2.11334000  |
| H | -1.17827300 | 2.73035900  | 2.99254500  |
| H | -0.07344000 | 0.72437900  | 2.02274900  |
| H | -4.46126700 | 2.28704600  | 0.23531300  |
| C | -3.49548800 | 0.05395000  | -1.03434200 |
| I | -0.93670900 | -1.27074700 | -0.38061700 |
| O | -2.75841600 | -0.97776200 | -1.40686300 |
| O | -4.55953500 | 0.33864100  | -1.54265700 |
| O | 0.68762000  | -1.23522300 | 0.87723200  |
| O | 2.93774800  | -2.51238800 | 1.51246100  |
| C | 3.02733400  | -1.33359600 | 0.84028100  |
| C | 1.85329300  | -0.64554800 | 0.47467900  |
| C | 4.25896300  | -0.79361800 | 0.51317900  |
| C | 1.93426500  | 0.55722300  | -0.21004800 |
| C | 4.35127100  | 0.41827300  | -0.18182400 |
| H | 5.15840600  | -1.33020300 | 0.79906600  |
| C | 3.18683600  | 1.09212600  | -0.54414700 |
| H | 1.03880100  | 1.10083300  | -0.49716200 |
| H | 1.98775300  | -2.68920700 | 1.63487400  |
| H | 5.32964700  | 0.81281300  | -0.42807600 |
| O | 3.15519000  | 2.27326300  | -1.21922600 |
| C | 4.40063500  | 2.84455200  | -1.57271900 |



|   |            |            |             |
|---|------------|------------|-------------|
| H | 4.97088200 | 2.18223300 | -2.23475000 |
| H | 4.17137100 | 3.77100200 | -2.10051900 |
| H | 5.00227100 | 3.07259000 | -0.68498400 |

### TS<sub>34</sub>

E(SMD/M06-2X/BS1) = -927.0844897 au

H(SMD/M06-2X/BS1) = -926.839376 au

G(SMD/M06-2X/BS1) = -926.908888 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1213.759337 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.71371300  | 2.93802600  | 0.15816800  |
| C | 0.66546300  | 1.13670800  | -1.68746300 |
| C | 1.94258000  | 1.57279100  | 0.34627900  |
| C | 0.97867700  | 3.40687000  | -0.92594700 |
| C | 0.46076400  | 2.50508800  | -1.85409400 |
| C | 1.39059900  | 0.69507100  | -0.58290900 |
| H | 0.81874700  | 4.47289100  | -1.05548800 |
| H | -0.10267600 | 2.85867000  | -2.71232700 |
| H | 0.26427200  | 0.42746700  | -2.40389000 |
| H | 2.14348800  | 3.61704700  | 0.88758500  |
| C | 2.82572000  | 1.11696000  | 1.51621500  |
| I | 1.66076400  | -1.37940600 | -0.34239700 |
| O | 3.16065200  | -0.09992600 | 1.50074500  |
| O | 3.14132600  | 1.98083500  | 2.34753400  |
| O | -0.85220100 | -1.65549100 | -1.43654100 |
| O | -1.44732100 | -3.07572400 | 0.65526500  |
| C | -2.08272800 | -1.94936600 | 0.49515900  |
| C | -1.71631300 | -1.14229600 | -0.68578500 |
| C | -3.03959900 | -1.49579400 | 1.40865300  |
| C | -2.34368300 | 0.12878600  | -0.86607300 |
| C | -3.62719100 | -0.27681600 | 1.17376600  |
| H | -3.29820000 | -2.09311200 | 2.27503400  |
| C | -3.29125900 | 0.54369100  | 0.03078300  |
| H | -2.09738600 | 0.73042100  | -1.73265000 |
| H | -0.83669800 | -3.18272600 | -0.11334700 |
| H | -4.37203800 | 0.07601100  | 1.87832900  |
| O | -3.88475300 | 1.72457600  | -0.19626000 |
| C | -4.88618200 | 2.19037200  | 0.70637800  |
| H | -5.21074200 | 3.15107100  | 0.30842600  |
| H | -5.73747700 | 1.50353800  | 0.73949700  |
| H | -4.47674700 | 2.33254500  | 1.71112900  |

### TS<sub>35</sub>

E(SMD/M06-2X/BS1) = -927.0913613 au

H(SMD/M06-2X/BS1) = -926.846447 au  
G(SMD/M06-2X/BS1) = -926.912567 au  
E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1213.7646998 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.35073500  | 2.41197800  | 1.04330100  |
| C | 0.03350400  | -0.28076100 | 1.71480700  |
| C | -0.73626700 | 1.72402400  | 0.52129100  |
| C | 1.27571600  | 1.77858900  | 1.88248400  |
| C | 1.09815800  | 0.44746900  | 2.24591100  |
| C | -0.84396600 | 0.36218600  | 0.83423000  |
| H | 2.10951100  | 2.34334500  | 2.28908500  |
| H | 1.78778100  | -0.03527800 | 2.93093700  |
| H | -0.12405600 | -1.31826100 | 1.99576500  |
| H | 0.44448100  | 3.46489900  | 0.79731900  |
| C | -1.82665400 | 2.47861900  | -0.26534200 |
| I | -2.20816600 | -0.81090600 | -0.16440800 |
| O | -2.92506000 | 1.87115300  | -0.36137100 |
| O | -1.51993900 | 3.60679400  | -0.67950800 |
| O | -0.32553600 | -1.97657600 | -1.19480200 |
| C | 1.33831500  | -0.27048100 | -1.33772900 |
| C | 0.81302300  | -1.49771400 | -0.85142700 |
| C | 2.57562100  | 0.15843200  | -0.91425000 |
| C | 1.57299800  | -2.26233500 | 0.11318600  |
| C | 3.33108800  | -0.64459100 | -0.00666800 |
| C | 2.84799900  | -1.84181300 | 0.48858800  |
| H | 3.42862200  | -2.43088500 | 1.18935100  |
| O | 1.03323700  | -3.36896900 | 0.60106400  |
| H | 0.15307900  | -3.47395000 | 0.17908600  |
| H | 0.74996400  | 0.32221400  | -2.03047600 |
| O | 3.02134800  | 1.33331800  | -1.40460900 |
| C | 4.22265800  | 1.87146200  | -0.86906300 |
| H | 5.08528600  | 1.24065000  | -1.10864000 |
| H | 4.34753600  | 2.84582700  | -1.34109400 |
| H | 4.14713100  | 1.99909200  | 0.21665900  |
| H | 4.31349800  | -0.31575600 | 0.31350300  |

### TS<sub>36</sub>-H,H,OMe,H

E(SMD/M06-2X/BS1) = -927.1024655 au  
H(SMD/M06-2X/BS1) = -926.858966 au  
G(SMD/M06-2X/BS1) = -926.92499 au  
E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1213.775109 au

|   |             |            |            |
|---|-------------|------------|------------|
| C | -1.51474000 | 2.63870400 | 0.69351500 |
| C | 0.01116300  | 0.61019700 | 1.86155900 |
| C | -1.78396200 | 1.31846600 | 0.33807600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.48508700 | 2.95060900  | 1.58043500  |
| C | 0.28329600  | 1.94182600  | 2.15935500  |
| C | -1.01296200 | 0.32213400  | 0.95238000  |
| H | -0.28096800 | 3.98934000  | 1.82125100  |
| H | 1.08448400  | 2.18468100  | 2.84921400  |
| H | 0.57648400  | -0.19027900 | 2.32680700  |
| H | -2.11503300 | 3.42432700  | 0.24525600  |
| C | -2.83721900 | 1.03638300  | -0.73877800 |
| I | -1.32882200 | -1.66933200 | 0.50824900  |
| O | -2.45617200 | 0.23801300  | -1.65482800 |
| O | -3.91887200 | 1.61184600  | -0.62808900 |
| O | 0.00335200  | -1.57296000 | -1.19453800 |
| O | -0.13527800 | 0.98156300  | -2.29907300 |
| C | 0.91875600  | 0.56957000  | -1.61868100 |
| C | 1.01571000  | -0.72721900 | -1.03405200 |
| C | 2.04597300  | 1.40563800  | -1.52071700 |
| C | 2.16512900  | -1.11075600 | -0.31483900 |
| C | 3.18018000  | 1.01267000  | -0.83584100 |
| H | 1.99264400  | 2.38891200  | -1.97635100 |
| C | 3.24986900  | -0.26042400 | -0.22169700 |
| H | 2.19384500  | -2.09066500 | 0.15208100  |
| H | -1.01563100 | 0.50437500  | -2.04716900 |
| H | 4.01420400  | 1.70192800  | -0.76769200 |
| O | 4.32600700  | -0.70874600 | 0.47073300  |
| C | 5.45563600  | 0.14479700  | 0.55554400  |
| H | 6.20372600  | -0.40417400 | 1.12804400  |
| H | 5.85736800  | 0.37541500  | -0.43755300 |
| H | 5.21370100  | 1.07743000  | 1.07770200  |

### 37

E(SMD/M06-2X/BS1) = -495.7743758 au

H(SMD/M06-2X/BS1) = -495.644476 au

G(SMD/M06-2X/BS1) = -495.688153 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -495.9821159 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.66468600 | -0.65491700 | 0.00040600  |
| C | -1.33809200 | 0.86038800  | -0.00057800 |
| C | -0.52923000 | -1.59766900 | -0.00195700 |
| C | 0.05865500  | 1.23924900  | 0.00049700  |
| C | 0.73311600  | -1.14797200 | -0.00187400 |
| H | -0.76002200 | -2.65814700 | -0.00312100 |
| C | 1.03818800  | 0.29709800  | -0.00011900 |
| H | 0.31270600  | 2.29371200  | 0.00130200  |
| H | 1.55497600  | -1.85509900 | -0.00314400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -2.81923100 | -1.02377400 | 0.00323000  |
| O | 2.30492700  | 0.72162400  | 0.00079100  |
| C | 3.38561400  | -0.21263300 | 0.00093800  |
| H | 3.36972400  | -0.83589300 | -0.89743400 |
| H | 4.28947300  | 0.39548000  | 0.00276000  |
| H | 3.36754400  | -0.83800700 | 0.89780600  |
| O | -2.26517000 | 1.65173400  | -0.00177700 |

### 38

E(SMD/M06-2X/BS1) = -431.3831957 au

H(SMD/M06-2X/BS1) = -431.267597 au

G(SMD/M06-2X/BS1) = -431.313262 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -717.8529099 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.66793400 | 0.05404900  | -0.00694100 |
| C | -0.74416800 | -1.94961600 | 0.07660100  |
| C | -1.31291100 | 0.40551600  | 0.01402600  |
| C | -3.06318500 | -1.27593000 | 0.04260100  |
| C | -2.09700800 | -2.27790600 | 0.08895200  |
| C | -0.35035700 | -0.61182300 | 0.04415200  |
| H | -4.11827800 | -1.52827900 | 0.04091600  |
| H | -2.39006000 | -3.32241800 | 0.12387700  |
| H | 0.00492700  | -2.73383300 | 0.08556500  |
| H | -3.40631800 | 0.84840800  | -0.05180000 |
| C | -1.03378600 | 1.88235900  | -0.01917500 |
| I | 1.72477000  | -0.23186800 | -0.07280200 |
| O | -0.13915400 | 2.36714100  | 0.85373600  |
| O | -1.62517900 | 2.63390600  | -0.75292500 |
| H | 0.22767000  | 1.65686300  | 1.41216900  |

### TS<sub>25</sub>

E(SMD/M06-2X/BS1) = -927.0053342 au

H(SMD/M06-2X/BS1) = -926.761438 au

G(SMD/M06-2X/BS1) = -926.829717 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1213.679412 au

|   |             |            |             |
|---|-------------|------------|-------------|
| C | -3.17672300 | 2.08493000 | 0.44706800  |
| C | -1.81935400 | 0.94316500 | -1.70899800 |
| C | -2.54816200 | 0.85223600 | 0.62697400  |
| C | -3.14132700 | 2.73720700 | -0.78243500 |
| C | -2.46865000 | 2.16653600 | -1.86233700 |
| C | -1.87006700 | 0.31542800 | -0.46488100 |
| H | -3.64253400 | 3.69294200 | -0.90253500 |
| H | -2.44224300 | 2.67050200 | -2.82321000 |
| H | -1.27104600 | 0.49856200 | -2.53243000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.69849600 | 2.50961100  | 1.29835500  |
| C | -2.64996800 | 0.13450700  | 1.98501700  |
| I | -0.87272600 | -1.52565600 | -0.25797700 |
| O | -2.17025200 | -1.03134000 | 2.00831300  |
| O | -3.19693400 | 0.76259100  | 2.90077500  |
| O | 0.61603300  | -1.09778700 | 0.68581400  |
| O | 0.77718900  | -0.72702600 | -2.09807000 |
| C | 1.64996500  | -0.21637600 | -1.34758700 |
| C | 1.66201800  | 1.20383400  | -1.04636600 |
| C | 2.66829000  | -1.03630400 | -0.72565000 |
| C | 2.65570900  | 1.74067300  | -0.29494400 |
| H | 0.88077000  | 1.82398700  | -1.47564800 |
| C | 3.68088700  | -0.49107100 | 0.02641700  |
| H | 2.63057500  | -2.10377300 | -0.91742900 |
| C | 3.68030700  | 0.89950400  | 0.24828200  |
| H | 2.70771800  | 2.80277900  | -0.07988200 |
| H | 4.44327600  | -1.12426200 | 0.46233000  |
| O | 4.59196800  | 1.53336900  | 0.95925700  |
| C | 5.66197200  | 0.78492700  | 1.54846000  |
| H | 6.27738700  | 1.51711600  | 2.06794800  |
| H | 5.26776200  | 0.05414400  | 2.25924700  |
| H | 6.24790000  | 0.28455000  | 0.77317900  |

### TS<sub>32</sub>

E(SMD/M06-2X/BS1) = -927.0266526 au

H(SMD/M06-2X/BS1) = -926.78264 au

G(SMD/M06-2X/BS1) = -926.847235 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1213.69734 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.24871700 | 2.63820900  | 0.62487800  |
| C | 2.21656000  | 1.92507500  | -0.52775900 |
| C | 0.21834900  | 1.32764800  | 0.74295200  |
| C | 0.50924800  | 3.58109600  | -0.05910500 |
| C | 1.73504300  | 3.22541900  | -0.63786900 |
| C | 1.44323200  | 1.00636700  | 0.17383000  |
| H | 0.14842600  | 4.60059400  | -0.15295300 |
| H | 2.31364400  | 3.96893600  | -1.17736600 |
| H | 3.15874300  | 1.61061400  | -0.96789300 |
| H | -1.20993600 | 2.88999400  | 1.06250700  |
| C | -0.56966800 | 0.23046000  | 1.41820600  |
| I | 2.10252300  | -0.96037000 | 0.30696200  |
| O | 0.05378700  | -0.89973400 | 1.44325500  |
| O | -1.69595400 | 0.45580300  | 1.85676000  |
| O | 0.41005600  | -1.45758500 | -1.57167800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.67537800 | -1.90738700 | -0.56994500 |
| C | -0.75026400 | -1.05733200 | -1.29228400 |
| C | -2.91694700 | -1.47101400 | -0.22286400 |
| C | -1.19605700 | 0.27422400  | -1.65980500 |
| C | -3.30008400 | -0.14116500 | -0.56510600 |
| H | -3.59032800 | -2.10965500 | 0.33515600  |
| C | -2.44577000 | 0.70082400  | -1.33465300 |
| H | -2.80673400 | 1.68915100  | -1.59831700 |
| O | -4.45535200 | 0.38675900  | -0.23603300 |
| C | -5.36629100 | -0.35640000 | 0.58528900  |
| H | -4.89148500 | -0.60868800 | 1.53640500  |
| H | -6.21260800 | 0.30728400  | 0.75165300  |
| H | -5.69546300 | -1.26029500 | 0.06696600  |
| H | -0.50375800 | 0.90571300  | -2.20934500 |
| H | -1.33140100 | -2.89977000 | -0.29804800 |
| O | 3.59591700  | -0.74154700 | -0.70134500 |

### 33

E(SMD/M06-2X/BS1) = -927.0416006 au

H(SMD/M06-2X/BS1) = -926.798614 au

G(SMD/M06-2X/BS1) = -926.86562 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1213.707779 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.37168700  | -1.11548800 | -1.80691400 |
| C | -0.85206500 | 0.57443500  | -2.18532000 |
| C | 0.33475200  | -1.10867000 | -0.87547700 |
| C | 1.29575200  | -0.28520300 | -2.92190700 |
| C | 0.19361700  | 0.55319700  | -3.10858800 |
| C | -0.74343000 | -0.26723100 | -1.08977200 |
| H | 2.09966800  | -0.28587900 | -3.65104900 |
| H | 0.14540500  | 1.19927800  | -3.97940400 |
| H | -1.71475100 | 1.21923100  | -2.31361700 |
| H | 2.22289300  | -1.76983800 | -1.64223100 |
| C | 0.34237000  | -1.95931700 | 0.36543800  |
| I | -2.23081000 | -0.37488600 | 0.38867000  |
| O | -0.73086800 | -1.81870200 | 1.09155800  |
| O | 1.27895800  | -2.69581600 | 0.63134100  |
| O | -0.78087300 | 2.68114400  | 1.26769900  |
| C | 0.80129600  | 1.04372800  | 1.89827400  |
| C | 0.31589300  | 2.11709700  | 1.05287900  |
| C | 1.97865800  | 0.38758200  | 1.63995700  |
| C | 1.16057000  | 2.48483700  | -0.07074500 |
| C | 2.74673200  | 0.75686100  | 0.51044800  |
| H | 2.30059700  | -0.42384300 | 2.28243900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.32890100  | 1.82954900  | -0.32444100 |
| H | 2.95477600  | 2.08406400  | -1.17447700 |
| O | 3.87227700  | 0.14855400  | 0.13950500  |
| C | 4.27842400  | -1.02081700 | 0.85341200  |
| H | 3.48174700  | -1.77085300 | 0.83533800  |
| H | 5.15904000  | -1.39325300 | 0.33114500  |
| H | 4.54296900  | -0.77031800 | 1.88531300  |
| H | 0.81666000  | 3.29026200  | -0.71285300 |
| H | 0.18889200  | 0.76600500  | 2.75128600  |
| O | -3.29997900 | 0.90741500  | -0.48446200 |

### MECP1

E(SMD/M06-2X/BS1) = -927.026908 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.17663000 | 1.44225900  | 1.50573200  |
| C | 0.93568700  | 2.25808300  | -0.16401500 |
| C | -0.11639400 | 0.57358400  | 1.26228800  |
| C | -1.18259500 | 2.70733700  | 0.91911100  |
| C | -0.12895400 | 3.11726700  | 0.09592800  |
| C | 0.90803600  | 1.00022500  | 0.42717200  |
| H | -2.00794000 | 3.38693600  | 1.10804700  |
| H | -0.13972800 | 4.10778900  | -0.34772900 |
| H | 1.76803300  | 2.53678900  | -0.80365800 |
| H | -1.98473400 | 1.11530000  | 2.15322700  |
| C | -0.03600300 | -0.81972600 | 1.84550200  |
| I | 2.41203300  | -0.36183000 | -0.01023200 |
| O | 0.97180100  | -1.49200000 | 1.39532500  |
| O | -0.87238800 | -1.20524500 | 2.65256800  |
| O | 0.71643300  | -1.35152800 | -1.70197600 |
| C | -1.32374000 | -1.82070400 | -0.61238900 |
| C | -0.46932000 | -1.00063200 | -1.43853400 |
| C | -2.60260800 | -1.43831100 | -0.30834000 |
| C | -1.00851400 | 0.24792600  | -1.93456500 |
| C | -3.09312000 | -0.20474100 | -0.80839700 |
| H | -3.22415400 | -2.06243200 | 0.32221600  |
| C | -2.28211200 | 0.62693300  | -1.63317700 |
| H | -2.70741100 | 1.55762200  | -1.99519700 |
| O | -4.30767500 | 0.25334100  | -0.56500300 |
| C | -5.20150900 | -0.52388400 | 0.23990000  |
| H | -4.78664300 | -0.66943700 | 1.24115100  |
| H | -6.12010000 | 0.05743900  | 0.29730300  |
| H | -5.39827900 | -1.48940500 | -0.23466200 |
| H | -0.36738500 | 0.86378000  | -2.55784500 |
| H | -0.91023600 | -2.74671600 | -0.22629300 |

O 3.33026400 0.73613300 -1.12986000

**22'**

E(SMD/M06-2X/BS1) = -1003.439667 au

H(SMD/M06-2X/BS1) = -1003.16642 au

G(SMD/M06-2X/BS1) = -1003.23982 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1290.157789 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.05125000  | 1.87358600  | -1.02598600 |
| C | 2.03256500  | -0.65952800 | -1.73619500 |
| C | 2.19553800  | 1.20279500  | -0.15809200 |
| C | 3.39249900  | 1.28215900  | -2.24165800 |
| C | 2.89433000  | 0.02575400  | -2.59340500 |
| C | 1.71184200  | -0.03846000 | -0.54050900 |
| H | 4.05831900  | 1.80231900  | -2.92273000 |
| H | 3.17548100  | -0.42411700 | -3.53991700 |
| H | 1.63009700  | -1.63750300 | -1.98228400 |
| H | 3.44245200  | 2.84401600  | -0.73790700 |
| C | 1.80307900  | 1.73745400  | 1.19611900  |
| I | 0.40442100  | -0.96009500 | 0.80202300  |
| O | 1.04375400  | 0.91144800  | 1.86915100  |
| O | 2.18233900  | 2.82524000  | 1.58459400  |
| O | -2.19129500 | -2.83391400 | -1.01622200 |
| C | -3.36313600 | -1.00791000 | -0.02014900 |
| C | -2.39536900 | -1.48974100 | -0.89752200 |
| C | -3.56158900 | 0.36382000  | 0.14424600  |
| C | -1.62544600 | -0.57189700 | -1.62780500 |
| C | -2.77112100 | 1.27490900  | -0.56296700 |
| H | -4.32199200 | 0.70577800  | 0.83690000  |
| C | -1.80246400 | 0.79652900  | -1.45347100 |
| H | -1.19683700 | 1.50950200  | -2.00498300 |
| O | -2.87160900 | 2.62429300  | -0.45655600 |
| C | -3.82283600 | 3.13320000  | 0.46179600  |
| H | -3.60919200 | 2.79803600  | 1.48348200  |
| H | -3.73960500 | 4.21933900  | 0.41350700  |
| H | -4.84153700 | 2.83529300  | 0.18780800  |
| H | -0.88317900 | -0.94054100 | -2.33166600 |
| H | -3.95610100 | -1.71744900 | 0.54857900  |
| O | 1.67964800  | -1.60519600 | 2.08559000  |
| H | 1.92473200  | -0.83287800 | 2.63726400  |
| O | 0.36738700  | -2.52628600 | -0.05625100 |
| H | -1.23357800 | -2.97747400 | -0.84410900 |

**TS**<sub>22'-23'</sub>



E(SMD/M06-2X/BS1) = -1003.416970 au  
H(SMD/M06-2X/BS1) = -1003.147838 au  
G(SMD/M06-2X/BS1) = -1003.217722 au  
E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1290.131936 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.02695000 | 2.01553000  | 0.90635300  |
| C | -2.64397700 | -0.77180300 | 1.13747200  |
| C | -2.01408100 | 1.38916800  | 0.18512900  |
| C | -3.84397500 | 1.25219300  | 1.73714600  |
| C | -3.65652000 | -0.12681600 | 1.85061800  |
| C | -1.85489000 | 0.02254400  | 0.32525300  |
| H | -4.63570300 | 1.73332800  | 2.30192600  |
| H | -4.30255900 | -0.71065600 | 2.49809100  |
| H | -2.48131400 | -1.84160500 | 1.21046300  |
| H | -3.16225400 | 3.08752100  | 0.80473500  |
| C | -1.09058000 | 2.12370700  | -0.74789900 |
| I | -0.32214500 | -0.76946500 | -0.86134100 |
| O | -0.22416300 | 1.33254700  | -1.33836300 |
| O | -1.16443100 | 3.32341400  | -0.91583500 |
| O | 1.25025300  | -2.91391900 | 1.23096900  |
| C | 3.05073100  | -1.55142500 | 0.47110100  |
| C | 1.76853000  | -1.74967000 | 1.07078600  |
| C | 3.56985800  | -0.29226600 | 0.27723500  |
| C | 1.02725800  | -0.55195700 | 1.37524000  |
| C | 2.85098100  | 0.87620800  | 0.65469200  |
| H | 4.55290200  | -0.19921700 | -0.17267900 |
| C | 1.60648900  | 0.73678800  | 1.22538700  |
| H | 1.05527900  | 1.62156800  | 1.53157900  |
| O | 3.33145500  | 2.13777400  | 0.50100700  |
| C | 4.63095400  | 2.28699600  | -0.04345500 |
| H | 4.68728100  | 1.89044700  | -1.06374100 |
| H | 4.82586000  | 3.35966400  | -0.06533800 |
| H | 5.38689300  | 1.79592800  | 0.58040000  |
| H | 0.14608300  | -0.66149200 | 2.00377400  |
| H | 3.62198400  | -2.43022100 | 0.18850200  |
| O | -1.71254600 | -0.95444400 | -2.23170500 |
| H | -1.28296600 | -1.18269500 | -3.08099000 |
| O | -0.68778200 | -2.52739000 | -0.25525500 |
| H | 0.07692800  | -2.81995500 | 0.43747400  |

**23'**

E(SMD/M06-2X/BS1) = -1003.429846 au  
H(SMD/M06-2X/BS1) = -1003.157994 au  
G(SMD/M06-2X/BS1) = -1003.226116 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1290.139601 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.12074700 | 2.05238600  | 1.77889800  |
| C | 1.24151600  | 2.10429600  | 0.23579600  |
| C | -0.48327700 | 0.86123700  | 1.43591100  |
| C | -0.57769800 | 3.26114600  | 1.35347000  |
| C | 0.59770600  | 3.28771900  | 0.59838800  |
| C | 0.66674300  | 0.91792200  | 0.66832900  |
| H | -1.06809100 | 4.19331500  | 1.61445600  |
| H | 1.01781700  | 4.23732700  | 0.28298100  |
| H | 2.14465500  | 2.11412900  | -0.36440200 |
| H | -2.02858400 | 2.01385900  | 2.37240000  |
| C | -0.98345600 | -0.48955400 | 1.86247400  |
| I | 1.40484100  | -0.96961900 | 0.11669600  |
| O | -0.21668800 | -1.47472300 | 1.45186000  |
| O | -1.98924000 | -0.62605700 | 2.53083900  |
| O | 1.16227600  | 0.84492700  | -2.84144800 |
| C | -0.11942400 | -0.83871900 | -1.76009500 |
| C | 0.08126500  | 0.51164500  | -2.30435200 |
| C | -1.42647900 | -1.21110000 | -1.24190400 |
| C | -0.99887600 | 1.46529100  | -2.11714800 |
| C | -2.38520800 | -0.26365700 | -1.06866200 |
| H | -1.58363300 | -2.24208100 | -0.94673300 |
| C | -2.15541400 | 1.09130300  | -1.52144200 |
| H | -2.96023500 | 1.80603700  | -1.36933300 |
| O | -3.60752500 | -0.45380100 | -0.52002600 |
| C | -3.87872000 | -1.75621300 | -0.02923800 |
| H | -3.14614500 | -2.04688500 | 0.73166000  |
| H | -4.87276500 | -1.71280200 | 0.41660900  |
| H | -3.87613200 | -2.48956400 | -0.84466200 |
| H | -0.84074300 | 2.47902500  | -2.47114900 |
| H | 0.41605500  | -1.61442300 | -2.31201100 |
| O | 2.72846400  | -0.18068900 | -1.04050500 |
| O | 2.72059800  | -0.81276700 | 1.60087600  |
| H | 2.92482700  | 0.12543800  | 1.77751500  |
| H | 2.28572500  | 0.18911000  | -1.86754200 |

**TS<sub>23'-24'</sub>**

E(SMD/M06-2X/BS1) = -1079.812382 au

H(SMD/M06-2X/BS1) = -1079.518951 au

G(SMD/M06-2X/BS1) = -1079.591937 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1366.570755 au

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -2.00392900 | -2.23340200 | 0.84440200 |
|---|-------------|-------------|------------|

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.18718900  | -0.84267100 | 1.94451300  |
| C | -1.06909100 | -1.63028500 | 0.00648800  |
| C | -1.84237100 | -2.14359100 | 2.22529000  |
| C | -0.75596800 | -1.45756600 | 2.77097400  |
| C | -0.00503500 | -0.95608000 | 0.57885100  |
| H | -2.56784700 | -2.60984000 | 2.88412300  |
| H | -0.64012600 | -1.39294700 | 3.84805700  |
| H | 1.02797500  | -0.29232700 | 2.35326500  |
| H | -2.84440500 | -2.75978600 | 0.40291800  |
| C | -1.17791500 | -1.65167800 | -1.49627400 |
| I | 1.29353900  | -0.04158300 | -0.77896700 |
| O | -0.22107400 | -0.99562800 | -2.08994200 |
| O | -2.09214700 | -2.23231600 | -2.05806800 |
| O | 1.38403800  | 3.51065900  | -0.14785100 |
| C | 0.45856900  | 2.75044900  | 0.06330000  |
| C | -1.46558500 | 1.41913400  | -0.91945300 |
| C | -0.23654000 | 2.67312200  | 1.36184900  |
| C | -2.10371100 | 1.50906300  | 0.27145900  |
| H | -1.93899500 | 1.00633500  | -1.80116500 |
| C | -1.44501700 | 2.09287800  | 1.44368100  |
| H | -1.99771100 | 2.06023800  | 2.37869200  |
| O | -3.36155500 | 1.11493900  | 0.53205700  |
| C | -4.08156500 | 0.51869700  | -0.53844000 |
| H | -3.55907400 | -0.36551100 | -0.92065300 |
| H | -5.04868500 | 0.22825000  | -0.12870900 |
| H | -4.22563100 | 1.23669100  | -1.35364100 |
| H | 0.23196200  | 3.15702200  | 2.21253900  |
| O | 2.31255200  | 0.77106400  | 0.57758600  |
| O | 2.47044500  | -2.00922500 | -0.23224900 |
| H | 3.00012200  | 0.00379000  | 1.13789500  |
| O | 3.57525500  | -0.98655300 | 1.62432800  |
| H | 4.53358200  | -0.89355700 | 1.49256900  |
| H | 3.14101700  | -1.64192700 | 0.76439700  |
| H | 3.08812200  | -2.20091800 | -0.95901900 |
| C | -0.05454600 | 1.81171200  | -1.00299000 |
| H | 0.27509800  | 2.12619500  | -1.99483200 |

## 24'

E(SMD/M06-2X/BS1) = -927.0401605 au

H(SMD/M06-2X/BS1) = -926.794673 au

G(SMD/M06-2X/BS1) = -926.860367 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1213.707139 au

|   |             |            |            |
|---|-------------|------------|------------|
| C | -1.72685600 | 2.43260800 | 0.65331400 |
|---|-------------|------------|------------|

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.74093800  | 2.69973400  | -0.68111700 |
| C | -0.75474200 | 1.44549200  | 0.79351600  |
| C | -1.46205700 | 3.55071600  | -0.13596500 |
| C | -0.23931500 | 3.68587100  | -0.79861600 |
| C | 0.44781800  | 1.61385700  | 0.12602500  |
| H | -2.21697100 | 4.32309500  | -0.24466700 |
| H | -0.05019700 | 4.55836800  | -1.41576100 |
| H | 1.69234200  | 2.75820300  | -1.20173400 |
| H | -2.67864400 | 2.30707700  | 1.16032800  |
| C | -0.96571400 | 0.17898700  | 1.59311400  |
| I | 1.82385000  | 0.04218800  | 0.24141700  |
| O | 0.07658900  | -0.58135600 | 1.61994400  |
| O | -2.04447800 | -0.04289900 | 2.13265200  |
| O | 1.46610600  | -3.33868900 | -0.05015000 |
| C | -0.86695200 | -3.04429300 | 0.16176200  |
| C | 0.47932800  | -2.67169000 | -0.30465000 |
| C | -1.94060300 | -2.30127800 | -0.14643200 |
| C | 0.59422400  | -1.40090800 | -1.13011700 |
| C | -1.82016100 | -1.10653100 | -0.99141400 |
| H | -2.92056800 | -2.58921700 | 0.21731700  |
| C | -0.62458500 | -0.73782100 | -1.52464800 |
| H | -0.57886200 | 0.11725400  | -2.19121700 |
| O | -2.90031800 | -0.38754300 | -1.32412200 |
| C | -4.09631800 | -0.53657100 | -0.55563400 |
| H | -3.87708200 | -0.45979100 | 0.51277600  |
| H | -4.73969400 | 0.28911000  | -0.85989100 |
| H | -4.59667000 | -1.48310700 | -0.78081900 |
| H | 1.38548200  | -1.45746000 | -1.88051000 |
| H | -0.94241900 | -3.94137400 | 0.76721600  |
| O | 2.93575100  | 0.66209000  | -1.03244400 |

### 16-*p*-Cl

E(SMD/M06-2X/BS1) = -766.906331 au

H(SMD/M06-2X/BS1) = -766.802487 au

G(SMD/M06-2X/BS1) = -766.841193 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -767.073519 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.81849600  | 0.01771100  | -0.00011400 |
| C | 1.11147600  | 1.22275500  | -0.00013400 |
| C | 1.12884400  | -1.19619400 | -0.00011400 |
| C | -0.27765200 | 1.21483700  | -0.00008100 |
| H | 1.65966600  | 2.15913100  | -0.00025300 |
| C | -0.26291600 | -1.20716100 | -0.00014300 |
| H | 1.67734800  | -2.13462000 | -0.00011700 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.95406900 | -0.00176600 | -0.00009900 |
| H  | -0.82937700 | 2.14894100  | -0.00001200 |
| H  | -0.80025000 | -2.14958400 | -0.00019200 |
| O  | 3.17265000  | 0.08756600  | 0.00023800  |
| H  | 3.54081300  | -0.81238400 | 0.00062400  |
| Cl | -2.70673400 | -0.01253500 | 0.00012700  |

### 16-*p*-C(O)CH<sub>3</sub>

E(SMD/M06-2X/BS1) = -459.930083 au

H(SMD/M06-2X/BS1) = -459.776375 au

G(SMD/M06-2X/BS1) = -459.82025 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -460.1233007 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.13805500  | -0.02759700 | -0.00000400 |
| C | 1.48317000  | 1.21040300  | 0.00094200  |
| C | 1.39943600  | -1.21391900 | -0.00084400 |
| C | 0.09984800  | 1.24952300  | 0.00099100  |
| H | 2.07560500  | 2.11967000  | 0.00163800  |
| C | 0.01094600  | -1.15923600 | -0.00083200 |
| H | 1.91273100  | -2.17210300 | -0.00155000 |
| C | -0.65749000 | 0.06948500  | 0.00004900  |
| H | -0.42002100 | 2.20227000  | 0.00157800  |
| H | -0.54716400 | -2.09034400 | -0.00138400 |
| O | 3.48993000  | -0.01552900 | -0.00004500 |
| H | 3.82109700  | -0.93030700 | 0.00001100  |
| C | -2.14601400 | 0.17192700  | -0.00046300 |
| C | -2.95364000 | -1.10433900 | 0.00166900  |
| H | -4.01529700 | -0.85417900 | 0.00198900  |
| H | -2.72071600 | -1.70929800 | -0.88077400 |
| H | -2.71929100 | -1.70653400 | 0.88575800  |
| O | -2.69403200 | 1.26094800  | -0.00199500 |

### 16-*p*-NO<sub>2</sub>

E(SMD/M06-2X/BS1) = -511.769692 au

H(SMD/M06-2X/BS1) = -511.651681 au

G(SMD/M06-2X/BS1) = -511.693512 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -511.991177 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.06890100  | 0.01756800  | 0.00009500  |
| C | 1.36604800  | 1.22995600  | 0.00000800  |
| C | 1.38125300  | -1.20251500 | 0.00005900  |
| C | -0.01715000 | 1.22325900  | -0.00020400 |
| H | 1.91978500  | 2.16236300  | 0.00005100  |
| C | -0.00418200 | -1.21178100 | 0.00006700  |
| H | 1.93332200  | -2.13818500 | 0.00012200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.68647200 | 0.00081000  | -0.00005600 |
| H | -0.57789300 | 2.14998000  | -0.00028800 |
| H | -0.55276900 | -2.14577400 | 0.00009400  |
| O | 3.41378600  | 0.08619300  | 0.00002200  |
| H | 3.78841000  | -0.81240000 | -0.00050100 |
| N | -2.14200400 | -0.00829500 | 0.00007300  |
| O | -2.71062000 | -1.08945300 | -0.00016700 |
| O | -2.72406800 | 1.06554700  | 0.00016800  |

### 16-*p*-CN

E(SMD/M06-2X/BS1) = -399.5581966 au

H(SMD/M06-2X/BS1) = -399.445267 au

G(SMD/M06-2X/BS1) = -399.484958 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -399.7252147 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.70790400  | 0.01697000  | -0.00003200 |
| C | 1.00494600  | 1.22771600  | 0.00004800  |
| C | 1.02075600  | -1.20218000 | -0.00001000 |
| C | -0.37884800 | 1.21889200  | 0.00013100  |
| H | 1.55841300  | 2.16053300  | -0.00002400 |
| C | -0.36525300 | -1.21025300 | 0.00009300  |
| H | 1.57326200  | -2.13782900 | 0.00005700  |
| C | -1.07125900 | -0.00088700 | 0.00012300  |
| H | -0.93057300 | 2.15304700  | 0.00025200  |
| H | -0.90447600 | -2.15167500 | 0.00015200  |
| O | 3.05497500  | 0.08564500  | -0.00024000 |
| H | 3.42736700  | -0.81354300 | 0.00075100  |
| C | -2.50502400 | -0.01075900 | -0.00000600 |
| N | -3.66330300 | -0.01895500 | -0.00019200 |

### 16-*p*-CH3

E(SMD/M06-2X/BS1) = -346.6340525 au

H(SMD/M06-2X/BS1) = -346.492244 au

G(SMD/M06-2X/BS1) = -346.532584 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -346.778884 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.43930200  | 0.02017800  | -0.00000700 |
| C | 0.72329300  | 1.22045000  | -0.00000300 |
| C | 0.75333600  | -1.19297400 | 0.00000300  |
| C | -0.66538000 | 1.19426300  | 0.00004800  |
| H | 1.26796200  | 2.15961700  | -0.00003600 |
| C | -0.64131900 | -1.19881000 | 0.00005400  |
| H | 1.30669600  | -2.12934600 | -0.00002500 |
| C | -1.37626600 | -0.01297400 | 0.00008000  |
| H | -1.21293500 | 2.13409300  | 0.00008200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.16470400 | -2.15171500 | 0.00009100  |
| O | 2.79766700  | 0.09651900  | -0.00001900 |
| H | 3.16499200  | -0.80329500 | -0.00018000 |
| C | -2.88361100 | -0.01865000 | -0.00006400 |
| H | -3.27333600 | -1.04032600 | 0.00274700  |
| H | -3.28317700 | 0.49747600  | 0.87984600  |
| H | -3.28296400 | 0.49244100  | -0.88303700 |

### 16-H

E(SMD/M06-2X/BS1) = -307.3382647 au

H(SMD/M06-2X/BS1) = -307.225947 au

G(SMD/M06-2X/BS1) = -307.261224 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -307.4691009 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.94025300 | -0.02764200 | -0.00004200 |
| C | -0.21747300 | -1.22325300 | 0.00004200  |
| C | -0.26950100 | 1.19704900  | -0.00005900 |
| C | 1.17288100  | -1.18632600 | -0.00007600 |
| H | -0.75757200 | -2.16488500 | 0.00022000  |
| C | 1.12360500  | 1.21938100  | 0.00005500  |
| H | -0.83735800 | 2.12460500  | -0.00011100 |
| C | 1.85299300  | 0.03231400  | 0.00001000  |
| H | 1.72893200  | -2.11922100 | -0.00003100 |
| H | 1.63796000  | 2.17584700  | 0.00012300  |
| O | -2.29630200 | -0.11520700 | -0.00000400 |
| H | -2.67285200 | 0.78096100  | 0.00019200  |
| H | 2.93780200  | 0.05521500  | 0.00004900  |

### 16-*o*-OMe

E(SMD/M06-2X/BS1) = -421.8165134 au

H(SMD/M06-2X/BS1) = -421.668119 au

G(SMD/M06-2X/BS1) = -421.709264 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -421.9960591 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.47733800 | 0.98852200  | 0.00000700  |
| C | 0.44611500  | -0.07505500 | 0.00004100  |
| C | -1.83816800 | 0.72392200  | -0.00000700 |
| C | -0.00333800 | -1.38907700 | 0.00000700  |
| C | -2.29020300 | -0.59909100 | -0.00002800 |
| H | -2.53110600 | 1.55966600  | -0.00002700 |
| C | -1.37952600 | -1.64763500 | 0.00001800  |
| H | 0.70382100  | -2.21131500 | -0.00004500 |
| H | -3.35686000 | -0.79970700 | -0.00003300 |
| O | -0.02850900 | 2.26927900  | -0.00009600 |
| H | 0.94425700  | 2.23813700  | -0.00001800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.72584600 | -2.67606100 | 0.00003600  |
| O | 1.74732700  | 0.32797100  | 0.00031200  |
| C | 2.74105200  | -0.68449400 | -0.00016900 |
| H | 2.66095600  | -1.31112900 | -0.89514100 |
| H | 3.70117600  | -0.16856800 | -0.00026700 |
| H | 2.66149300  | -1.31157500 | 0.89455000  |

### 16-*o*-NO<sub>2</sub>

E(SMD/M06-2X/BS1) = -511.7596789 au

H(SMD/M06-2X/BS1) = -511.641736 au

G(SMD/M06-2X/BS1) = -511.683805 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -511.98067 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.44596400  | 0.97952300  | 0.04834400  |
| C | -0.23612600 | -0.24711700 | -0.01382400 |
| C | 1.84637700  | 0.94131900  | 0.04405200  |
| C | 0.45071000  | -1.46013200 | -0.07319100 |
| C | 2.52810500  | -0.26364900 | -0.03026300 |
| H | 2.39316300  | 1.87896600  | 0.10240300  |
| C | 1.83467600  | -1.47512300 | -0.09066700 |
| H | -0.12373900 | -2.37795200 | -0.11278600 |
| H | 3.61346200  | -0.25627400 | -0.03805100 |
| O | -0.22480500 | 2.14055600  | 0.14431600  |
| H | 0.42234700  | 2.86134400  | 0.24762900  |
| H | 2.36816700  | -2.41674700 | -0.15050100 |
| N | -1.69280100 | -0.30848800 | -0.01750500 |
| O | -2.31725200 | 0.65955600  | -0.41222300 |
| O | -2.21319600 | -1.34746700 | 0.36380000  |

### 16-*m*-OMe

E(SMD/M06-2X/BS1) = -421.817200 au

H(SMD/M06-2X/BS1) = -421.669101 au

G(SMD/M06-2X/BS1) = -421.710244 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -421.9970666 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.64826700  | -0.34275500 | -0.00000600 |
| C | 0.41249300  | -0.97866100 | 0.00003200  |
| C | 1.72955500  | 1.05526900  | -0.00002800 |
| C | -0.76305100 | -0.21748600 | 0.00005100  |
| H | 0.33844200  | -2.06274300 | -0.00000600 |
| C | 0.55461800  | 1.79206000  | -0.00000300 |
| H | 2.70341400  | 1.53278300  | -0.00012500 |
| C | -0.70077900 | 1.17789700  | 0.00003200  |
| H | 0.60760200  | 2.87685500  | -0.00001300 |
| O | 2.81582100  | -1.03658700 | 0.00001200  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.62130000  | -1.98900300 | -0.00026800 |
| O | -1.91535600 | -0.93083500 | 0.00005800  |
| H | -1.59868900 | 1.78317500  | 0.00010400  |
| C | -3.13201000 | -0.20333900 | -0.00007000 |
| H | -3.22070500 | 0.42391400  | -0.89416800 |
| H | -3.92904000 | -0.94748600 | -0.00017000 |
| H | -3.22060200 | 0.42398000  | 0.89404000  |

### 16-*m*-NO<sub>2</sub>

E(SMD/M06-2X/BS1) = -511.7664884 au

H(SMD/M06-2X/BS1) = -511.648647 au

G(SMD/M06-2X/BS1) = -511.691129 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -511.9877681 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.73515200  | -0.46833100 | -0.00007700 |
| C | 2.06259900  | 0.89252400  | 0.00008800  |
| C | 0.40018600  | -0.86621400 | -0.00011800 |
| C | 1.05858600  | 1.85222500  | 0.00025600  |
| H | 3.10960400  | 1.17753100  | 0.00007800  |
| C | -0.57342300 | 0.12544700  | 0.00003800  |
| H | 0.12027400  | -1.91409600 | -0.00041400 |
| C | -0.28490300 | 1.48188600  | 0.00022700  |
| H | 1.32344800  | 2.90412100  | 0.00039400  |
| O | 2.75717500  | -1.35460300 | -0.00025700 |
| H | 2.40324300  | -2.26082400 | -0.00038600 |
| H | -1.07992400 | 2.21618700  | 0.00044900  |
| N | -1.98105500 | -0.29472400 | -0.00000100 |
| O | -2.22114700 | -1.49009500 | 0.00076200  |
| O | -2.83583300 | 0.57406400  | -0.00082800 |

### TS<sub>24-26</sub>-*p*-Cl

E(SMD/M06-2X/BS1) = -1272.115189 au

H(SMD/M06-2X/BS1) = -1271.915491 au

G(SMD/M06-2X/BS1) = -1271.977873 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1558.767715 au

|   |             |            |             |
|---|-------------|------------|-------------|
| C | 2.54053800  | 2.60586700 | 0.13847300  |
| C | 0.25635300  | 1.49866500 | -1.08381400 |
| C | 2.39231300  | 1.22467900 | 0.07455600  |
| C | 1.55431500  | 3.43037100 | -0.40486100 |
| C | 0.42326500  | 2.88370800 | -1.01165400 |
| C | 1.25454500  | 0.71224100 | -0.53030900 |
| H | 1.66906300  | 4.50854700 | -0.35705200 |
| H | -0.33607200 | 3.53465400 | -1.43310100 |
| H | -0.61259300 | 1.04499300 | -1.54996400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 3.42513800  | 3.01833200  | 0.61332000  |
| C  | 3.40417700  | 0.25304200  | 0.63375400  |
| I  | 1.06713700  | -1.35904400 | -0.50355000 |
| O  | 3.07209100  | -0.98846800 | 0.44660700  |
| O  | 4.41544500  | 0.65164600  | 1.18910500  |
| O  | -0.62988100 | -1.32001600 | -1.18280500 |
| O  | -0.05277200 | -1.08774300 | 1.61307900  |
| C  | -1.19478600 | -0.65960600 | 1.23292200  |
| C  | -1.55538800 | 0.72779100  | 1.35259700  |
| C  | -2.08824800 | -1.54398300 | 0.54042700  |
| C  | -2.78157500 | 1.15835500  | 0.92969800  |
| H  | -0.85243400 | 1.40083700  | 1.83417000  |
| C  | -3.34168400 | -1.08985200 | 0.10984200  |
| H  | -1.84832300 | -2.59962400 | 0.50772400  |
| C  | -3.66018900 | 0.23689400  | 0.30261200  |
| H  | -3.08863000 | 2.19125500  | 1.05318900  |
| H  | -4.04168400 | -1.76643300 | -0.36689700 |
| Cl | -5.20785900 | 0.82496500  | -0.22626800 |

### TS<sub>24-26</sub>-*p*-C(O)CH<sub>3</sub>

E(SMD/M06-2X/BS1) = -965.1346012 au

H(SMD/M06-2X/BS1) = -964.885146 au

G(SMD/M06-2X/BS1) = -964.953035 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1251.811934 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.56911500  | 2.70877200  | 0.06969500  |
| C | 0.33576000  | 1.44850200  | -1.09841200 |
| C | 2.50112300  | 1.32041400  | 0.03037500  |
| C | 1.52806800  | 3.46434400  | -0.47115800 |
| C | 0.42242000  | 2.84183500  | -1.05134500 |
| C | 1.38634700  | 0.73200800  | -0.54743300 |
| H | 1.57951600  | 4.54805700  | -0.44269200 |
| H | -0.37995100 | 3.43984800  | -1.47143900 |
| H | -0.51224600 | 0.93790800  | -1.54363200 |
| H | 3.43521000  | 3.17996000  | 0.52355200  |
| C | 3.57747600  | 0.42010300  | 0.58741300  |
| I | 1.32672300  | -1.34649000 | -0.48254100 |
| O | 3.31673400  | -0.84254400 | 0.42484800  |
| O | 4.57205500  | 0.88558200  | 1.11940400  |
| O | -0.38068500 | -1.42361100 | -1.13590400 |
| O | 0.23750000  | -1.10377600 | 1.64841200  |
| C | -0.93399200 | -0.74437000 | 1.28327100  |
| C | -1.37858800 | 0.61678500  | 1.40619600  |
| C | -1.77148500 | -1.68349800 | 0.59157600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.63098200 | 0.96663100  | 0.98506700  |
| H | -0.71307000 | 1.32873100  | 1.88520000  |
| C | -3.05065700 | -1.29235000 | 0.16562900  |
| H | -1.47670100 | -2.72566300 | 0.57728200  |
| C | -3.47587000 | 0.00882400  | 0.35095100  |
| H | -2.97830300 | 1.98522600  | 1.12322000  |
| H | -3.71450200 | -2.00615100 | -0.30955400 |
| C | -4.85859300 | 0.37635600  | -0.12347600 |
| O | -5.55213400 | -0.45903700 | -0.67052700 |
| C | -5.34199000 | 1.78485000  | 0.09985100  |
| H | -4.67638100 | 2.50071300  | -0.39413800 |
| H | -6.35105200 | 1.88472700  | -0.30122400 |
| H | -5.34549400 | 2.02246400  | 1.16903700  |

### TS<sub>24-26-p-NO<sub>2</sub></sub>

E(SMD/M06-2X/BS1) = -1016.970993 au

H(SMD/M06-2X/BS1) = -1016.757418 au

G(SMD/M06-2X/BS1) = -1016.823564 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1303.676102 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.57782900  | 2.67502300  | 0.06098300  |
| C | 0.32200100  | 1.45250400  | -1.10690600 |
| C | 2.48568200  | 1.28830300  | 0.02163500  |
| C | 1.54900200  | 3.44764200  | -0.47933700 |
| C | 0.43276600  | 2.84415900  | -1.05916200 |
| C | 1.36050700  | 0.71928600  | -0.55536200 |
| H | 1.61854100  | 4.53026900  | -0.45050500 |
| H | -0.35966800 | 3.45561200  | -1.47857500 |
| H | -0.53503100 | 0.95836200  | -1.55325600 |
| H | 3.45163900  | 3.13195000  | 0.51453500  |
| C | 3.54431500  | 0.36911100  | 0.57897900  |
| I | 1.27317200  | -1.35751900 | -0.47852200 |
| O | 3.25785500  | -0.89112200 | 0.41820400  |
| O | 4.54846700  | 0.81133000  | 1.10951200  |
| O | -0.44260700 | -1.40853600 | -1.12089900 |
| O | 0.21568100  | -1.08227100 | 1.65040100  |
| C | -0.95161000 | -0.69805900 | 1.29518500  |
| C | -1.37133400 | 0.66944300  | 1.43466400  |
| C | -1.78931800 | -1.61542600 | 0.57708600  |
| C | -2.60988800 | 1.05428400  | 1.00708400  |
| H | -0.69847400 | 1.36362400  | 1.92833200  |
| C | -3.06430500 | -1.20381400 | 0.13957100  |
| H | -1.53134900 | -2.66670000 | 0.57726400  |
| C | -3.42919100 | 0.09976800  | 0.35565300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.96788900 | 2.06770100  | 1.13885400  |
| H | -3.73831500 | -1.89709500 | -0.34733100 |
| N | -4.75976400 | 0.53261600  | -0.09790500 |
| O | -5.44855300 | -0.27245800 | -0.69876700 |
| O | -5.09808600 | 1.67594800  | 0.15370400  |

**TS<sub>24-26</sub>-p-CN**

E(SMD/M06-2X/BS1) = -904.7611186 au

H(SMD/M06-2X/BS1) = -904.552481 au

G(SMD/M06-2X/BS1) = -904.615926 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1191.411932 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.43078500  | 2.61195800  | 0.12571500  |
| C | 0.13399100  | 1.50704600  | -1.07758800 |
| C | 2.28123600  | 1.23114300  | 0.05991300  |
| C | 1.43905900  | 3.43706900  | -0.40619000 |
| C | 0.30218400  | 2.89169000  | -1.00328500 |
| C | 1.13738400  | 0.72034400  | -0.53439500 |
| H | 1.55415200  | 4.51510500  | -0.35741000 |
| H | -0.46106300 | 3.54348100  | -1.41608300 |
| H | -0.73965000 | 1.05666300  | -1.53779800 |
| H | 3.32016200  | 3.02348100  | 0.59224600  |
| C | 3.29762800  | 0.25813100  | 0.60524100  |
| I | 0.96282500  | -1.35226700 | -0.50704700 |
| O | 2.96244600  | -0.98490000 | 0.41510200  |
| O | 4.31421400  | 0.64955900  | 1.15285400  |
| O | -0.74508300 | -1.31697400 | -1.16777200 |
| O | -0.11418400 | -1.08724200 | 1.62065600  |
| C | -1.26059200 | -0.65034800 | 1.26012500  |
| C | -1.62524600 | 0.73088100  | 1.41985300  |
| C | -2.13328400 | -1.52086800 | 0.52582300  |
| C | -2.84582900 | 1.16945600  | 0.99433600  |
| H | -0.92719300 | 1.38893100  | 1.92814100  |
| C | -3.38737400 | -1.05261500 | 0.09286200  |
| H | -1.90831300 | -2.57952800 | 0.49827700  |
| C | -3.72355100 | 0.26772000  | 0.32040600  |
| H | -3.15730000 | 2.19716900  | 1.14656200  |
| H | -4.07882600 | -1.71969500 | -0.40930500 |
| C | -5.00375300 | 0.75264700  | -0.12029100 |
| N | -6.03238200 | 1.14792400  | -0.47328800 |

**TS<sub>24-26</sub>-H**

E(SMD/M06-2X/BS1) = -812.5475602 au

H(SMD/M06-2X/BS1) = -812.339403 au

G(SMD/M06-2X/BS1) = -812.398734 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1099.163087 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.60784800  | 2.15274900  | 0.14523500  |
| C | 0.18017700  | 1.55826000  | -1.15405800 |
| C | 2.15009000  | 0.84009300  | 0.10372800  |
| C | 1.85896800  | 3.16314100  | -0.45936300 |
| C | 0.65708900  | 2.87017600  | -1.10453800 |
| C | 0.94959900  | 0.58231700  | -0.54043500 |
| H | 2.21570400  | 4.18772100  | -0.42975100 |
| H | 0.08436700  | 3.66371200  | -1.57381000 |
| H | -0.75132900 | 1.30012700  | -1.64797900 |
| H | 3.54441700  | 2.36692500  | 0.65035600  |
| C | 2.89184000  | -0.31898700 | 0.72707200  |
| I | 0.28964400  | -1.38937300 | -0.48365500 |
| O | 2.29524100  | -1.45762900 | 0.54948000  |
| O | 3.94472100  | -0.14102600 | 1.31968000  |
| O | -1.32800400 | -0.98458300 | -1.22898100 |
| O | -0.79848900 | -0.81532200 | 1.58239500  |
| C | -1.80701600 | -0.15362900 | 1.15476200  |
| C | -1.84990200 | 1.28193100  | 1.22822200  |
| C | -2.86037400 | -0.84129600 | 0.46245000  |
| C | -2.94481000 | 1.95359800  | 0.75575700  |
| H | -1.02295600 | 1.79144700  | 1.71412300  |
| C | -3.96752400 | -0.12566400 | -0.01595800 |
| H | -2.85046300 | -1.92482400 | 0.46110700  |
| C | -4.00354600 | 1.24666100  | 0.12526600  |
| H | -3.00887600 | 3.03289400  | 0.85032300  |
| H | -4.78493000 | -0.65255400 | -0.49615500 |
| H | -4.85947700 | 1.80369700  | -0.24389700 |

### TS<sub>24-26</sub>-*p*-CH<sub>3</sub>

E(SMD/M06-2X/BS1) = -851.8471447 au

H(SMD/M06-2X/BS1) = -851.609599 au

G(SMD/M06-2X/BS1) = -851.673297 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1138.477873 au

|   |             |            |             |
|---|-------------|------------|-------------|
| C | 2.48981700  | 2.48222200 | 0.15087900  |
| C | 0.17338000  | 1.51718500 | -1.12769700 |
| C | 2.24980900  | 1.11335200 | 0.09786700  |
| C | 1.57928000  | 3.36511400 | -0.43124400 |
| C | 0.43173700  | 2.88855700 | -1.06588600 |
| C | 1.09880800  | 0.67103400 | -0.53679200 |
| H | 1.76601500  | 4.43356800 | -0.39152800 |
| H | -0.26883800 | 3.58441400 | -1.51650500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.71085300 | 1.11541000  | -1.61265000 |
| H | 3.38610300  | 2.83886800  | 0.64856100  |
| C | 3.17627500  | 0.08376100  | 0.70211300  |
| I | 0.75972200  | -1.38119400 | -0.49987400 |
| O | 2.76592900  | -1.13261200 | 0.52545600  |
| O | 4.19655800  | 0.42641100  | 1.28100800  |
| O | -0.90567300 | -1.23535100 | -1.23070700 |
| O | -0.40157000 | -1.02250800 | 1.58514600  |
| C | -1.50312200 | -0.51860800 | 1.17863700  |
| C | -1.75883800 | 0.89578800  | 1.26528500  |
| C | -2.47400700 | -1.34575000 | 0.52038600  |
| C | -2.95518100 | 1.39822100  | 0.83912000  |
| H | -1.00151300 | 1.52274000  | 1.72698500  |
| C | -3.68448700 | -0.80050900 | 0.08988200  |
| H | -2.29627300 | -2.41409100 | 0.48455500  |
| C | -3.93840200 | 0.55587000  | 0.23834000  |
| H | -3.17382800 | 2.45758800  | 0.94501300  |
| H | -4.43203300 | -1.44059600 | -0.36843100 |
| C | -5.23264800 | 1.16305100  | -0.21119200 |
| H | -5.04738800 | 1.95546100  | -0.94540100 |
| H | -5.89377800 | 0.41782200  | -0.65842200 |
| H | -5.74940200 | 1.62885600  | 0.63573300  |

### TS<sub>24-26</sub>-*o*-OMe

E(SMD/M06-2X/BS1) = -927.0315037 au

H(SMD/M06-2X/BS1) = -926.787487 au

G(SMD/M06-2X/BS1) = -926.852606 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1213.696646 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.43725100 | 2.20944900  | 0.31389600  |
| C | -0.21575100 | 1.04655300  | 1.59757600  |
| C | -2.14633000 | 0.86455900  | 0.10719400  |
| C | -1.62753400 | 2.96832300  | 1.15902700  |
| C | -0.52846700 | 2.39207300  | 1.79958700  |
| C | -1.04298800 | 0.32704500  | 0.74926400  |
| H | -1.85397500 | 4.01731900  | 1.32276100  |
| H | 0.09133400  | 2.99218700  | 2.45881800  |
| H | 0.63504300  | 0.56945100  | 2.07412900  |
| H | -3.29474100 | 2.64470600  | -0.18982800 |
| C | -2.96161800 | -0.03377100 | -0.79411300 |
| I | -0.59206600 | -1.65592700 | 0.30895200  |
| O | -2.51580900 | -1.24886500 | -0.83986900 |
| O | -3.93746300 | 0.40264400  | -1.38848400 |
| O | 0.99766600  | -1.59589500 | 1.19594900  |

|   |            |             |             |
|---|------------|-------------|-------------|
| O | 0.74251100 | -0.87253900 | -1.56911700 |
| C | 1.78150300 | -0.43654800 | -0.98371800 |
| C | 1.95189200 | 0.99678200  | -0.75417600 |
| C | 2.78152000 | -1.33198900 | -0.47223500 |
| C | 3.09700600 | 1.45446700  | -0.12100600 |
| C | 3.92036800 | -0.84517400 | 0.14315600  |
| H | 2.63791800 | -2.38956100 | -0.66191000 |
| C | 4.05746200 | 0.53226900  | 0.31976600  |
| H | 3.26462600 | 2.51344600  | 0.03379300  |
| H | 4.68785800 | -1.52170600 | 0.50111000  |
| H | 4.94544700 | 0.91794300  | 0.81233800  |
| O | 0.98893200 | 1.75834400  | -1.25920200 |
| C | 1.13506800 | 3.17109600  | -1.14267000 |
| H | 0.23710400 | 3.60074400  | -1.58507600 |
| H | 1.21212900 | 3.47048400  | -0.09323300 |
| H | 2.02078100 | 3.50880600  | -1.69088000 |

### TS<sub>24-26-o-NO<sub>2</sub></sub>

E(SMD/M06-2X/BS1) = -1016.967857 au

H(SMD/M06-2X/BS1) = -1016.754259 au

G(SMD/M06-2X/BS1) = -1016.81961 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1303.671062 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.22676500  | 2.23051400  | -0.54969900 |
| C | 0.05462700  | 0.87287800  | -1.72609400 |
| C | 2.02133000  | 0.88377400  | -0.27192400 |
| C | 1.35650200  | 2.89372000  | -1.41529800 |
| C | 0.28407400  | 2.22135700  | -2.00329800 |
| C | 0.93757400  | 0.24938700  | -0.85731400 |
| H | 1.51400500  | 3.94498400  | -1.63388500 |
| H | -0.38654200 | 2.74867400  | -2.67394900 |
| H | -0.78017400 | 0.32999800  | -2.15808500 |
| H | 3.06378500  | 2.74192400  | -0.08514800 |
| C | 2.90447000  | 0.07993600  | 0.64907100  |
| I | 0.63745500  | -1.72380600 | -0.27203500 |
| O | 2.54404100  | -1.16823000 | 0.73601600  |
| O | 3.85336400  | 0.59066200  | 1.21904600  |
| O | -1.01589100 | -1.79967200 | -1.05646600 |
| O | -0.54734000 | -0.81263000 | 1.59004500  |
| C | -1.62567300 | -0.41817400 | 1.03627800  |
| C | -1.92866500 | 0.95552300  | 0.70068100  |
| C | -2.51391800 | -1.41158600 | 0.50366600  |
| C | -3.07435500 | 1.29015500  | 0.03227100  |
| C | -3.69557300 | -1.04625700 | -0.17367200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.35758300 | -2.43447100 | 0.82323400  |
| C | -3.96352300 | 0.28026200  | -0.41104600 |
| H | -3.29542900 | 2.33429500  | -0.15564500 |
| H | -4.38207500 | -1.81820100 | -0.50352800 |
| H | -4.86940000 | 0.57585400  | -0.92925500 |
| N | -1.05216000 | 2.04623200  | 1.13323000  |
| O | -0.23545900 | 1.82361100  | 2.00708700  |
| O | -1.20226700 | 3.13202100  | 0.59424500  |

### TS<sub>24-26</sub>-*m*-OMe

E(SMD/M06-2X/BS1) = -927.0250686 au

H(SMD/M06-2X/BS1) = -926.781104 au

G(SMD/M06-2X/BS1) = -926.846341 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1213.689849 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.80032200  | 2.91550200  | 0.03644400  |
| C | -0.06076900 | 1.25528000  | -1.27282500 |
| C | 1.96502800  | 1.53419600  | 0.06676200  |
| C | 0.71226300  | 3.46451700  | -0.64207100 |
| C | -0.21051000 | 2.64327400  | -1.29202300 |
| C | 1.02981200  | 0.74598800  | -0.58507200 |
| H | 0.58133800  | 4.54167100  | -0.66648700 |
| H | -1.05371500 | 3.08157700  | -1.81641700 |
| H | -0.76396700 | 0.59098800  | -1.76515600 |
| H | 2.52566400  | 3.54218900  | 0.54564100  |
| C | 3.10755400  | 0.84938500  | 0.77913400  |
| I | 1.29742700  | -1.31179400 | -0.41887400 |
| O | 3.07461600  | -0.44297000 | 0.66611400  |
| O | 3.94962800  | 1.49952200  | 1.37881800  |
| O | -0.29024900 | -1.69570000 | -1.23315700 |
| O | -0.00998400 | -1.20570000 | 1.58131000  |
| C | -1.19085400 | -1.04536500 | 1.10429100  |
| C | -1.82961800 | 0.23033000  | 1.11217400  |
| C | -1.81226800 | -2.13665200 | 0.40825200  |
| C | -3.08191600 | 0.37763700  | 0.56149200  |
| H | -1.33398000 | 1.06782100  | 1.59263800  |
| C | -3.09115200 | -1.95952000 | -0.13871400 |
| H | -1.35366500 | -3.11601300 | 0.46305100  |
| C | -3.71550500 | -0.73152700 | -0.07318800 |
| H | -3.59302600 | -2.79100300 | -0.62131400 |
| H | -4.70407400 | -0.61725400 | -0.50331600 |
| O | -3.64554500 | 1.60271700  | 0.64150100  |
| C | -4.93749800 | 1.78817400  | 0.07992900  |
| H | -5.67966900 | 1.14761500  | 0.56822500  |



|   |             |            |             |
|---|-------------|------------|-------------|
| H | -5.19058000 | 2.83346000 | 0.25724600  |
| H | -4.93503500 | 1.59373800 | -0.99798400 |

**TS<sub>24-26-m-NO<sub>2</sub></sub>**

E(SMD/M06-2X/BS1) = -1016.972747 au

H(SMD/M06-2X/BS1) = -1016.75911 au

G(SMD/M06-2X/BS1) = -1016.824592 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1303.67758 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.39498100  | 3.01394100  | -0.09224700 |
| C | -0.17125100 | 1.03249100  | -1.34244100 |
| C | 1.78183200  | 1.68061100  | -0.02079500 |
| C | 0.23009800  | 3.35655200  | -0.78103500 |
| C | -0.54603500 | 2.37766500  | -1.40143900 |
| C | 0.98644700  | 0.73017300  | -0.64256900 |
| H | -0.07494500 | 4.39660000  | -0.83566000 |
| H | -1.44847000 | 2.65605200  | -1.93622300 |
| H | -0.75477400 | 0.25028900  | -1.81774700 |
| H | 2.00691300  | 3.76646200  | 0.39489900  |
| C | 3.01605900  | 1.20923100  | 0.70776800  |
| I | 1.56459100  | -1.24613100 | -0.35713800 |
| O | 3.18204700  | -0.08019200 | 0.64104500  |
| O | 3.75124900  | 1.99633100  | 1.27869300  |
| O | 0.03332400  | -1.89861200 | -1.12367400 |
| O | 0.23686600  | -1.15689900 | 1.62839900  |
| C | -0.94038800 | -1.17936500 | 1.12624100  |
| C | -1.72630400 | 0.01731900  | 1.03028400  |
| C | -1.40376900 | -2.36579400 | 0.46726200  |
| C | -2.95175200 | -0.06447300 | 0.43417500  |
| H | -1.35485500 | 0.93827300  | 1.46539600  |
| C | -2.68225200 | -2.38878200 | -0.12972700 |
| H | -0.85213900 | -3.28517000 | 0.62090300  |
| C | -3.45129900 | -1.25200500 | -0.15422000 |
| H | -3.05366400 | -3.30631300 | -0.57118000 |
| H | -4.43542800 | -1.24639400 | -0.60684200 |
| N | -3.77095700 | 1.15025300  | 0.35517400  |
| O | -3.30140000 | 2.18465800  | 0.79536700  |
| O | -4.87426900 | 1.05696100  | -0.15470500 |

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E(SMD/M06-2X/BS1) = -306.4745852 au

H(SMD/M06-2X/BS1) = -306.374618 au

G(SMD/M06-2X/BS1) = -306.410765 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -306.5931478 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.04438600 | 0.00000000  | 0.00011600  |
| C | -0.28223500 | -1.28424200 | 0.00039600  |
| C | -0.28223400 | 1.28424200  | 0.00039600  |
| C | 1.07181300  | -1.25948400 | 0.00013100  |
| H | -0.86135300 | -2.20274500 | 0.00060200  |
| C | 1.07181400  | 1.25948400  | 0.00013100  |
| H | -0.86135300 | 2.20274500  | 0.00060200  |
| C | 1.73677600  | 0.00000000  | -0.00049000 |
| H | 1.66171000  | -2.16806600 | 0.00017900  |
| H | 1.66171100  | 2.16806600  | 0.00017900  |
| O | -2.25674100 | 0.00000100  | -0.00053800 |
| H | 2.82393300  | 0.00000000  | -0.00133900 |

### 7-*p*-Cl

E(SMD/M06-2X/BS1) = -766.0416407 au

H(SMD/M06-2X/BS1) = -765.949962 au

G(SMD/M06-2X/BS1) = -765.989218 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -766.1998253 au

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.89456400  | 0.00000000  | 0.00004100  |
| C  | 1.12924900  | -1.27970300 | -0.00050300 |
| C  | 1.12924800  | 1.27970300  | -0.00050300 |
| C  | -0.22106300 | -1.26695100 | -0.00074500 |
| H  | 1.70069400  | -2.20279700 | -0.00060200 |
| C  | -0.22106400 | 1.26695100  | -0.00074500 |
| H  | 1.70069600  | 2.20279600  | -0.00060200 |
| C  | -0.88734600 | 0.00000000  | -0.00030900 |
| H  | -0.81082200 | -2.17662600 | -0.00095500 |
| H  | -0.81082300 | 2.17662600  | -0.00095600 |
| O  | 3.10650000  | 0.00000000  | 0.00118500  |
| Cl | -2.56313400 | 0.00000000  | 0.00060200  |

### 7-*p*-C(O)CH<sub>3</sub>

E(SMD/M06-2X/BS1) = -459.0528255 au

H(SMD/M06-2X/BS1) = -458.911682 au

G(SMD/M06-2X/BS1) = -458.9566 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -459.233851 au

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 2.22667400 | -0.05440800 | -0.01399200 |
| C | 1.41321500 | -1.29379500 | 0.15767500  |
| C | 1.51470000 | 1.24843200  | -0.15276500 |
| C | 0.05998400 | -1.21533800 | 0.17428800  |
| H | 1.95208500 | -2.23102600 | 0.25860500  |
| C | 0.16138100 | 1.27930000  | -0.12121800 |
| H | 2.12433800 | 2.13878300  | -0.27447900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.56042100 | 0.05792500  | 0.01995600  |
| H | -0.55049400 | -2.10290900 | 0.29322300  |
| H | -0.39498400 | 2.20464200  | -0.21352400 |
| O | 3.43781100  | -0.10850200 | -0.03814400 |
| C | -2.08617000 | 0.16936800  | 0.03308600  |
| O | -2.54653100 | 1.24380000  | 0.34566800  |
| C | -2.89418100 | -1.03680300 | -0.31905500 |
| H | -2.51435200 | -1.50234300 | -1.23417900 |
| H | -2.82186100 | -1.77562700 | 0.48788100  |
| H | -3.93606000 | -0.74198800 | -0.44557300 |

### 7-*p*-NO<sub>2</sub>

E(SMD/M06-2X/BS1) = -510.8710293 au

H(SMD/M06-2X/BS1) = -510.765977 au

G(SMD/M06-2X/BS1) = -510.809102 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -511.0812535 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.15094900 | 0.00002300  | -0.00005200 |
| C | -1.39061400 | -1.27149600 | -0.19618300 |
| C | -1.39057600 | 1.27157000  | 0.19584100  |
| C | -0.03189200 | -1.25408800 | -0.18382200 |
| H | -1.96481700 | -2.18196100 | -0.34043600 |
| C | -0.03185400 | 1.25408600  | 0.18353100  |
| H | -1.96475000 | 2.18205500  | 0.34006300  |
| C | 0.58814200  | -0.00002000 | -0.00008600 |
| H | 0.56760400  | -2.14799800 | -0.31404400 |
| H | 0.56769300  | 2.14796400  | 0.31378400  |
| O | -3.36215600 | -0.00000600 | 0.00034900  |
| O | 2.60333200  | 0.91396400  | -0.58715900 |
| O | 2.60316000  | -0.91400600 | 0.58742200  |
| N | 2.06943400  | -0.00001800 | 0.00005100  |

### 7-*p*-CN

E(SMD/M06-2X/BS1) = -398.6697034 au

H(SMD/M06-2X/BS1) = -398.569696 au

G(SMD/M06-2X/BS1) = -398.610703 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -398.8241948 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.80480400  | 0.00000000  | 0.00001800  |
| C | 1.04397300  | -1.28290900 | -0.00069200 |
| C | 1.04397300  | 1.28290900  | -0.00069200 |
| C | -0.31209900 | -1.26497800 | -0.00094400 |
| H | 1.61733600  | -2.20495700 | -0.00076900 |
| C | -0.31209900 | 1.26497900  | -0.00094400 |
| H | 1.61733700  | 2.20495600  | -0.00076800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.97113100 | 0.00000000  | -0.00050600 |
| H | -0.90315300 | -2.17311200 | -0.00121800 |
| H | -0.90315300 | 2.17311300  | -0.00121800 |
| O | 3.01708400  | 0.00000000  | 0.00177700  |
| C | -2.40411100 | 0.00000000  | 0.00046700  |
| N | -3.56069900 | 0.00000000  | 0.00135900  |

### 7-*p*-CH<sub>3</sub>

E(SMD/M06-2X/BS1) = -345.7863844 au

H(SMD/M06-2X/BS1) = -345.658367 au

G(SMD/M06-2X/BS1) = -345.696983 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -345.9206646 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.52996400 | -0.00000600 | 0.00303400  |
| C | -0.76257600 | -1.27809500 | -0.00277200 |
| C | -0.76259000 | 1.27809400  | -0.00277300 |
| C | 0.58496500  | -1.25786500 | -0.01610600 |
| H | -1.33707100 | -2.19929400 | 0.00235800  |
| C | 0.58495300  | 1.25788200  | -0.01610300 |
| H | -1.33709600 | 2.19928500  | 0.00235300  |
| C | 1.28668100  | 0.00001300  | -0.02498900 |
| H | 1.17096100  | -2.17055300 | -0.02266900 |
| H | 1.17093800  | 2.17057700  | -0.02266800 |
| O | -2.74274100 | -0.00001000 | 0.01489800  |
| C | 2.74985700  | 0.00000400  | 0.00731600  |
| H | 3.17591300  | 0.90816600  | -0.42347100 |
| H | 3.01445700  | -0.00027700 | 1.08315100  |
| H | 3.17587700  | -0.90798800 | -0.42387700 |

### 7-*p*-OMe

E(SMD/M06-2X/BS1) = -420.9917102 au

H(SMD/M06-2X/BS1) = -420.854603 au

G(SMD/M06-2X/BS1) = -420.896096 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -421.1602184 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.92774800  | -0.15027400 | -0.00017200 |
| C | 0.96404700  | -1.29019500 | 0.00046800  |
| C | 1.37224800  | 1.23053300  | 0.00019400  |
| C | -0.36263200 | -1.08460000 | 0.00093800  |
| H | 1.38921800  | -2.28898100 | 0.00054700  |
| C | 0.04752700  | 1.42883200  | 0.00047100  |
| H | 2.08240100  | 2.05128000  | 0.00025200  |
| C | -0.84633300 | 0.28211500  | 0.00045500  |
| H | -1.06557600 | -1.90898000 | 0.00150200  |
| H | -0.40695100 | 2.41354800  | 0.00065400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 3.12356100  | -0.35155700 | -0.00098600 |
| O | -2.08662400 | 0.57927200  | -0.00020400 |
| C | -3.12972800 | -0.43795100 | -0.00080100 |
| H | -3.03789500 | -1.04143300 | 0.90261300  |
| H | -4.05866700 | 0.12527200  | -0.00259600 |
| H | -3.03529500 | -1.04318400 | -0.90277100 |

### 7-*o*-OMe

E(SMD/M06-2X/BS1) = -420.9830112 au

H(SMD/M06-2X/BS1) = -420.846344 au

G(SMD/M06-2X/BS1) = -420.888147 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -421.1504064 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.57001700  | 1.07379300  | 0.00001000  |
| C | 1.97327200  | 0.62044400  | -0.00029300 |
| C | -0.51637300 | -0.01738900 | 0.00002700  |
| C | 2.24277100  | -0.69394700 | -0.00020700 |
| H | 2.73870800  | 1.38924600  | -0.00046900 |
| C | -0.16464600 | -1.38024600 | 0.00026300  |
| C | 1.16925000  | -1.68180100 | 0.00018600  |
| H | 3.26327200  | -1.05912500 | -0.00039400 |
| H | -0.91747100 | -2.15915800 | 0.00048700  |
| O | 0.22871200  | 2.23091500  | 0.00035600  |
| H | 1.45930400  | -2.72836100 | 0.00044200  |
| O | -1.69718600 | 0.45658400  | -0.00013100 |
| C | -2.84851500 | -0.43367500 | -0.00019400 |
| H | -3.71096300 | 0.22707100  | -0.00065100 |
| H | -2.81959200 | -1.04665200 | -0.90212000 |
| H | -2.82011400 | -1.04609500 | 0.90214400  |

### 7-*o*-NO<sub>2</sub>

E(SMD/M06-2X/BS1) = -510.8706857 au

H(SMD/M06-2X/BS1) = -510.766397 au

G(SMD/M06-2X/BS1) = -510.807992 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -511.0825003 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.40678500 | 1.02179600  | -0.00763200 |
| C | 0.25631200  | -0.32385500 | 0.00295200  |
| C | -1.89886000 | 1.03051500  | -0.00823900 |
| C | -0.43605000 | -1.47385000 | 0.00955100  |
| C | -2.58428000 | -0.14149800 | 0.00145400  |
| H | -2.38044100 | 2.00369000  | -0.01599100 |
| C | -1.86750800 | -1.36634900 | 0.01046500  |
| H | 0.03745800  | -2.44967600 | 0.01445000  |
| H | -3.66725400 | -0.16609300 | 0.00164600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.25400700  | 2.03184400  | -0.01589900 |
| H | -2.43413000 | -2.29378800 | 0.01675500  |
| N | 1.71854700  | -0.27730500 | 0.00270100  |
| O | 2.25233000  | -0.28069600 | -1.08327200 |
| O | 2.24835900  | -0.20534200 | 1.08828600  |

### 7-*m*-OMe

E(SMD/M06-2X/BS1) = -420.9488233 au

H(SMD/M06-2X/BS1) = -420.812963 au

G(SMD/M06-2X/BS1) = -420.854993 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -421.1167961 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.71817300  | -0.48127200 | 0.00022600  |
| C | 0.36978700  | -1.08727400 | 0.00007200  |
| C | 1.84759100  | 1.00923800  | 0.00070000  |
| C | -0.73928000 | -0.29212800 | 0.00005600  |
| H | 0.29932400  | -2.17027500 | -0.00019500 |
| C | 0.72372900  | 1.76605000  | -0.00032300 |
| H | 2.85019900  | 1.42466200  | 0.00155500  |
| C | -0.54543900 | 1.13062200  | -0.00034300 |
| H | 0.75910900  | 2.84873500  | -0.00069300 |
| O | 2.71348400  | -1.17693000 | -0.00055300 |
| H | -1.42143500 | 1.77451100  | -0.00037300 |
| O | -1.94160200 | -0.86598800 | 0.00039700  |
| C | -3.11065700 | -0.03962700 | -0.00010500 |
| H | -3.14767000 | 0.58154400  | -0.89968400 |
| H | -3.95044200 | -0.73240800 | 0.00040600  |
| H | -3.14757100 | 0.58291500  | 0.89853100  |

### 7- *m*-NO<sub>2</sub>

E(SMD/M06-2X/BS1) = -510.8789208 au

H(SMD/M06-2X/BS1) = -510.77471 au

G(SMD/M06-2X/BS1) = -510.815335 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -511.0887729 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.79080200 | -0.63920800 | -0.01058900 |
| C | -2.19903800 | 0.79863100  | 0.00490500  |
| C | -0.33021300 | -0.97029100 | -0.00920100 |
| C | -1.25605600 | 1.77815500  | 0.02172100  |
| H | -3.26549500 | 1.00595700  | 0.00306200  |
| C | 0.53959800  | 0.05827600  | 0.00441700  |
| H | -0.02924600 | -2.01386500 | -0.01949500 |
| C | 0.10916800  | 1.41506500  | 0.01967400  |
| H | -1.51987700 | 2.82841700  | 0.03487400  |
| O | -2.61663300 | -1.52290700 | -0.02157500 |

|   |            |             |             |
|---|------------|-------------|-------------|
| H | 0.86740200 | 2.19468200  | 0.03219400  |
| N | 1.99211400 | -0.21236500 | -0.00049400 |
| O | 2.33317400 | -1.37345600 | 0.05581800  |
| O | 2.72926900 | 0.74981400  | -0.06333600 |

### 16'-H,H,H,H

E(SMD/M06-2X/BS1) = -382.5301549 au  
H(SMD/M06-2X/BS1) = -382.412495 au  
G(SMD/M06-2X/BS1) = -382.450354 au  
E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -382.7009558 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.53684700  | 0.70325000  | -0.00003200 |
| C | 0.53702700  | -0.70332400 | -0.00012500 |
| C | -0.67214900 | 1.38917400  | 0.00003000  |
| C | -0.67206500 | -1.38920400 | 0.00001400  |
| C | -1.88436800 | 0.69448800  | -0.00003300 |
| H | -0.65952200 | 2.47707000  | 0.00007500  |
| C | -1.88428500 | -0.69459500 | 0.00002100  |
| H | -0.65951500 | -2.47710000 | 0.00010600  |
| H | -2.81809400 | 1.24735600  | -0.00004500 |
| O | 1.74851300  | 1.31951400  | 0.00011100  |
| H | 1.60554900  | 2.28093100  | -0.00040100 |
| H | -2.81793800 | -1.24762200 | 0.00012000  |
| O | 1.74869500  | -1.31934300 | -0.00003500 |
| H | 1.60582300  | -2.28073800 | 0.00028200  |

### 16-OMe,H,H,H

E(SMD/M06-2X/BS1) -497.0082305 au  
H(SMD/M06-2X/BS1) = -496.854547 au  
G(SMD/M06-2X/BS1) = -496.898515 au  
E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -497.2279339 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.62202700  | -0.07707900 | 0.00002000  |
| C | 0.38275000  | -0.71675400 | -0.00003600 |
| C | 1.68194800  | 1.31874500  | 0.00003100  |
| C | -0.79137500 | 0.04939900  | -0.00009100 |
| C | 0.50946600  | 2.06582000  | -0.00002400 |
| H | 2.65288300  | 1.80713400  | 0.00008700  |
| C | -0.73856300 | 1.44182500  | -0.00007900 |
| H | 0.56495200  | 3.14951000  | -0.00001300 |
| O | 2.72519700  | -0.87185000 | 0.00011800  |
| H | 3.51369700  | -0.30391900 | -0.00014000 |
| O | 0.32634900  | -2.07450300 | -0.00002600 |
| H | -0.61596800 | -2.31728800 | 0.00001300  |
| O | -1.92613500 | -0.70461400 | -0.00021200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.16567900 | -0.01463600 | 0.00020800  |
| H | -3.26751000 | 0.60905000  | -0.89449800 |
| H | -3.94043600 | -0.78139300 | 0.00043800  |
| H | -3.26690500 | 0.60900500  | 0.89501400  |
| H | -1.64743200 | 2.03171900  | -0.00011600 |

### 16-H,H,OMe,H

E(SMD/M06-2X/BS1) = -497.0065637 au

H(SMD/M06-2X/BS1) = -496.853142 au

G(SMD/M06-2X/BS1) = -496.896899 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -497.2261363 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.53179600  | -0.61903800 | 0.00002600  |
| C | 1.21653200  | 0.75392700  | 0.00002900  |
| C | 0.49970900  | -1.54169000 | -0.00007800 |
| C | -0.10854700 | 1.15892600  | -0.00005100 |
| C | -0.84356900 | -1.14315800 | 0.00001600  |
| H | 0.74201000  | -2.60196500 | -0.00011200 |
| C | -1.14555500 | 0.21457800  | 0.00000100  |
| H | -1.62062200 | -1.89753600 | 0.00000800  |
| O | 2.85342000  | -0.95421500 | -0.00005800 |
| H | 2.92211000  | -1.92335500 | 0.00083000  |
| O | 2.25833700  | 1.62476300  | -0.00009300 |
| H | 1.90534300  | 2.53047400  | 0.00056600  |
| H | -0.35828400 | 2.21690700  | -0.00024900 |
| O | -2.40500300 | 0.72853400  | 0.00014800  |
| C | -3.47484300 | -0.19794000 | -0.00006100 |
| H | -4.39043200 | 0.39455300  | -0.00009100 |
| H | -3.45352000 | -0.83259800 | -0.89392700 |
| H | -3.45377900 | -0.83276500 | 0.89370700  |

### 16-H,H,CN,H

E(SMD/M06-2X/BS1) = -474.7496099 au

H(SMD/M06-2X/BS1) = -474.631379 au

G(SMD/M06-2X/BS1) = -474.673643 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -474.9564426 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.94500600  | 0.80983800  | 0.00003500  |
| C | 1.45786900  | -0.50478000 | 0.00007000  |
| C | -0.42478500 | 1.00926400  | -0.00003500 |
| C | 0.58758100  | -1.59080500 | 0.00003700  |
| C | -1.29218000 | -0.09538000 | -0.00005900 |
| H | -0.82517400 | 2.01909800  | -0.00006400 |
| C | -0.78973400 | -1.39648100 | -0.00002500 |
| H | 0.99681900  | -2.59770300 | 0.00006600  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.85082200  | 1.81659900  | 0.00005300  |
| H | 1.37847200  | 2.66685800  | 0.00021800  |
| O | 2.80150100  | -0.62876800 | 0.00012800  |
| H | 3.03249000  | -1.57420800 | 0.00022600  |
| H | -1.46444800 | -2.24507700 | -0.00004600 |
| C | -2.70970800 | 0.12345800  | -0.00012400 |
| N | -3.85443300 | 0.29967100  | -0.00017700 |

### 16-H,H,H,CN

E(SMD/M06-2X/BS1) = -474.7473504 au

H(SMD/M06-2X/BS1) = -474.629203 au

G(SMD/M06-2X/BS1) = -474.671553 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -474.9535282 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.04610600 | -0.65887600 | 0.00002000  |
| C | -1.41656700 | -0.33743700 | 0.00008000  |
| C | 0.88684900  | 0.38533800  | -0.00005800 |
| C | -1.80993300 | 0.99324800  | 0.00007300  |
| C | 0.48328700  | 1.73221500  | -0.00005100 |
| C | -0.86627400 | 2.02701900  | 0.00001400  |
| H | -2.87226400 | 1.22580000  | 0.00012300  |
| H | 1.23637900  | 2.51204500  | -0.00010000 |
| O | 0.27973900  | -1.96649800 | 0.00000200  |
| H | 1.24793500  | -2.07531500 | 0.00021100  |
| O | -2.27944800 | -1.38107900 | 0.00012600  |
| H | -3.18874600 | -1.03555300 | 0.00030600  |
| H | -1.20091500 | 3.05823000  | 0.00001700  |
| C | 2.27721700  | 0.03998600  | -0.00013300 |
| N | 3.38920700  | -0.28479200 | -0.00017800 |

### TS<sub>36</sub>-H,H,H,H

E(SMD/M06-2X/BS1) = -812.62734443 au

H(SMD/M06-2X/BS1) = -812.419806 au

G(SMD/M06-2X/BS1) = -812.479864 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1099.2511247 au

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -1.01100700 | 2.70331100  | 0.52269300 |
| C | 0.18828700  | 0.62959600  | 1.96056800 |
| C | -1.28841100 | 1.39050500  | 0.14814100 |
| C | -0.12821700 | 2.98448000  | 1.56516600 |
| C | 0.47884800  | 1.95291800  | 2.27886800 |
| C | -0.68613600 | 0.37159000  | 0.89937800 |
| H | 0.08756000  | 4.01717500  | 1.82116900 |
| H | 1.16664900  | 2.17154600  | 3.08873400 |
| H | 0.62480500  | -0.18669700 | 2.52631500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.48511400 | 3.50716900  | -0.03176400 |
| C | -2.16071900 | 1.13580500  | -1.08538400 |
| I | -1.04642200 | -1.61140500 | 0.45558800  |
| O | -1.67832800 | 0.29306700  | -1.91135300 |
| O | -3.21116700 | 1.76922800  | -1.17079700 |
| O | 0.55280200  | -1.65677600 | -1.00474200 |
| O | 0.74551500  | 0.86937800  | -2.16588700 |
| C | 1.66239500  | 0.41282500  | -1.34011100 |
| C | 1.57957600  | -0.86644800 | -0.71231200 |
| C | 2.82462500  | 1.18012100  | -1.11643900 |
| C | 2.59246400  | -1.29483300 | 0.17666000  |
| C | 3.81537000  | 0.72732400  | -0.26865300 |
| H | 2.90028300  | 2.14256700  | -1.61194000 |
| C | 3.70729000  | -0.51698500 | 0.38927700  |
| H | -0.19941400 | 0.45248000  | -2.05011400 |
| H | 4.69086500  | 1.34655100  | -0.09754100 |
| H | 4.49373200  | -0.85056500 | 1.05725000  |
| H | 2.46423700  | -2.25619800 | 0.66683200  |

### TS<sub>36</sub>-OMe,H,H,H

E(SMD/M06-2X/BS1) = -927.101384332 au

H(SMD/M06-2X/BS1) = -926.857802 au

G(SMD/M06-2X/BS1) = -926.923505 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1213.77452877 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.00631200 | 2.66742400  | 0.94859300  |
| C | -0.22354300 | 0.12965700  | 2.09839900  |
| C | -0.84134400 | 1.73305400  | 0.33946600  |
| C | 0.73613100  | 2.33912400  | 2.08234700  |
| C | 0.63561400  | 1.07216600  | 2.65495700  |
| C | -0.94064900 | 0.47431600  | 0.94715900  |
| H | 1.39852700  | 3.07832100  | 2.52218000  |
| H | 1.21273900  | 0.81745400  | 3.53752100  |
| H | -0.33829400 | -0.85146700 | 2.54685900  |
| H | 0.06958700  | 3.65516300  | 0.50474400  |
| C | -1.53154000 | 2.09660300  | -0.97930300 |
| I | -2.14024000 | -0.99222100 | 0.12879100  |
| O | -1.42013300 | 1.21661800  | -1.89428900 |
| O | -2.09801000 | 3.18672100  | -1.03442300 |
| O | -0.57539300 | -1.65798700 | -1.18173000 |
| O | 0.99537600  | 0.52892500  | -1.85373600 |
| C | 1.41904300  | -0.40926900 | -1.03413600 |
| C | 0.64727300  | -1.53887200 | -0.66101400 |
| C | 2.75879700  | -0.32864200 | -0.54869700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.15416800  | -2.51209200 | 0.23223100  |
| C | 3.24582000  | -1.30105600 | 0.30544500  |
| C | 2.44090500  | -2.39606900 | 0.69458200  |
| H | -0.03506000 | 0.62437700  | -1.89579600 |
| H | 2.85424800  | -3.14023900 | 1.36680100  |
| H | 0.50889500  | -3.33772300 | 0.51636700  |
| O | 3.44334700  | 0.75927400  | -0.96577300 |
| C | 4.75132000  | 0.92906800  | -0.44760600 |
| H | 5.12783300  | 1.85773600  | -0.87682200 |
| H | 4.73598900  | 1.01176400  | 0.64562200  |
| H | 5.40668800  | 0.10051000  | -0.73995500 |
| H | 4.25597800  | -1.22906300 | 0.69160500  |

### TS<sub>36</sub>-H,H,CN,H

E(SMD/M06-2X/BS1) = -904.84490268 au

H(SMD/M06-2X/BS1) = -904.639538 au

G(SMD/M06-2X/BS1) = -904.704453 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1191.5065345 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.19897500  | 2.38221800  | -0.59070200 |
| C | 0.29214600  | 0.82835800  | -1.92721800 |
| C | 2.04190600  | 1.05097900  | -0.21798900 |
| C | 1.40253900  | 2.94152400  | -1.59065800 |
| C | 0.44621000  | 2.17409800  | -2.25103400 |
| C | 1.09248500  | 0.29227800  | -0.91599100 |
| H | 1.53023800  | 3.98683800  | -1.85339700 |
| H | -0.17408100 | 2.61297000  | -3.02506400 |
| H | -0.42599300 | 0.20703400  | -2.45137600 |
| H | 2.94002100  | 2.98420300  | -0.07409200 |
| C | 2.85411900  | 0.49505100  | 0.94124100  |
| I | 0.86962100  | -1.72742000 | -0.51818900 |
| O | 2.15541700  | -0.07868800 | 1.86830900  |
| O | 4.06767300  | 0.61570000  | 0.92622200  |
| O | -0.40316700 | -1.47836400 | 1.07507700  |
| O | 0.06067000  | 1.04555200  | 2.12963700  |
| C | -1.04840600 | 0.77403000  | 1.52850700  |
| C | -1.33037100 | -0.49573100 | 0.93471500  |
| C | -2.08564600 | 1.74622100  | 1.46303400  |
| C | -2.52640800 | -0.74959100 | 0.26818200  |
| C | -3.27567100 | 1.49048400  | 0.82449500  |
| H | -1.89587000 | 2.71129000  | 1.92116900  |
| C | -3.50842500 | 0.23537600  | 0.21547300  |
| H | 1.03998900  | 0.36770600  | 1.96698900  |
| H | -4.04496800 | 2.25482400  | 0.77640100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.74725000 | -0.02027700 | -0.45328900 |
| N | -5.75158100 | -0.22218600 | -0.99544200 |
| H | -2.68017800 | -1.72003500 | -0.19503600 |

**TS<sub>36</sub>-H,H,H,CN**

E(SMD/M06-2X/BS1) = -904.8425577 au

H(SMD/M06-2X/BS1) = -904.635569 au

G(SMD/M06-2X/BS1) = -904.699966 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1191.502158 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.33819900 | 1.94139300  | 0.85904700  |
| C | -0.16833700 | 0.57747600  | 1.97875000  |
| C | -1.99957100 | 0.69372400  | 0.34204100  |
| C | -1.59386200 | 2.51744700  | 1.88885300  |
| C | -0.50663800 | 1.84466200  | 2.44345600  |
| C | -0.91754200 | 0.02520800  | 0.93318400  |
| H | -1.86531700 | 3.50079000  | 2.25995200  |
| H | 0.07173400  | 2.29508600  | 3.24293600  |
| H | 0.65344100  | 0.02272000  | 2.41991700  |
| H | -3.18352000 | 2.46921700  | 0.42846000  |
| C | -2.75916400 | 0.15054600  | -0.86729200 |
| I | -0.35450300 | -1.83987400 | 0.25861400  |
| O | -2.01352600 | -0.19580200 | -1.85018900 |
| O | -3.98225900 | 0.10278700  | -0.80233300 |
| O | 0.91718800  | -0.96817000 | -1.27785500 |
| O | -0.23047800 | 1.45192800  | -2.08372500 |
| C | 0.86740700  | 1.40799700  | -1.38189400 |
| C | 1.46288700  | 0.18698000  | -0.94335400 |
| C | 1.55393800  | 2.61372200  | -1.09264500 |
| C | 2.66134500  | 0.22778700  | -0.17301700 |
| C | 2.72457400  | 2.61711500  | -0.36678300 |
| H | 1.10943600  | 3.53895900  | -1.44445000 |
| C | 3.29780000  | 1.41996600  | 0.10782600  |
| H | -0.90651500 | 0.61239100  | -1.98654500 |
| H | 3.21575300  | 3.55949500  | -0.14752500 |
| H | 4.21606100  | 1.43009900  | 0.68317800  |
| C | 3.18542900  | -1.02207000 | 0.29943900  |
| N | 3.58996700  | -2.03615500 | 0.68352300  |

**7'**

E(SMD/M06-2X/BS1) = -381.6951397 au

H(SMD/M06-2X/BS1) = -381.588964 au

G(SMD/M06-2X/BS1) = -381.627028 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -381.8520385 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.45675200  | 0.90226900  | -0.00019500 |
| C | 0.70607900  | -0.61426700 | -0.00007700 |
| C | -0.95004200 | 1.34650300  | 0.00005100  |
| C | -0.35920400 | -1.51929400 | 0.00020300  |
| C | -1.93139200 | 0.43070300  | 0.00028500  |
| H | -1.12791300 | 2.41638800  | 0.00001600  |
| C | -1.62616600 | -0.99459300 | 0.00034600  |
| H | -0.18192700 | -2.59014700 | 0.00028100  |
| H | -2.97498200 | 0.72271800  | 0.00044600  |
| O | 1.40891600  | 1.64235500  | -0.00030000 |
| H | -2.46712200 | -1.68228700 | 0.00054200  |
| O | 1.95193600  | -0.92628200 | -0.00029300 |
| H | 2.08897000  | -1.90318700 | -0.00022200 |

### 7'-OMe,H,H,H

E(SMD/M06-2X/BS1) = -496.1707827 au

H(SMD/M06-2X/BS1) = -496.028641 au

G(SMD/M06-2X/BS1) = -496.072634 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -496.3765479 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.58616400 | 0.72158000  | -0.00001900 |
| C | -0.43111700 | 1.65160900  | -0.00016700 |
| C | -1.27211500 | -0.76383900 | -0.00004300 |
| C | 0.82454900  | 1.19019100  | -0.00009400 |
| H | -0.66092800 | 2.71192700  | -0.00024100 |
| C | 0.01502200  | -1.20936400 | 0.00005800  |
| C | 1.06159900  | -0.25652400 | -0.00001100 |
| H | 1.67307200  | 1.86381900  | -0.00011200 |
| O | -2.73187200 | 1.10037300  | 0.00024400  |
| O | -2.34543700 | -1.51205900 | -0.00008800 |
| H | -2.10966100 | -2.46364500 | -0.00016300 |
| H | 2.07214700  | -0.60822378 | -0.00000218 |
| O | 0.34114932  | -2.60167897 | 0.00008040  |
| C | 1.62828999  | -2.79044129 | 0.59382924  |
| H | 1.78004755  | -3.83070433 | 0.79313417  |
| H | 2.38523886  | -2.44172093 | -0.07723150 |
| H | 1.68268839  | -2.24014028 | 1.50985850  |

### 7'-H,H,OMe,H

E(SMD/M06-2X/BS1) = -496.1727988 au

H(SMD/M06-2X/BS1) = -496.030638 au

G(SMD/M06-2X/BS1) = -496.075099 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -496.3795917 au

|   |            |            |             |
|---|------------|------------|-------------|
| C | 1.25638900 | 0.90850500 | -0.00009400 |
|---|------------|------------|-------------|

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.14206700 | 1.27352500  | 0.00002400  |
| C | 1.58089800  | -0.59769000 | 0.00008600  |
| C | -1.09870500 | 0.31126300  | -0.00004500 |
| C | 0.55733900  | -1.56526100 | -0.00052000 |
| C | -0.72748800 | -1.11740000 | -0.00053900 |
| H | 0.78994600  | -2.62544600 | -0.00073900 |
| O | 2.19380900  | 1.67635200  | -0.00036700 |
| O | 2.83141500  | -0.85741500 | 0.00073700  |
| H | 3.01496600  | -1.82825700 | 0.00074000  |
| H | -1.51978600 | -1.86010500 | -0.00097300 |
| H | -0.39791700 | 2.32660800  | 0.00005800  |
| O | -2.37321400 | 0.68151500  | 0.00014800  |
| C | -3.42510900 | -0.29282800 | 0.00035300  |
| H | -4.34616000 | 0.28730200  | 0.00060800  |
| H | -3.38249000 | -0.91210300 | -0.89937800 |
| H | -3.38217800 | -0.91229700 | 0.89994400  |

#### 7'-H,H,CN,H

E(SMD/M06-2X/BS1) = -473.8964518 au

H(SMD/M06-2X/BS1) = -473.789603 au

G(SMD/M06-2X/BS1) = -473.831656 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -474.089787 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.97293100  | 0.95371300  | -0.00021000 |
| C | -0.49766700 | 1.09571400  | -0.00027200 |
| C | 1.53489000  | -0.47365900 | 0.00028000  |
| C | -1.25599200 | -0.01678500 | -0.00025300 |
| H | -0.90901800 | 2.09942200  | -0.00037100 |
| C | 0.68281700  | -1.58985700 | 0.00026500  |
| C | -0.66154800 | -1.35807100 | -0.00002600 |
| H | 1.08373500  | -2.59833400 | 0.00051400  |
| O | 1.73903700  | 1.88261400  | 0.00021100  |
| O | 2.81305600  | -0.51289300 | 0.00057900  |
| H | 3.16226700  | -1.43750500 | 0.00083900  |
| H | -1.34362100 | -2.20375100 | 0.00002200  |
| C | -2.69163900 | 0.07975400  | -0.00040500 |
| N | -3.84469500 | 0.14822100  | -0.00051400 |

#### 7'-H,H,H,CN

E(SMD/M06-2X/BS1) = -473.8976133 au

H(SMD/M06-2X/BS1) = -473.790932 au

G(SMD/M06-2X/BS1) = -473.833839 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -474.0905926 au

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -0.01657300 | -0.75926300 | 0.00005100 |
|---|-------------|-------------|------------|

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.97653800  | 0.34445000  | -0.00019700 |
| C | -1.49135900 | -0.33736100 | 0.00023600  |
| C | 0.56101900  | 1.62525100  | -0.00008200 |
| C | -1.86590600 | 1.01652100  | 0.00041900  |
| C | -0.86423300 | 1.94545400  | 0.00023800  |
| H | 1.27039100  | 2.44548900  | -0.00021500 |
| H | -2.91294100 | 1.30380200  | 0.00065300  |
| O | 0.26371600  | -1.92811100 | 0.00015900  |
| O | -2.29233500 | -1.33366100 | 0.00022900  |
| H | -3.24111300 | -1.05573500 | 0.00038800  |
| H | -1.12854900 | 2.99836800  | 0.00032700  |
| C | 2.35901700  | -0.02978700 | -0.00049800 |
| N | 3.47002000  | -0.34704900 | -0.00075200 |

### 27-H,H,H,H

E(SMD/M06-2X/BS1) = -812.669286777 au

H(SMD/M06-2X/BS1) = -812.458258 au

G(SMD/M06-2X/BS1) = -812.518979 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1099.2894053 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.52301200  | 1.65419000  | 0.00887100  |
| C | 0.83779400  | 1.77210000  | -0.84320500 |
| C | 2.71061300  | 0.52512500  | 0.09616900  |
| C | 2.99619900  | 2.83652200  | -0.50011000 |
| C | 1.66591000  | 2.89283900  | -0.92211500 |
| C | 1.39392300  | 0.61323700  | -0.32694900 |
| H | 3.62106200  | 3.72058000  | -0.57116200 |
| H | 1.26314300  | 3.81829500  | -1.32099300 |
| H | -0.19381400 | 1.80708200  | -1.17502900 |
| H | 4.55401600  | 1.58589300  | 0.34133000  |
| C | 3.20263200  | -0.78525200 | 0.62801300  |
| I | 0.36975900  | -1.19883600 | -0.10558500 |
| O | 2.27993900  | -1.73068300 | 0.62292100  |
| O | 4.33777100  | -0.95480600 | 1.02123900  |
| O | -1.29046700 | -0.30724000 | -0.92438900 |
| O | -3.79039700 | -0.85583800 | -1.63768800 |
| C | -3.58966100 | -0.12247000 | -0.51571900 |
| C | -2.27654500 | 0.16816300  | -0.10165300 |
| C | -4.67087000 | 0.34638500  | 0.22084600  |
| C | -2.06294600 | 0.91864500  | 1.04940600  |
| C | -4.44971900 | 1.09745400  | 1.37621700  |
| H | -5.67529900 | 0.11141900  | -0.11758100 |
| C | -3.15210700 | 1.38184300  | 1.79146500  |
| H | -2.90781200 | -1.06966100 | -1.99167700 |

|   |             |            |            |
|---|-------------|------------|------------|
| H | -5.29798400 | 1.45751700 | 1.94982700 |
| H | -2.97774300 | 1.96515200 | 2.68973500 |
| H | -1.04699000 | 1.13789800 | 1.36747800 |

### 27-OMe,H,H,H

E(SMD/M06-2X/BS1) = -927.142763575 au

H(SMD/M06-2X/BS1) = -926.895760 au

G(SMD/M06-2X/BS1) = -926.962124 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1213.81218020 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 4.04916400  | 1.71122200  | 0.02788400  |
| C | 1.37433300  | 1.76627200  | -0.86202100 |
| C | 3.25868000  | 0.56663800  | 0.11521400  |
| C | 3.50577900  | 2.87756800  | -0.50025600 |
| C | 2.18069200  | 2.90266200  | -0.94129500 |
| C | 1.94648100  | 0.62395400  | -0.32659300 |
| H | 4.11358900  | 3.77342000  | -0.57165000 |
| H | 1.76493500  | 3.81564200  | -1.35535400 |
| H | 0.34671800  | 1.77671000  | -1.20747500 |
| H | 5.07648900  | 1.66727200  | 0.37547600  |
| C | 3.76964300  | -0.72868400 | 0.66623600  |
| I | 0.95393800  | -1.20483300 | -0.09936000 |
| O | 2.86707600  | -1.69289600 | 0.65634200  |
| O | 4.90250800  | -0.87057500 | 1.07700900  |
| O | -0.71144300 | -0.35214700 | -0.94391800 |
| O | -3.19286100 | -0.97098000 | -1.67266300 |
| C | -3.00570800 | -0.21766600 | -0.56003900 |
| C | -1.71554800 | 0.10979800  | -0.13362200 |
| C | -4.11888100 | 0.24247800  | 0.16036000  |
| C | -1.51861400 | 0.88089300  | 1.01376800  |
| C | -3.92257000 | 1.01165700  | 1.30881100  |
| C | -2.62680900 | 1.32188400  | 1.72707900  |
| H | -2.30167500 | -1.16877700 | -2.01393900 |
| H | -2.48651300 | 1.92057800  | 2.62120900  |
| H | -0.51148600 | 1.12637300  | 1.33800100  |
| O | -5.32595900 | -0.12099400 | -0.33918000 |
| C | -6.47082900 | 0.32291000  | 0.36669100  |
| H | -7.33155100 | -0.06309600 | -0.18042100 |
| H | -6.48586500 | -0.06884400 | 1.39040800  |
| H | -6.52138600 | 1.41759100  | 0.39736200  |
| H | -4.77143300 | 1.37051400  | 1.87843700  |

### 27-H,H,CN,H

E(SMD/M06-2X/BS1) = -904.88871185 au



H(SMD/M06-2X/BS1) = -904.677253 au  
G(SMD/M06-2X/BS1) = -904.742504 au  
E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1191.5449998 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.47717900 | 1.81729300  | 0.65891900  |
| C | -0.92292500 | 1.10070100  | 1.61576900  |
| C | -2.81251000 | 0.71509900  | 0.12450800  |
| C | -2.86729100 | 2.55959800  | 1.66448400  |
| C | -1.60297000 | 2.20212400  | 2.13801200  |
| C | -1.55625800 | 0.38894500  | 0.61037200  |
| H | -3.37592600 | 3.42031900  | 2.08570600  |
| H | -1.13558000 | 2.78384300  | 2.92599100  |
| H | 0.05496000  | 0.81500900  | 1.98634100  |
| H | -4.46024500 | 2.07365300  | 0.27675400  |
| C | -3.40237900 | -0.13734500 | -0.95404400 |
| I | -0.75979200 | -1.29086900 | -0.35058300 |
| O | -2.61468700 | -1.13643100 | -1.32184500 |
| O | -4.49398200 | 0.06609900  | -1.43981000 |
| O | 0.91043000  | -1.11996900 | 0.85839600  |
| O | 3.23481700  | -2.21172000 | 1.47547000  |
| C | 3.24489900  | -1.06684300 | 0.76838500  |
| C | 2.01700900  | -0.46809300 | 0.40830800  |
| C | 4.45180700  | -0.47961400 | 0.40336600  |
| C | 2.01408500  | 0.71226800  | -0.31660100 |
| C | 4.45329000  | 0.70208900  | -0.32792300 |
| H | 5.37986900  | -0.96094100 | 0.69278100  |
| C | 3.23865800  | 1.29329200  | -0.68638800 |
| H | 2.29912800  | -2.44567700 | 1.62580900  |
| H | 5.38933600  | 1.16483600  | -0.62045300 |
| C | 3.23668300  | 2.51262600  | -1.44169000 |
| N | 3.23658100  | 3.49725800  | -2.05179500 |
| H | 1.07924200  | 1.18750000  | -0.59999600 |

## 27-H,H,H,CN

E(SMD/M06-2X/BS1) = -904.886614133 au  
H(SMD/M06-2X/BS1) = -904.675228 au  
G(SMD/M06-2X/BS1) = -904.740140 au  
E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1191.54211693 au

|   |            |            |             |
|---|------------|------------|-------------|
| C | 3.93770600 | 1.11120100 | -0.18565100 |
| C | 1.32562500 | 1.61726400 | -1.12320100 |
| C | 2.92403300 | 0.17803900 | 0.02584100  |
| C | 3.64772400 | 2.29074700 | -0.86211100 |
| C | 2.35383100 | 2.53856700 | -1.32634700 |
| C | 1.64937500 | 0.45536700 | -0.44255100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.42992500  | 3.02312600  | -1.03162300 |
| H | 2.13589200  | 3.46097600  | -1.85514100 |
| H | 0.31966200  | 1.80335000  | -1.47926200 |
| H | 4.93539600  | 0.89558100  | 0.18339900  |
| C | 3.15821600  | -1.11447300 | 0.73975900  |
| I | 0.31618000  | -1.09679000 | -0.00276600 |
| O | 2.07045200  | -1.86809900 | 0.83334000  |
| O | 4.23414400  | -1.44519800 | 1.18730400  |
| O | -1.16435000 | 0.02527300  | -0.98470600 |
| O | -3.33842400 | -1.29476100 | -1.84677900 |
| C | -3.46268300 | -0.45534700 | -0.79544200 |
| C | -2.32750700 | 0.22872900  | -0.32419200 |
| C | -4.69785000 | -0.26526900 | -0.18793500 |
| C | -2.46938900 | 1.10199400  | 0.76301700  |
| C | -4.81903400 | 0.60208700  | 0.89947700  |
| H | -5.55715500 | -0.80560800 | -0.57229000 |
| C | -3.71488900 | 1.29063800  | 1.38055500  |
| H | -2.41542200 | -1.23058200 | -2.15549100 |
| H | -5.78716500 | 0.74004000  | 1.36855100  |
| H | -3.79700100 | 1.97095900  | 2.22068100  |
| C | -1.31159300 | 1.80747200  | 1.23061600  |
| N | -0.37109200 | 2.37317300  | 1.60050100  |

H<sub>2</sub>O

E(SMD/M06-2X/BS1) = -76.3802305 au

H(SMD/M06-2X/BS1) = -76.355226 au

G(SMD/M06-2X/BS1) = -76.376671 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -76.4341177 au

|   |            |             |             |
|---|------------|-------------|-------------|
| O | 0.00000000 | 0.00000000  | 0.11977800  |
| H | 0.00000000 | 0.76105000  | -0.47911100 |
| H | 0.00000000 | -0.76105000 | -0.47911100 |

(H<sub>2</sub>O)<sub>3</sub>

E(SMD/M06-2X/BS1) = -229.158957 au

H(SMD/M06-2X/BS1) = -229.080423 au

G(SMD/M06-2X/BS1) = -229.120496 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -229.3148003 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.64174800  | 0.02318900  | -0.00029100 |
| O | 2.45700600  | -0.50865700 | -0.00030300 |
| H | 2.13542100  | -1.42114200 | 0.00224000  |
| O | -0.00240800 | 0.99125900  | 0.00010100  |
| H | -0.02825900 | 1.58415700  | -0.77019300 |
| H | -0.02810700 | 1.58402200  | 0.77050300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.52915100 | -0.15491300 | 0.00007300  |
| O | -2.34726600 | -0.68230600 | 0.00002700  |
| H | -3.05030800 | -0.01768100 | -0.00093000 |

### 1\_OAc

E(SMD/M06-2X/BS1) = -734.2264719 au

H(SMD/M06-2X/BS1) = -734.061321 au

G(SMD/M06-2X/BS1) = -734.118945 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1020.826565 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.90485700  | 1.50113100  | 0.08440400  |
| C | 0.18367400  | 1.97302800  | -0.49211000 |
| C | 1.98615000  | 0.45745300  | 0.13200800  |
| C | 2.46179200  | 2.77830400  | -0.24814100 |
| C | 1.11643800  | 3.01012300  | -0.53867600 |
| C | 0.65105300  | 0.71522400  | -0.14499100 |
| H | 3.16858500  | 3.60053400  | -0.28814500 |
| H | 0.78414900  | 4.00714400  | -0.80839800 |
| H | -0.85550000 | 2.15668700  | -0.73931300 |
| H | 3.94829600  | 1.29934300  | 0.30386400  |
| C | 2.38561100  | -0.95038900 | 0.45496200  |
| I | -0.50854500 | -1.03432100 | -0.06115500 |
| O | 1.36770300  | -1.80393300 | 0.41824300  |
| O | 3.51850000  | -1.27437300 | 0.72307900  |
| O | -2.16210800 | 0.11437000  | -0.54906200 |
| O | -0.45595400 | -1.67301100 | -1.70514400 |
| C | -2.63678300 | 0.74290300  | 0.52780200  |
| O | -2.04168600 | 0.70699000  | 1.59140600  |
| C | -3.92054900 | 1.47735500  | 0.27930900  |
| H | -3.76036200 | 2.23775900  | -0.49096800 |
| H | -4.67540400 | 0.77941500  | -0.09266000 |
| H | -4.26196400 | 1.94700900  | 1.20126200  |

### 1\_OAc

E(SMD/M06-2X/BS1) = -1156.042639 au

H(SMD/M06-2X/BS1) = -1155.728182 au

G(SMD/M06-2X/BS1) = -1155.806054 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1442.808587 au

|   |             |            |            |
|---|-------------|------------|------------|
| C | -1.44470700 | 1.10087000 | 2.54191900 |
| C | 0.36432400  | 2.28154800 | 0.72490500 |
| C | -0.70304700 | 0.30075700 | 1.67414000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.28349800 | 2.48253900  | 2.49767000  |
| C | -0.38055800 | 3.06685300  | 1.60520800  |
| C | 0.16531800  | 0.91218700  | 0.78784600  |
| H | -1.85895400 | 3.11357300  | 3.16700300  |
| H | -0.25302600 | 4.14445500  | 1.59130300  |
| H | 1.06348600  | 2.72237800  | 0.02283200  |
| H | -2.13394100 | 0.63015900  | 3.23569500  |
| C | -0.80096400 | -1.19766700 | 1.65054000  |
| I | 1.03872900  | -0.41529600 | -0.57632500 |
| O | -0.00251500 | -1.75005900 | 0.76215900  |
| O | -1.54018700 | -1.81224700 | 2.39298300  |
| O | -0.40832400 | 2.05510400  | -2.51664700 |
| C | -0.89042200 | -0.18832700 | -1.88305400 |
| C | -1.17515900 | 1.27663400  | -1.93078600 |
| C | -1.90922600 | -1.07414200 | -1.31820300 |
| C | -2.34934000 | 1.75655200  | -1.21277100 |
| C | -2.97094200 | -0.55367100 | -0.65707800 |
| H | -1.75143300 | -2.14277600 | -1.39728900 |
| C | -3.18027500 | 0.88658800  | -0.60375100 |
| H | -4.05192500 | 1.23535700  | -0.05625200 |
| O | -3.93687200 | -1.25138300 | -0.02778100 |
| C | -3.77749100 | -2.66243800 | 0.00577600  |
| H | -2.82896000 | -2.93279000 | 0.48200800  |
| H | -4.60942400 | -3.04713200 | 0.59561700  |
| H | -3.82001200 | -3.08229700 | -1.00579500 |
| H | -2.51833200 | 2.82805000  | -1.19199800 |
| H | -0.43954500 | -0.54182600 | -2.81431200 |
| O | 1.83772000  | 1.02052100  | -1.59158900 |
| O | 2.70560700  | -0.10260800 | 0.78149700  |
| H | 1.13757100  | 1.48836000  | -2.12478500 |
| C | 3.81855000  | -0.65141800 | 0.33520200  |
| O | 3.89457700  | -1.23913500 | -0.73308600 |
| C | 4.98709000  | -0.48143000 | 1.27577900  |
| H | 5.17320000  | 0.58392400  | 1.43840000  |
| H | 4.74485500  | -0.92793000 | 2.24426500  |
| H | 5.87583800  | -0.95499800 | 0.85818700  |

**TS**<sub>26-37</sub>

E(SMD/M06-2X/BS1) = -927.0452983 au

H(SMD/M06-2X/BS1) = -926.80473 au

G(SMD/M06-2X/BS1) = -926.870302 au

E(SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1213.714239 au

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.05806700  | 2.40760700  | 0.24712100  |
| C | 3.77906700  | -0.14267800 | -0.61382300 |
| C | 2.12015900  | 1.37901800  | 0.34185700  |
| C | 4.34698700  | 2.16808700  | -0.22488700 |
| C | 4.71027400  | 0.89439900  | -0.65405300 |
| C | 2.50940400  | 0.10996400  | -0.10166500 |
| H | 5.06421200  | 2.98164300  | -0.27065300 |
| H | 5.70687800  | 0.70613600  | -1.04015900 |
| H | 4.03927600  | -1.13006000 | -0.98301600 |
| H | 2.75773300  | 3.40379400  | 0.55664400  |
| C | 0.72521600  | 1.70976700  | 0.86891900  |
| I | 1.14821600  | -1.49235300 | -0.01654900 |
| O | 0.16796000  | 0.78513400  | 1.57517800  |
| O | 0.24894400  | 2.80454600  | 0.58826300  |
| O | -0.16460800 | -0.34357800 | -0.93486600 |
| O | -1.14563700 | -2.50798500 | 0.24525700  |
| C | -1.91184200 | -1.51350000 | 0.20556400  |
| C | -1.37170200 | -0.22329700 | -0.21181600 |
| C | -3.29314000 | -1.50971500 | 0.60101200  |
| C | -2.26793900 | 0.81470800  | -0.68681000 |
| H | -0.94726700 | 0.29551700  | 0.86811400  |
| C | -4.08356600 | -0.43281800 | 0.31152400  |
| H | -3.71642600 | -2.41294300 | 1.02721100  |
| C | -3.58578900 | 0.74352600  | -0.35115200 |
| H | -1.85531000 | 1.69080500  | -1.17586700 |
| O | -4.37945900 | 1.80153100  | -0.67487700 |
| H | -5.13512800 | -0.48547500 | 0.57437700  |
| C | -5.76725700 | 1.70092800  | -0.40480000 |
| H | -6.21006800 | 2.62729200  | -0.77217700 |
| H | -6.22066500 | 0.85278800  | -0.93074400 |
| H | -5.96394000 | 1.61204400  | 0.66978800  |