

## Supporting Information

DFT Study of Ni/NHC-Catalyzed C–H Alkylation of Fluoroarenes with Alkenes to  
Synthesize Fluorotetralins: Mechanism, Chemoselectivity of C–H vs C–F Bond  
Activation, and Regio-, and Enantioselectivities of C–H Bond Activation

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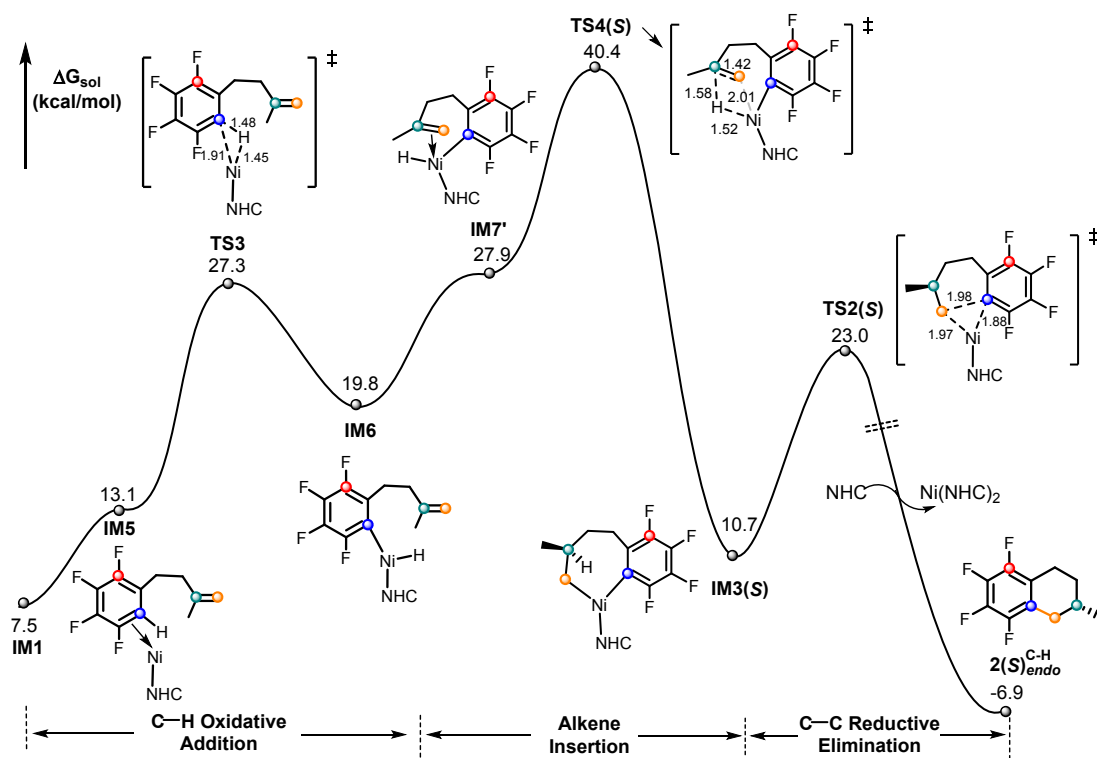
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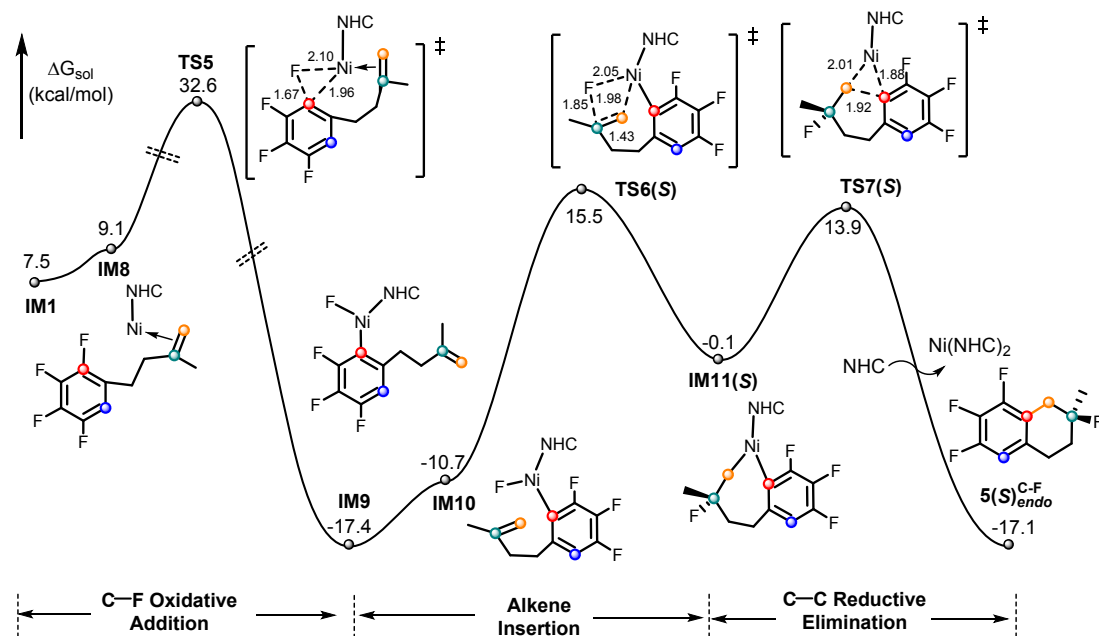
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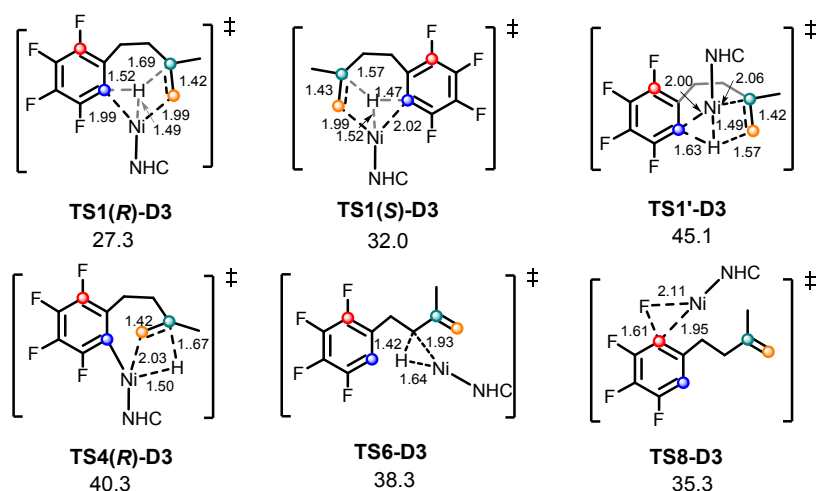
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**Figure S1.** Calculated Gibbs energy profile for the formation of the *S*-type fluorotetralin product  $2(S)^{\text{C-H}}_{\text{endo}}$  according to the stepwise oxidative addition/alkene insertion mechanism. Note that in **IM7'**, the double bond coordinates to the Ni center from its *Re*-face.



**Figure S2.** Calculated Gibbs energy profile with schematic geometries for the formation of the hypothetical *S*-type C–F bond activation product **5(S)<sup>C-F</sup><sub>endo</sub>**.



**Figure S3.** Calculated relative Gibbs energies of several key transition state structures by performing the dispersion-corrected B3LYP-D3(BJ) calculations.

To calibrate the results, geometrical optimization calculations were also performed using the dispersion-corrected B3LYP-D3(BJ) functional with the implicit solvation model for several key transition state structures including TS1(*R*), TS1(*S*), TS1', TS4(*R*), TS6, and TS8. The relative Gibbs energies of these transition states are refined to 40.3, 27.3, 32.0, 45.1, 38.3 and 35.7 kcal/mol, which are comparable with those obtained from the B3LYP calculations, 24.7, 28.8, 42.6, 38.3, 35.9 and 32.6 kcal/mol, respectively. More important, the dispersion-corrected B3LYP-D3(BJ) calculations give consistent the conclusions with the B3LYP calculations for the decisive reaction pathway as well as the enantio-, regio- and chemoselectivities, confirming the reliability of the B3LYP calculations.

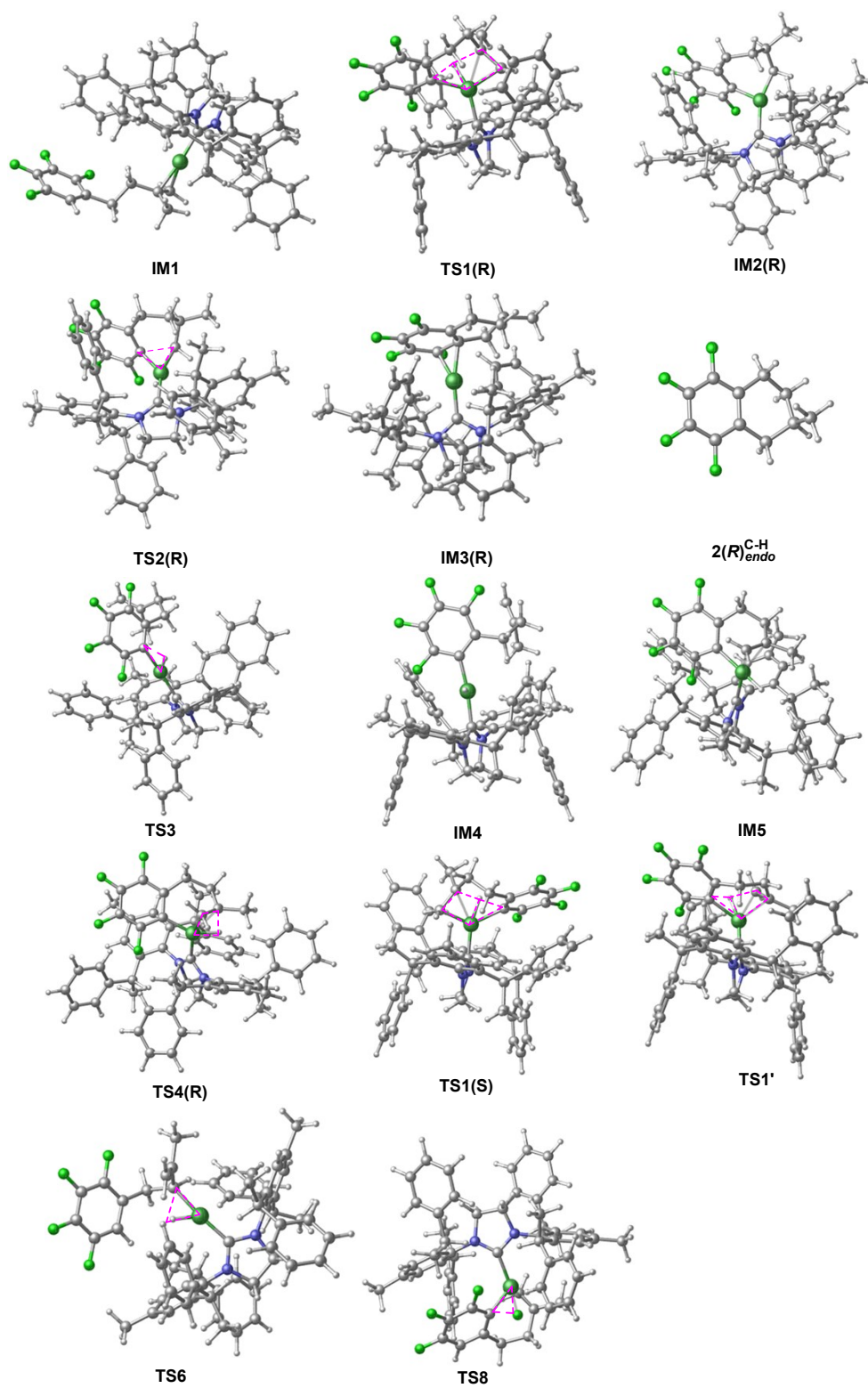
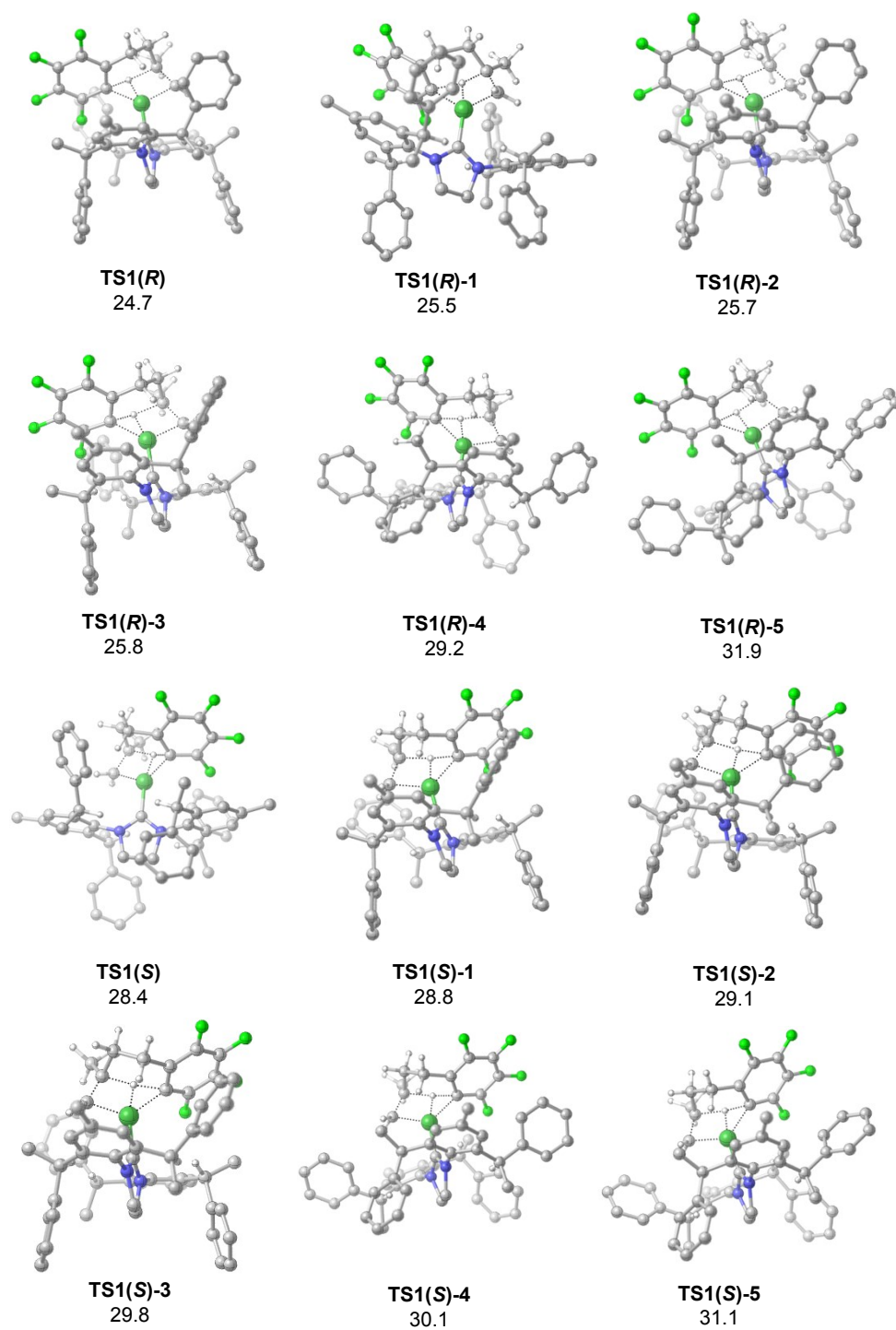


Figure S4. 3D models of some key intermediates and transition states



**Figure S5.** Selected diastereomeric transition state structures with relative Gibbs energies within ~ 6 kcal/mol.

## Cartesian Coordinates of All Structures Involved in This Work

### Ni(cod)<sub>2</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| Ni | -0.00000100 | 0.00000800  | 0.00000000  |
| C  | -2.24878500 | 1.83618400  | -0.60112900 |
| C  | -1.39612000 | 1.53789000  | 0.61521500  |
| C  | -1.53887500 | 0.47031600  | 1.48148800  |
| C  | -2.24865300 | -1.83619000 | 0.60153700  |
| C  | -1.39621600 | -1.53789100 | -0.61496500 |
| C  | -1.53912600 | -0.47031800 | -1.48121400 |
| C  | -2.63807800 | -0.58257900 | 1.41994400  |
| C  | -2.63832200 | 0.58257400  | -1.41949000 |
| C  | 2.24866700  | -1.83632400 | -0.60109500 |
| C  | 1.39621200  | -1.53773800 | 0.61532500  |
| C  | 1.53911800  | -0.46996600 | 1.48133100  |
| C  | 2.24879900  | 1.83631800  | 0.60068700  |
| C  | 1.39611500  | 1.53773700  | -0.61557600 |
| C  | 1.53886700  | 0.46996400  | -1.48160500 |
| C  | 2.63831700  | 0.58290800  | 1.41936800  |
| C  | 2.63807300  | -0.58291200 | -1.41982200 |
| H  | -1.67945200 | 2.51531800  | -1.24722100 |
| H  | -3.15780400 | 2.39005700  | -0.31519000 |
| H  | -0.77910100 | 2.36769100  | 0.95479900  |
| H  | -1.00190800 | 0.53127100  | 2.42457800  |
| H  | -3.15770700 | -2.39009700 | 0.31577100  |
| H  | -1.67918100 | -2.51529400 | 1.24753900  |
| H  | -0.77925700 | -2.36769000 | -0.95466200 |
| H  | -1.00232700 | -0.53128200 | -2.42439900 |
| H  | -3.55354700 | -0.13903400 | 1.01660100  |
| H  | -2.88792800 | -0.89426100 | 2.44075400  |
| H  | -2.88832500 | 0.89426600  | -2.44026000 |
| H  | -3.55373100 | 0.13902100  | -1.01601900 |
| H  | 1.67922100  | -2.51560700 | -1.24693100 |
| H  | 3.15773200  | -2.39013700 | -0.31518100 |
| H  | 0.77925100  | -2.36745800 | 0.95521000  |
| H  | 1.00231300  | -0.53070700 | 2.42452700  |
| H  | 3.15782900  | 2.39009700  | 0.31459900  |
| H  | 1.67949100  | 2.51563200  | 1.24661300  |
| H  | 0.77909400  | 2.36745900  | -0.95534800 |
| H  | 1.00189400  | 0.53069500  | -2.42470600 |
| H  | 3.55373300  | 0.13925600  | 1.01602400  |
| H  | 2.88830200  | 0.89485100  | 2.44006600  |
| H  | 2.88790600  | -0.89484600 | -2.44055900 |
| H  | 3.55354900  | -0.13926800 | -1.01660600 |



## NHC

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.00004800  | -0.00003000 | -0.31719300 |
| C | -0.75210600 | -0.15049800 | 1.94846300  |
| C | 0.75218200  | 0.15053900  | 1.94846100  |
| H | -1.34180400 | 0.69691700  | 2.31876600  |
| H | -1.01443600 | -1.03675800 | 2.52856800  |
| H | 1.01450700  | 1.03681500  | 2.52854200  |
| H | 1.34188100  | -0.69686500 | 2.31879000  |
| N | 1.01793500  | 0.36259200  | 0.49663400  |
| N | -1.01785700 | -0.36258700 | 0.49664100  |
| C | 2.31841200  | 0.73952700  | 0.02119600  |
| C | 2.60467000  | 2.10685400  | -0.21434900 |
| C | 3.29523100  | -0.24605000 | -0.21093700 |
| C | 3.88303500  | 2.44928100  | -0.66082000 |
| C | 4.56039600  | 0.15031500  | -0.66579300 |
| C | 4.87852100  | 1.48831900  | -0.88559000 |
| H | 4.11644400  | 3.49062500  | -0.85886100 |
| H | 5.30729900  | -0.61245300 | -0.87121700 |
| C | -2.31833400 | -0.73953200 | 0.02120900  |
| C | -3.29517000 | 0.24602800  | -0.21094400 |
| C | -2.60457700 | -2.10686900 | -0.21429600 |
| C | -4.56033200 | -0.15037000 | -0.66578100 |
| C | -3.88293600 | -2.44932400 | -0.66076100 |
| C | -4.87843600 | -1.48838300 | -0.88555200 |
| H | -5.30725300 | 0.61238100  | -0.87120700 |
| H | -4.11633100 | -3.49067700 | -0.85877500 |
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| C | 1.52734000  | 3.17220600  | -0.01535400 |
| C | -3.01771000 | 1.73608500  | 0.00104700  |
| C | -1.52723400 | -3.17220200 | -0.01526600 |
| H | -0.58303600 | -2.72178900 | -0.33665800 |
| H | 1.98319800  | -1.82522100 | 0.34194000  |
| H | 0.58314500  | 2.72181300  | -0.33677900 |
| H | -1.98318700 | 1.82526300  | 0.34190300  |
| C | 3.09407300  | -2.49873500 | -1.32592300 |
| C | 4.08394400  | -3.44858500 | -1.60593100 |
| C | 2.12423100  | -2.23546500 | -2.30978600 |
| C | 4.10938400  | -4.11739700 | -2.83494100 |
| H | 4.84317800  | -3.68180600 | -0.86642800 |
| C | 2.14653000  | -2.90432600 | -3.53249100 |
| H | 1.35034700  | -1.49743600 | -2.10521500 |
| C | 3.14213100  | -3.84910100 | -3.80218700 |
| H | 4.88736200  | -4.85061800 | -3.03016500 |
| H | 1.38537900  | -2.68836400 | -4.27748900 |

|   |              |              |              |
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| H | 3. 16031000  | -4. 37007700 | -4. 75531800 |
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| H | 4. 97514000  | -2. 22772000 | 0. 87792100  |
| H | 3. 74213000  | -1. 76623500 | 2. 04957000  |
| H | 3. 68553500  | -3. 36790500 | 1. 29294800  |
| C | 1. 34237400  | 3. 58800800  | 1. 44659800  |
| C | 2. 41952200  | 3. 68411600  | 2. 33890100  |
| C | 0. 06565700  | 3. 94433300  | 1. 90707600  |
| C | 2. 22515300  | 4. 11888200  | 3. 65244700  |
| H | 3. 41605900  | 3. 40817500  | 2. 00682500  |
| C | -0. 13284900 | 4. 37928100  | 3. 21872200  |
| H | -0. 78024800 | 3. 88498000  | 1. 22607900  |
| C | 0. 94859200  | 4. 46696200  | 4. 09855800  |
| H | 3. 07373500  | 4. 18309600  | 4. 32817000  |
| H | -1. 13153700 | 4. 64632700  | 3. 55327100  |
| H | 0. 79756700  | 4. 80147600  | 5. 12088000  |
| C | 1. 73380400  | 4. 43051900  | -0. 88641600 |
| H | 1. 86353800  | 4. 16344000  | -1. 93987100 |
| H | 0. 85878300  | 5. 08159800  | -0. 80371100 |
| H | 2. 60321100  | 5. 01332600  | -0. 56646400 |
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| C | -2. 12429800 | 2. 23567200  | -2. 30977100 |
| C | -4. 08420300 | 3. 44845700  | -1. 60587300 |
| C | -2. 14669800 | 2. 90457900  | -3. 53244800 |
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| C | -4. 10974800 | 4. 11731000  | -2. 83485800 |
| H | -4. 84347500 | 3. 68152800  | -0. 86636200 |
| C | -3. 14245100 | 3. 84920400  | -3. 80211300 |
| H | -1. 38550500 | 2. 68877500  | -4. 27744800 |
| H | -4. 88784300 | 4. 85041500  | -3. 03005500 |
| H | -3. 16071000 | 4. 37021500  | -4. 75522300 |
| C | -3. 91033800 | 2. 31100900  | 1. 11596500  |
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| H | -3. 68554100 | 3. 36782400  | 1. 29303400  |
| H | -4. 97512700 | 2. 22762400  | 0. 87798900  |
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| C | 0. 13287200  | -4. 37926400 | 3. 21885700  |
| H | 0. 78032500  | -3. 88495600 | 1. 22623300  |
| C | -0. 94859400 | -4. 46695700 | 4. 09866100  |
| H | -3. 07374600 | -4. 18311300 | 4. 32821100  |

|   |             |             |             |
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| H | -0.79759500 | -4.80147100 | 5.12098800  |
| C | -1.73364300 | -4.43051700 | -0.88633800 |
| H | -0.85860400 | -5.08157000 | -0.80361800 |
| H | -2.60303900 | -5.01335100 | -0.56640600 |
| H | -1.86336300 | -4.16343600 | -1.93979400 |
| C | 6.25379300  | 1.90173200  | -1.35497200 |
| C | -6.25370400 | -1.90182800 | -1.35491700 |
| H | -6.83105900 | -1.04198000 | -1.70537700 |
| H | -6.19469100 | -2.62805800 | -2.17243500 |
| H | -6.82306600 | -2.37539300 | -0.54567000 |
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| H | 6.82317100  | 2.37529500  | -0.54573500 |

**cod**

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| C | 0.00024400  | -1.70256400 | -0.22380400 |
| H | 1.75757500  | -1.91878400 | 0.95926700  |
| H | 0.65507100  | -0.73041800 | 1.59803800  |
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| H | 1.83181300  | 1.82890100  | -1.17464400 |
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| H | 0.28079400  | -2.63069000 | -0.72223100 |
| C | -1.07504500 | 1.11293800  | 0.66505900  |
| H | -0.28083200 | 2.63057100  | -0.72254300 |
| C | -1.92380100 | 0.01875300  | -0.01795000 |
| H | -1.83179900 | -1.82903900 | -1.17449500 |
| H | -1.75757300 | 1.91884400  | 0.95911000  |
| H | -0.65509800 | 0.73046200  | 1.59791500  |
| H | -2.43330700 | 0.46405800  | -0.88440000 |
| H | -2.73596300 | -0.27472200 | 0.66535500  |

**Ni(NHC)**

|    |             |             |             |
|----|-------------|-------------|-------------|
| Ni | 0.00111500  | -0.00088900 | -2.04577300 |
| C  | 0.00018300  | -0.00057300 | -0.27311600 |
| C  | 0.44731400  | 0.62440200  | 1.97761900  |
| C  | -0.44937500 | -0.62474000 | 1.97735900  |
| H  | 1.36172900  | 0.47653500  | 2.55813900  |
| H  | -0.06581800 | 1.51032500  | 2.36589500  |
| H  | 0.06331700  | -1.51051300 | 2.36657500  |
| H  | -1.36447900 | -0.47668000 | 2.55675000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -0.75389000 | -0.79956400 | 0.54094500  |
| N | 0.75347000  | 0.79865500  | 0.54147000  |
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| C | -1.17350700 | -3.06890200 | -0.35638600 |
| C | -3.04805600 | -1.56671300 | 0.14312900  |
| C | -2.09951800 | -4.03932900 | -0.74416800 |
| C | -3.93331000 | -2.57821500 | -0.25442600 |
| C | -3.48351800 | -3.81927300 | -0.69681000 |
| H | -1.74160800 | -5.00041800 | -1.09954300 |
| H | -5.00154100 | -2.37701200 | -0.23255300 |
| C | 1.66200400  | 1.81332600  | 0.09110500  |
| C | 3.04776300  | 1.56707400  | 0.14593600  |
| C | 1.17274200  | 3.06791600  | -0.35577000 |
| C | 3.93275800  | 2.57885300  | -0.25082900 |
| C | 2.09873700  | 4.03891300  | -0.74283200 |
| C | 3.48257800  | 3.81916100  | -0.69547500 |
| H | 5.00117100  | 2.37885300  | -0.22607900 |
| H | 1.74072700  | 5.00041500  | -1.09695200 |
| C | -3.62404500 | -0.23123800 | 0.62034800  |
| C | 0.32601600  | -3.35127200 | -0.42248900 |
| C | 3.62391300  | 0.23257700  | 0.62570500  |
| C | -0.32677100 | 3.35030600  | -0.42171500 |
| H | -0.80584400 | 2.40979700  | -0.71459900 |
| H | -2.77939200 | 0.44302300  | 0.78614900  |
| H | 0.80507400  | -2.41101600 | -0.71626800 |
| H | 2.77945500  | -0.44213900 | 0.79068200  |
| C | -4.48250600 | 0.42096300  | -0.46812700 |
| C | -5.86614100 | 0.60235000  | -0.34863400 |
| C | -3.85468600 | 0.86657500  | -1.64496400 |
| C | -6.60325000 | 1.20633400  | -1.37347800 |
| H | -6.38441300 | 0.27809000  | 0.54771900  |
| C | -4.58641300 | 1.47167600  | -2.66550700 |
| H | -2.77922900 | 0.72903800  | -1.75826200 |
| C | -5.96827000 | 1.64345400  | -2.53490600 |
| H | -7.67594100 | 1.33525300  | -1.25703100 |
| H | -4.07784900 | 1.81102700  | -3.56422800 |
| H | -6.54025100 | 2.11471900  | -3.32912600 |
| C | -4.34761600 | -0.39916100 | 1.96980900  |
| H | -5.19480100 | -1.08815800 | 1.89674200  |
| H | -3.66379700 | -0.80775800 | 2.71937900  |
| H | -4.71944400 | 0.56233500  | 2.33823400  |
| C | 0.93179100  | -3.76882600 | 0.92046200  |
| C | 0.20547500  | -4.47258900 | 1.89117700  |
| C | 2.28389600  | -3.48956400 | 1.17749500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.80958100  | -4.88018900 | 3.08390100  |
| H | -0.84221800 | -4.69809700 | 1.71666300  |
| C | 2.89041800  | -3.89572900 | 2.36716900  |
| H | 2.86782500  | -2.95347400 | 0.43304100  |
| C | 2.15350800  | -4.59270300 | 3.32816100  |
| H | 0.22610100  | -5.42255300 | 3.82305900  |
| H | 3.93797300  | -3.66651500 | 2.54310200  |
| H | 2.62180700  | -4.90729600 | 4.25643200  |
| C | 0.71018500  | -4.38303800 | -1.50607700 |
| H | 0.29351700  | -4.10186700 | -2.47882100 |
| H | 1.79911100  | -4.42733000 | -1.59974100 |
| H | 0.36482400  | -5.39158900 | -1.25875800 |
| C | 4.48479300  | -0.42016300 | -0.46053500 |
| C | 5.86818600  | -0.60127800 | -0.33798700 |
| C | 3.85953600  | -0.86669400 | -1.63839600 |
| C | 6.60755700  | -1.20587900 | -1.36084100 |
| H | 6.38451500  | -0.27630100 | 0.55922500  |
| C | 4.59351000  | -1.47240200 | -2.65696400 |
| H | 2.78431000  | -0.72944900 | -1.75405900 |
| C | 5.97511200  | -1.64389400 | -2.52331100 |
| H | 7.68001600  | -1.33455700 | -1.24202300 |
| H | 4.08690300  | -1.81245300 | -3.55652300 |
| H | 6.54884100  | -2.11562700 | -3.31598800 |
| C | 4.34489800  | 0.40247700  | 1.97629700  |
| H | 3.65947400  | 0.81155500  | 2.72413300  |
| H | 4.71660100  | -0.55837600 | 2.34652100  |
| H | 5.19182000  | 1.09188600  | 1.90401800  |
| C | -0.93242800 | 3.76904300  | 0.92093900  |
| C | -0.20579700 | 4.47285800  | 1.89138200  |
| C | -2.28471600 | 3.49065300  | 1.17799400  |
| C | -0.80978400 | 4.88133000  | 3.08387300  |
| H | 0.84203200  | 4.69772200  | 1.71687600  |
| C | -2.89110300 | 3.89768100  | 2.36743600  |
| H | -2.86887500 | 2.95452100  | 0.43374700  |
| C | -2.15387900 | 4.59468500  | 3.32816900  |
| H | -0.22605800 | 5.42370200  | 3.82283000  |
| H | -3.93878800 | 3.66910000  | 2.54341700  |
| H | -2.62207600 | 4.90994100  | 4.25626600  |
| C | -0.71107000 | 4.38107400  | -1.50623200 |
| H | -1.79999800 | 4.42520800  | -1.59993200 |
| H | -0.36577900 | 5.38987000  | -1.25983700 |
| H | -0.29439600 | 4.09905800  | -2.47872800 |
| C | -4.44784900 | -4.90070400 | -1.12463100 |
| C | 4.44690900  | 4.89523900  | -1.13662700 |

|                     |             |             |             |
|---------------------|-------------|-------------|-------------|
| H                   | 5.47892800  | 4.63257500  | -0.88896900 |
| H                   | 4.39514700  | 5.05358500  | -2.22053800 |
| H                   | 4.21762300  | 5.85556700  | -0.66199500 |
| H                   | -5.48589600 | -4.57536400 | -1.01598200 |
| H                   | -4.29157900 | -5.18095000 | -2.17270000 |
| H                   | -4.31583300 | -5.81054100 | -0.52777000 |
| <b>Ni(cod)(NHC)</b> |             |             |             |
| H                   | -1.91199700 | 1.51025100  | 4.85104200  |
| C                   | -1.27109400 | 1.44578900  | 3.95736600  |
| C                   | 0.21915600  | 1.52189100  | 4.39012400  |
| H                   | -1.50787000 | 2.33144700  | 3.35609700  |
| C                   | -1.62864500 | 0.22890700  | 3.12996600  |
| C                   | 1.17461200  | 1.05601300  | 3.31001300  |
| H                   | 0.44781000  | 2.56188900  | 4.65089600  |
| H                   | 0.37225600  | 0.94404900  | 5.30594700  |
| C                   | -1.17392800 | -1.05646400 | 3.30986200  |
| H                   | -2.46837700 | 0.37176300  | 2.45300400  |
| C                   | 1.62931300  | -0.22922600 | 3.12913100  |
| H                   | 1.65599200  | 1.84124000  | 2.73042400  |
| C                   | -0.21798700 | -1.52305800 | 4.38924000  |
| H                   | -1.65566200 | -1.84131100 | 2.73005800  |
| C                   | 1.27211900  | -1.44659100 | 3.95598000  |
| H                   | 2.46878600  | -0.37166600 | 2.45176700  |
| H                   | -0.44648500 | -2.56325500 | 4.64935200  |
| H                   | -0.37075900 | -0.94589000 | 5.30554100  |
| H                   | 1.50877700  | -2.33190100 | 3.35415400  |
| H                   | 1.91331500  | -1.51147600 | 4.84941400  |
| Ni                  | 0.00005200  | 0.00012400  | 1.73248800  |
| C                   | -0.00005400 | 0.00002600  | -0.17519100 |
| C                   | -0.36892300 | 0.67034800  | -2.44002900 |
| C                   | 0.36869400  | -0.67012000 | -2.44010200 |
| H                   | -1.25952300 | 0.65640400  | -3.07194400 |
| H                   | 0.27093000  | 1.49863000  | -2.76586300 |
| H                   | -0.27117300 | -1.49837100 | -2.76598200 |
| H                   | 1.25926800  | -0.65612100 | -3.07205100 |
| N                   | 0.72299600  | -0.81951800 | -1.01135400 |
| N                   | -0.72316500 | 0.81961900  | -1.01125500 |
| C                   | 1.62882900  | -1.83734300 | -0.56731800 |
| C                   | 1.13785100  | -3.07483500 | -0.07852500 |
| C                   | 3.01941600  | -1.61250200 | -0.65580300 |
| C                   | 2.05815000  | -4.03153300 | 0.35972300  |
| C                   | 3.89797800  | -2.60775200 | -0.20747200 |
| C                   | 3.44177600  | -3.81708600 | 0.31264400  |
| H                   | 1.69470900  | -4.97848200 | 0.74638300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.96792500  | -2.42206000 | -0.25708000 |
| C | -1.62899500 | 1.83739400  | -0.56709600 |
| C | -3.01958100 | 1.61254900  | -0.65553200 |
| C | -1.13800600 | 3.07485300  | -0.07822600 |
| C | -3.89813400 | 2.60775700  | -0.20707500 |
| C | -2.05828900 | 4.03150100  | 0.36015200  |
| C | -3.44191900 | 3.81705100  | 0.31311000  |
| H | -4.96808200 | 2.42205000  | -0.25663600 |
| H | -1.69483700 | 4.97841700  | 0.74688300  |
| C | 3.60581500  | -0.34128200 | -1.28011400 |
| C | -0.35975000 | -3.37652900 | -0.06678800 |
| C | -3.60601700 | 0.34137300  | -1.27989100 |
| C | 0.35959600  | 3.37655600  | -0.06657500 |
| H | 0.86620000  | 2.43203400  | 0.15083700  |
| H | 2.77907500  | 0.36193400  | -1.41184100 |
| H | -0.86633200 | -2.43204300 | 0.15082000  |
| H | -2.77927200 | -0.36180000 | -1.41180700 |
| C | 4.61305000  | 0.34925900  | -0.35809000 |
| C | 6.00072000  | 0.25848900  | -0.53181100 |
| C | 4.13212900  | 1.11803800  | 0.71466500  |
| C | 6.87903800  | 0.90623600  | 0.34303900  |
| H | 6.41152100  | -0.31323900 | -1.35760500 |
| C | 5.00447900  | 1.76804300  | 1.58789800  |
| H | 3.05814000  | 1.19746300  | 0.86271600  |
| C | 6.38614300  | 1.66270900  | 1.40600800  |
| H | 7.95090400  | 0.82032600  | 0.18668800  |
| H | 4.60543300  | 2.35808000  | 2.40834100  |
| H | 7.06875300  | 2.16850800  | 2.08274300  |
| C | 4.17900200  | -0.65330000 | -2.67815500 |
| H | 4.97986500  | -1.39748100 | -2.63187200 |
| H | 3.40181000  | -1.06280000 | -3.32938000 |
| H | 4.57789900  | 0.25122300  | -3.14843200 |
| C | -0.88502000 | -3.86917100 | -1.42028600 |
| C | -0.10673200 | -4.63745900 | -2.29733800 |
| C | -2.21341400 | -3.59321600 | -1.78246400 |
| C | -0.63707800 | -5.11109700 | -3.50028400 |
| H | 0.92465500  | -4.86106200 | -2.04236300 |
| C | -2.74630000 | -4.06444300 | -2.98360000 |
| H | -2.83887400 | -3.00729200 | -1.11324500 |
| C | -1.95799400 | -4.82567200 | -3.85003100 |
| H | -0.01364900 | -5.70226900 | -4.16574200 |
| H | -3.77627400 | -3.83444200 | -3.24253400 |
| H | -2.36856600 | -5.19081300 | -4.78710600 |
| C | -0.78300800 | -4.36971700 | 1.03805100  |

|                            |             |             |             |
|----------------------------|-------------|-------------|-------------|
| H                          | -0.41350400 | -4.05032700 | 2.01757500  |
| H                          | -1.87468500 | -4.42484200 | 1.08395700  |
| H                          | -0.41675800 | -5.38243800 | 0.84351000  |
| C                          | -4.61308200 | -0.34927200 | -0.35776100 |
| C                          | -4.13194800 | -1.11773500 | 0.71512600  |
| C                          | -6.00077100 | -0.25890300 | -0.53150300 |
| C                          | -5.00412200 | -1.76783300 | 1.58846200  |
| H                          | -3.05793600 | -1.19683200 | 0.86318400  |
| C                          | -6.87891600 | -0.90674800 | 0.34345100  |
| H                          | -6.41172200 | 0.31258100  | -1.35739100 |
| C                          | -6.38581800 | -1.66291000 | 1.40654600  |
| H                          | -4.60491900 | -2.35762200 | 2.40900800  |
| H                          | -7.95080500 | -0.82115600 | 0.18708400  |
| H                          | -7.06829200 | -2.16878200 | 2.08336400  |
| C                          | -4.17942400 | 0.65350800  | -2.67781000 |
| H                          | -3.40236000 | 1.06315900  | -3.32909300 |
| H                          | -4.57830100 | -0.25099400 | -3.14814600 |
| H                          | -4.98035400 | 1.39760700  | -2.63132200 |
| C                          | 0.88472600  | 3.86941300  | -1.42005000 |
| C                          | 0.10635400  | 4.63788100  | -2.29687200 |
| C                          | 2.21306200  | 3.59347500  | -1.78244800 |
| C                          | 0.63656100  | 5.11171000  | -3.49980200 |
| H                          | -0.92499400 | 4.86147400  | -2.04172800 |
| C                          | 2.74581100  | 4.06489200  | -2.98357200 |
| H                          | 2.83859400  | 3.00741800  | -1.11341300 |
| C                          | 1.95742200  | 4.82629800  | -3.84976900 |
| H                          | 0.01306600  | 5.70301900  | -4.16507800 |
| H                          | 3.77574300  | 3.83489800  | -3.24267700 |
| H                          | 2.36788700  | 5.19158600  | -4.78683400 |
| C                          | 0.78295400  | 4.36955800  | 1.03839200  |
| H                          | 1.87463600  | 4.42467200  | 1.08421000  |
| H                          | 0.41669300  | 5.38231400  | 0.84405700  |
| H                          | 0.41353400  | 4.04999500  | 2.01789100  |
| C                          | 4.40282900  | -4.86546500 | 0.82246800  |
| C                          | -4.40294100 | 4.86543900  | 0.82297500  |
| H                          | -5.42146300 | 4.67822600  | 0.47180200  |
| H                          | -4.42941400 | 4.87808500  | 1.91951800  |
| H                          | -4.10929700 | 5.86899200  | 0.49782200  |
| H                          | 5.42110600  | -4.67897100 | 0.47019700  |
| H                          | 4.43034200  | -4.87718500 | 1.91899900  |
| H                          | 4.10844800  | -5.86916100 | 0.49844200  |
| <b>Ni(NHC)<sub>2</sub></b> |             |             |             |
| Ni                         | -0.00237300 | 0.00295900  | 0.00358400  |
| C                          | 0.10149600  | 1.90759300  | 0.02849300  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.64352900  | 4.16435200  | -0.56352400 |
| C | -0.21068000 | 4.18840500  | 0.68966500  |
| H | 1.68117700  | 4.42860900  | -0.34024900 |
| H | 0.26712200  | 4.82121300  | -1.34932900 |
| H | 0.22745600  | 4.78055300  | 1.49471900  |
| H | -1.21676100 | 4.56108700  | 0.47617700  |
| N | -0.25734400 | 2.75297500  | 1.05912500  |
| N | 0.54830400  | 2.74255900  | -0.97646600 |
| C | -0.61307000 | 2.42089000  | 2.41271400  |
| C | 0.41060600  | 2.13056800  | 3.35365400  |
| C | -1.94709100 | 2.56640400  | 2.85715700  |
| C | 0.05283200  | 1.89763500  | 4.68495800  |
| C | -2.24503800 | 2.33983300  | 4.20759600  |
| C | -1.26821700 | 1.98853400  | 5.13525500  |
| H | 0.82602400  | 1.66094600  | 5.40738800  |
| H | -3.27648400 | 2.44161900  | 4.53515900  |
| C | 0.86041800  | 2.41943400  | -2.34303700 |
| C | 2.19819100  | 2.45341400  | -2.79900300 |
| C | -0.19364800 | 2.25161700  | -3.28081200 |
| C | 2.46189000  | 2.23567200  | -4.15847500 |
| C | 0.12922200  | 2.02393200  | -4.62130800 |
| C | 1.44914600  | 2.00269500  | -5.08409300 |
| H | 3.49519900  | 2.24983400  | -4.49494900 |
| H | -0.66967400 | 1.88170500  | -5.34041200 |
| C | -3.08345000 | 3.06766100  | 1.95981700  |
| C | 1.88677800  | 2.16262600  | 2.95972500  |
| C | 3.38457000  | 2.82724500  | -1.90328300 |
| C | -1.65781100 | 2.41207800  | -2.87325600 |
| H | -1.77833400 | 1.93562100  | -1.89475300 |
| H | -2.74921100 | 2.97239100  | 0.92242400  |
| H | 1.96978300  | 1.70059300  | 1.97026900  |
| H | 3.05517400  | 2.72883100  | -0.86449100 |
| C | -4.34756400 | 2.21428300  | 2.09656300  |
| C | -5.52507700 | 2.68184400  | 2.69782600  |
| C | -4.33841500 | 0.90191200  | 1.60088300  |
| C | -6.65276400 | 1.86248000  | 2.80939500  |
| H | -5.57762500 | 3.69371000  | 3.08424100  |
| C | -5.46320900 | 0.08406400  | 1.70473400  |
| H | -3.43407400 | 0.52169600  | 1.13130000  |
| C | -6.62693600 | 0.55937800  | 2.31493200  |
| H | -7.55153300 | 2.24983200  | 3.28161900  |
| H | -5.43544200 | -0.92177800 | 1.29741300  |
| H | -7.50305200 | -0.07751700 | 2.39614400  |
| C | -3.34450500 | 4.56240000  | 2.24525300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.66421000 | 4.71745300  | 3.28020000  |
| H | -2.43798100 | 5.15273900  | 2.10014000  |
| H | -4.12041600 | 4.96083700  | 1.58371400  |
| C | 2.44022100  | 3.58902300  | 2.85232500  |
| C | 2.00341600  | 4.62815600  | 3.68698900  |
| C | 3.48814500  | 3.85818600  | 1.95849800  |
| C | 2.58744100  | 5.89616200  | 3.62227800  |
| H | 1.19779000  | 4.44539700  | 4.39165000  |
| C | 4.07675000  | 5.12268100  | 1.89236100  |
| H | 3.85391200  | 3.06254200  | 1.31424000  |
| C | 3.62528400  | 6.15029900  | 2.72375900  |
| H | 2.22935300  | 6.68583300  | 4.27734900  |
| H | 4.88733800  | 5.30397800  | 1.19187500  |
| H | 4.07841300  | 7.13616200  | 2.67292800  |
| C | 2.80112100  | 1.36499300  | 3.91383000  |
| H | 2.45437800  | 0.33522900  | 4.03037900  |
| H | 3.81555500  | 1.33530400  | 3.51074000  |
| H | 2.85941100  | 1.83298300  | 4.90159000  |
| C | 4.57057300  | 1.87496800  | -2.08196500 |
| C | 4.46500800  | 0.56063100  | -1.60377800 |
| C | 5.76962100  | 2.25406000  | -2.70302200 |
| C | 5.51755200  | -0.34407300 | -1.74064200 |
| H | 3.54261600  | 0.24798500  | -1.12029700 |
| C | 6.82453600  | 1.34785000  | -2.84885900 |
| H | 5.89638600  | 3.26380900  | -3.07758500 |
| C | 6.70357900  | 0.04452800  | -2.36893200 |
| H | 5.41651400  | -1.34973500 | -1.34438500 |
| H | 7.74201800  | 1.66788700  | -3.33527400 |
| H | 7.52381500  | -0.65949800 | -2.47570300 |
| C | 3.77041900  | 4.30216800  | -2.14846900 |
| H | 2.92288400  | 4.96509000  | -1.96596700 |
| H | 4.59102300  | 4.60935500  | -1.49213600 |
| H | 4.08242000  | 4.46208500  | -3.18495000 |
| C | -2.07401100 | 3.88117100  | -2.72671900 |
| C | -1.52766200 | 4.90045500  | -3.52010100 |
| C | -3.10430700 | 4.22057900  | -1.83613700 |
| C | -1.98792500 | 6.21624800  | -3.41807400 |
| H | -0.73359200 | 4.66431100  | -4.22208100 |
| C | -3.56930500 | 5.53306200  | -1.73283200 |
| H | -3.55454600 | 3.44331800  | -1.22370900 |
| C | -3.00929700 | 6.53957000  | -2.52307400 |
| H | -1.54615800 | 6.98881800  | -4.04171000 |
| H | -4.36882000 | 5.76847100  | -1.03572300 |
| H | -3.36626200 | 7.56233000  | -2.44334000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.64697700 | 1.72584300  | -3.83941300 |
| H | -3.65832300 | 1.78097700  | -3.43164500 |
| H | -2.66521500 | 2.21991300  | -4.81602200 |
| H | -2.39746800 | 0.67133200  | -3.98176200 |
| C | -1.62010200 | 1.70855600  | 6.57691900  |
| C | 1.75806400  | 1.73281600  | -6.53747700 |
| H | 2.73944200  | 2.12612500  | -6.81802000 |
| H | 1.76643600  | 0.65546800  | -6.74533100 |
| H | 1.00815700  | 2.18211600  | -7.19636400 |
| H | -2.50602700 | 2.26950300  | 6.88918600  |
| H | -1.83978200 | 0.64428500  | 6.72901000  |
| H | -0.79576200 | 1.96866300  | 7.24796800  |
| C | -0.10521900 | -1.90394900 | -0.01898300 |
| C | 0.21571200  | -4.20151900 | 0.57469700  |
| C | -0.64820000 | -4.14374100 | -0.67012400 |
| H | 1.22229600  | -4.56197900 | 0.34316500  |
| H | -0.21376300 | -4.82016300 | 1.36413600  |
| H | -0.27735300 | -4.77919600 | -1.47575700 |
| H | -1.68461900 | -4.41328800 | -0.44667800 |
| N | -0.55520800 | -2.71104100 | -1.04453100 |
| N | 0.25863400  | -2.77728500 | 0.98627800  |
| C | -0.86788900 | -2.35032100 | -2.40174300 |
| C | 0.18623400  | -2.15197100 | -3.33353500 |
| C | -2.20535600 | -2.37709700 | -2.85822000 |
| C | -0.13758500 | -1.89020400 | -4.66753700 |
| C | -2.47016400 | -2.12242000 | -4.21118200 |
| C | -1.45786200 | -1.86063200 | -5.12959300 |
| H | 0.66030100  | -1.72632400 | -5.38324000 |
| H | -3.50349300 | -2.13149000 | -4.54825100 |
| C | 0.61616700  | -2.48318200 | 2.34834400  |
| C | 1.94875100  | -2.64923600 | 2.78943300  |
| C | -0.40626300 | -2.21049200 | 3.29625900  |
| C | 2.24767400  | -2.45832900 | 4.14547900  |
| C | -0.04777800 | -2.01482300 | 4.63295500  |
| C | 1.27286000  | -2.12503100 | 5.08138800  |
| H | 3.27791700  | -2.57632600 | 4.47142100  |
| H | -0.82000200 | -1.79266800 | 5.36100500  |
| C | -3.38792100 | -2.78601700 | -1.97371900 |
| C | 1.65060700  | -2.31386000 | -2.92760600 |
| C | 3.08103300  | -3.14258000 | 1.88245800  |
| C | -1.88255800 | -2.22461600 | 2.90149100  |
| H | -1.96426800 | -1.72983600 | 1.92784600  |
| H | -3.05666700 | -2.72151700 | -0.93274800 |
| H | 1.76608000  | -1.86114200 | -1.93708000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.74840700  | -3.02429700 | 0.84679700  |
| C | -4.57911600 | -1.83386600 | -2.11958700 |
| C | -5.80514200 | -2.22295200 | -2.67821600 |
| C | -4.45029200 | -0.50962600 | -1.67455700 |
| C | -6.86432900 | -1.31732000 | -2.79614600 |
| H | -5.94963400 | -3.23953900 | -3.02648600 |
| C | -5.50609700 | 0.39461000  | -1.78507600 |
| H | -3.50612900 | -0.18847800 | -1.24103600 |
| C | -6.71959500 | -0.00408900 | -2.35166200 |
| H | -7.80288600 | -1.64533300 | -3.23469800 |
| H | -5.38586000 | 1.40924000  | -1.41783600 |
| H | -7.54205000 | 0.70010100  | -2.43831800 |
| C | -3.76452500 | -4.25432500 | -2.26649100 |
| H | -4.09478700 | -4.37763400 | -3.30242400 |
| H | -2.90687300 | -4.91398100 | -2.12405700 |
| H | -4.56891400 | -4.59525900 | -1.60687200 |
| C | 2.07784000  | -3.78313400 | -2.81794000 |
| C | 1.52691900  | -4.79015100 | -3.62362600 |
| C | 3.12447200  | -4.13260900 | -1.95030700 |
| C | 1.99825900  | -6.10430500 | -3.55563200 |
| H | 0.72163000  | -4.54563700 | -4.30943900 |
| C | 3.60110100  | -5.44311200 | -1.88166600 |
| H | 3.57943500  | -3.36359300 | -1.33093000 |
| C | 3.03582200  | -6.43773600 | -2.68349000 |
| H | 1.55272100  | -6.86736300 | -4.18823500 |
| H | 4.41413800  | -5.68620000 | -1.20304400 |
| H | 3.40191800  | -7.45901400 | -2.63048900 |
| C | 2.63809100  | -1.59566600 | -3.87228700 |
| H | 2.38159400  | -0.53967100 | -3.98834800 |
| H | 3.64813100  | -1.65406500 | -3.46141300 |
| H | 2.66403000  | -2.06406200 | -4.86131300 |
| C | 4.35321800  | -2.30387800 | 2.03703400  |
| C | 4.33522300  | -0.96122200 | 1.63017200  |
| C | 5.54658700  | -2.81373600 | 2.56833500  |
| C | 5.46682400  | -0.15551100 | 1.75170700  |
| H | 3.41741900  | -0.54731200 | 1.21853700  |
| C | 6.68184300  | -2.00696000 | 2.69675200  |
| H | 5.60611200  | -3.84852600 | 2.88683400  |
| C | 6.64732500  | -0.67405800 | 2.29049200  |
| H | 5.43136800  | 0.87590700  | 1.41496600  |
| H | 7.59300300  | -2.42748000 | 3.11361100  |
| H | 7.52878000  | -0.04655800 | 2.38572000  |
| C | 3.32589900  | -4.64513000 | 2.13886600  |
| H | 2.40924400  | -5.22000500 | 1.99635800  |

|          |             |             |             |
|----------|-------------|-------------|-------------|
| H        | 4.08643000  | -5.04405400 | 1.46007400  |
| H        | 3.65704000  | -4.82046300 | 3.16685200  |
| C        | -2.44035600 | -3.64511800 | 2.74769900  |
| C        | -1.99332500 | -4.71658000 | 3.53482000  |
| C        | -3.50243700 | -3.87799600 | 1.86020600  |
| C        | -2.58055500 | -5.98047700 | 3.42961400  |
| H        | -1.17759400 | -4.56257000 | 4.23465900  |
| C        | -4.09472900 | -5.13809300 | 1.75450900  |
| H        | -3.87665900 | -3.05724500 | 1.25328500  |
| C        | -3.63247300 | -6.19805800 | 2.53816700  |
| H        | -2.21423300 | -6.79538800 | 4.04822400  |
| H        | -4.91721000 | -5.29076200 | 1.06109400  |
| H        | -4.08875000 | -7.18039700 | 2.45649200  |
| C        | -2.79379500 | -1.45567100 | 3.88198200  |
| H        | -3.80825500 | -1.40863200 | 3.48073300  |
| H        | -2.85287000 | -1.95602400 | 4.85376300  |
| H        | -2.44250700 | -0.43184800 | 4.03261700  |
| C        | -1.76728400 | -1.55196000 | -6.57513000 |
| C        | 1.62519700  | -1.88563900 | 6.53022200  |
| H        | 2.54505500  | -2.40760200 | 6.80954200  |
| H        | 1.78421300  | -0.81765600 | 6.72522700  |
| H        | 0.82514500  | -2.22029100 | 7.19797200  |
| H        | -2.75019400 | -1.93470400 | -6.86452600 |
| H        | -1.77166200 | -0.46949300 | -6.75422600 |
| H        | -1.01944300 | -1.98640900 | -7.24623200 |
| <b>1</b> |             |             |             |
| C        | -2.72396000 | -0.10330400 | -0.12017000 |
| C        | -2.11648200 | -1.32915200 | 0.14161100  |
| C        | -0.75875200 | -1.41051000 | 0.41858800  |
| C        | 0.03699200  | -0.25691100 | 0.44274900  |
| C        | -0.58516800 | 0.96274000  | 0.17533500  |
| C        | 1.52152600  | -0.31003700 | 0.71934100  |
| H        | 1.75854300  | -1.25382000 | 1.22027500  |
| H        | 1.78716500  | 0.49694700  | 1.40969400  |
| C        | 2.37448400  | -0.18959200 | -0.57044300 |
| H        | 2.07698200  | -0.98264500 | -1.26459300 |
| H        | 2.13364000  | 0.76770400  | -1.05140000 |
| C        | 3.86511800  | -0.26779300 | -0.31344600 |
| C        | 4.58690800  | -1.31386800 | -0.73127800 |
| H        | 4.13276900  | -2.14126000 | -1.27039300 |
| H        | 5.65706200  | -1.37692300 | -0.55228000 |
| C        | -1.94704900 | 1.05134400  | -0.10203700 |
| C        | 4.49151700  | 0.89018000  | 0.42562600  |
| H        | 4.30861100  | 1.83504100  | -0.10207500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.06662700  | 1.00825900  | 1.43002600  |
| H | 5.57169200  | 0.76082900  | 0.53244000  |
| F | -2.87907600 | -2.43678300 | 0.12230500  |
| F | -4.03484100 | -0.02645800 | -0.38581400 |
| F | -2.51283300 | 2.23976800  | -0.35059300 |
| F | 0.13359800  | 2.10473300  | 0.18211600  |
| H | -0.32552000 | -2.38404900 | 0.62090200  |

**IM1**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 7.47206600  | 0.32810000  | -1.55113300 |
| C  | 6.63127100  | -0.76971500 | -1.70659000 |
| C  | 5.38187300  | -0.60357800 | -2.29619600 |
| C  | 4.91634400  | 0.64277300  | -2.71584600 |
| C  | 5.77631700  | 1.73802900  | -2.55247900 |
| H  | 5.46987400  | 2.73011500  | -2.86605400 |
| C  | 3.51505100  | 0.78920000  | -3.25905500 |
| H  | 3.31556800  | 0.00249900  | -3.99477900 |
| H  | 3.43521300  | 1.74802200  | -3.77957400 |
| C  | 2.44463700  | 0.69643900  | -2.13345700 |
| H  | 2.56776600  | -0.26668500 | -1.63089800 |
| H  | 2.65885800  | 1.47303700  | -1.38699400 |
| C  | 1.01468000  | 0.83606000  | -2.62799500 |
| C  | 0.28916600  | -0.29512500 | -3.03344800 |
| H  | 0.74734600  | -1.28467400 | -3.01302900 |
| H  | -0.56789100 | -0.19812700 | -3.69989700 |
| C  | 0.62189300  | 2.22292400  | -3.10331700 |
| Ni | -0.24533800 | 0.18204600  | -1.19878500 |
| C  | -1.25505100 | -0.06553000 | 0.40413000  |
| C  | -2.08907600 | 0.17963300  | 2.61819200  |
| C  | -2.85219500 | -0.95910000 | 1.92363600  |
| H  | -1.61223800 | -0.14703800 | 3.54511300  |
| H  | -2.72524400 | 1.04060700  | 2.84236500  |
| H  | -2.65539300 | -1.93724600 | 2.37248600  |
| H  | -3.93225400 | -0.79290500 | 1.92082500  |
| N  | -2.30811800 | -0.91185300 | 0.54516100  |
| N  | -1.07276100 | 0.54801200  | 1.60249000  |
| C  | -2.81939100 | -1.76768600 | -0.48903200 |
| C  | -2.16045800 | -2.98553000 | -0.79635600 |
| C  | -4.00048600 | -1.40364000 | -1.16379100 |
| C  | -2.70554700 | -3.79788200 | -1.79290100 |
| C  | -4.50549100 | -2.25860400 | -2.15299500 |
| C  | -3.87782200 | -3.45708700 | -2.48207400 |
| H  | -2.20676000 | -4.72655600 | -2.05089400 |
| H  | -5.40487700 | -1.96458300 | -2.68826600 |
| C  | -0.06048700 | 1.53018900  | 1.87472800  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 1. 07888900  | 1. 15975200  | 2. 61685100  |
| C | -0. 22972200 | 2. 86828000  | 1. 43445500  |
| C | 2. 05118500  | 2. 13112400  | 2. 89135500  |
| C | 0. 77285500  | 3. 79362800  | 1. 73347800  |
| C | 1. 92180700  | 3. 44813300  | 2. 45808400  |
| H | 2. 93875700  | 1. 83985600  | 3. 44727400  |
| H | 0. 66448600  | 4. 81957800  | 1. 39728700  |
| C | -4. 76535200 | -0. 11743100 | -0. 84416800 |
| C | -0. 88903200 | -3. 40226900 | -0. 05908700 |
| C | 1. 28229500  | -0. 25672000 | 3. 16363100  |
| C | -1. 47999400 | 3. 29494800  | 0. 66529700  |
| H | -1. 71924500 | 2. 47810300  | -0. 02353300 |
| H | -4. 15301300 | 0. 45837300  | -0. 14433300 |
| H | -0. 31968800 | -2. 48579200 | 0. 12367300  |
| H | 0. 49678700  | -0. 88622200 | 2. 73653200  |
| C | -4. 93202200 | 0. 75977700  | -2. 08922800 |
| C | -6. 17807300 | 1. 05139500  | -2. 65859900 |
| C | -3. 78456600 | 1. 30862900  | -2. 68905000 |
| C | -6. 27787900 | 1. 86284600  | -3. 79428400 |
| H | -7. 08634300 | 0. 65154700  | -2. 22027200 |
| C | -3. 88221100 | 2. 12025600  | -3. 81819300 |
| H | -2. 80546500 | 1. 08763700  | -2. 26651400 |
| C | -5. 13243000 | 2. 40079200  | -4. 37850600 |
| H | -7. 25628100 | 2. 07332900  | -4. 21757600 |
| H | -2. 98153200 | 2. 53486200  | -4. 26326000 |
| H | -5. 20989500 | 3. 03240400  | -5. 25884100 |
| C | -6. 09153200 | -0. 44216700 | -0. 13001200 |
| H | -6. 75862300 | -1. 03717000 | -0. 76144200 |
| H | -5. 90335000 | -1. 02315300 | 0. 77730100  |
| H | -6. 61802500 | 0. 47377000  | 0. 15645400  |
| C | -1. 15918900 | -4. 04406200 | 1. 30553500  |
| C | -2. 30079100 | -4. 81597600 | 1. 56250600  |
| C | -0. 20499100 | -3. 91030800 | 2. 32683500  |
| C | -2. 48636800 | -5. 43019000 | 2. 80409300  |
| H | -3. 05354900 | -4. 93265600 | 0. 78870000  |
| C | -0. 38704000 | -4. 52274700 | 3. 56788200  |
| H | 0. 69426400  | -3. 32713100 | 2. 14312500  |
| C | -1. 53199600 | -5. 28508100 | 3. 81261900  |
| H | -3. 38020300 | -6. 02206700 | 2. 98187800  |
| H | 0. 36513100  | -4. 40321000 | 4. 34294000  |
| H | -1. 67814400 | -5. 76040100 | 4. 77834400  |
| C | 0. 03295200  | -4. 32280600 | -0. 88880500 |
| H | 0. 24577000  | -3. 88441100 | -1. 86904000 |
| H | 0. 98134100  | -4. 46097900 | -0. 36170600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.40190300 | -5.31570700 | -1.03934100 |
| C | 2.61122300  | -0.85759100 | 2.69660900  |
| C | 3.71176400  | -1.03986100 | 3.54450500  |
| C | 2.73986500  | -1.24819700 | 1.35302700  |
| C | 4.90799800  | -1.58382800 | 3.06357200  |
| H | 3.64693100  | -0.76142500 | 4.59129900  |
| C | 3.92724700  | -1.79988000 | 0.87312300  |
| H | 1.89999600  | -1.10211900 | 0.67612700  |
| C | 5.02180200  | -1.96470500 | 1.72724600  |
| H | 5.74890500  | -1.70956500 | 3.74020300  |
| H | 4.00468700  | -2.09524700 | -0.16798300 |
| H | 5.95013400  | -2.38022100 | 1.34609900  |
| C | 1.10220800  | -0.27308500 | 4.69477400  |
| H | 0.10863400  | 0.09358400  | 4.96769700  |
| H | 1.21222200  | -1.28778600 | 5.09035100  |
| H | 1.82986500  | 0.37102100  | 5.19752700  |
| C | -2.70311000 | 3.50071400  | 1.56374100  |
| C | -2.59832500 | 3.97907200  | 2.87738600  |
| C | -3.98514600 | 3.26480400  | 1.04292300  |
| C | -3.74022800 | 4.20549900  | 3.65052800  |
| H | -1.61694300 | 4.16929600  | 3.30164500  |
| C | -5.12782700 | 3.49055000  | 1.81243100  |
| H | -4.08713000 | 2.90730100  | 0.02102800  |
| C | -5.00930700 | 3.96034900  | 3.12282300  |
| H | -3.63574500 | 4.57319200  | 4.66773500  |
| H | -6.10961700 | 3.29910700  | 1.38800300  |
| H | -5.89629600 | 4.13391200  | 3.72532600  |
| C | -1.27590800 | 4.55398400  | -0.20555400 |
| H | -2.15925200 | 4.71156400  | -0.83088100 |
| H | -1.14273400 | 5.45523000  | 0.40085200  |
| H | -0.40729200 | 4.44572000  | -0.86214100 |
| C | -4.43805800 | -4.37361700 | -3.54428400 |
| C | 2.99052000  | 4.47770500  | 2.74076600  |
| H | 3.56258100  | 4.71219000  | 1.83489600  |
| H | 2.55503500  | 5.41730800  | 3.09691200  |
| H | 3.69791500  | 4.12289000  | 3.49512200  |
| H | -5.27203000 | -3.90679000 | -4.07516700 |
| H | -3.67402800 | -4.64131900 | -4.28212700 |
| H | -4.80309000 | -5.31069500 | -3.10698400 |
| C | 7.03231600  | 1.57711200  | -1.98334100 |
| F | 4.60108000  | -1.70056600 | -2.42893000 |
| F | 7.02189600  | -1.97917500 | -1.27710600 |
| F | 8.67917900  | 0.17777600  | -0.98878100 |
| F | 7.85499500  | 2.63054200  | -1.83092700 |



|            |              |              |              |
|------------|--------------|--------------|--------------|
| H          | 1. 20560700  | 2. 53206100  | -3. 98367600 |
| H          | -0. 43461300 | 2. 26824100  | -3. 38212300 |
| H          | 0. 79952900  | 2. 97574000  | -2. 32561100 |
| <b>IM2</b> |              |              |              |
| C          | 4. 54366000  | 1. 97066800  | -0. 50592900 |
| C          | 3. 38201400  | 2. 45940300  | -1. 09369300 |
| C          | 2. 75471200  | 1. 78125400  | -2. 12872500 |
| C          | 3. 28831100  | 0. 58627500  | -2. 62913000 |
| C          | 4. 45719400  | 0. 11230300  | -2. 03100800 |
| C          | 2. 70969000  | -0. 16756700 | -3. 80913500 |
| H          | 2. 70656300  | -1. 23684300 | -3. 57590300 |
| H          | 3. 42054700  | -0. 05922900 | -4. 63986400 |
| C          | 1. 32510600  | 0. 26806200  | -4. 30214700 |
| H          | 1. 30192200  | 1. 36138700  | -4. 41643800 |
| H          | 1. 22819900  | -0. 11129200 | -5. 33326200 |
| C          | 0. 08703100  | -0. 19489200 | -3. 53351900 |
| C          | 0. 04814900  | -1. 41914800 | -2. 83264000 |
| H          | 0. 94082900  | -2. 02551700 | -2. 69411600 |
| H          | -0. 88234500 | -1. 98404300 | -2. 77110300 |
| Ni         | -0. 04360000 | 0. 01867400  | -1. 51716600 |
| H          | 1. 84609400  | 2. 20140600  | -2. 54005300 |
| C          | -0. 67475300 | -0. 16249300 | 0. 29695400  |
| C          | -2. 33700200 | -0. 33343000 | 1. 99347900  |
| C          | -1. 03072700 | -0. 92193200 | 2. 51965900  |
| H          | -2. 57159900 | 0. 62710700  | 2. 46856100  |
| H          | -3. 18939300 | -1. 00307200 | 2. 11276000  |
| H          | -0. 74021400 | -0. 52417000 | 3. 49164400  |
| H          | -1. 07248500 | -2. 01700600 | 2. 58268700  |
| N          | -0. 06752900 | -0. 51434900 | 1. 46497500  |
| N          | -2. 01380500 | -0. 12956900 | 0. 56152500  |
| C          | 1. 34406900  | -0. 62620100 | 1. 70735000  |
| C          | 2. 02899300  | 0. 48022100  | 2. 27357600  |
| C          | 2. 00790800  | -1. 85401400 | 1. 50238300  |
| C          | 3. 38698700  | 0. 33806700  | 2. 57182500  |
| C          | 3. 36241600  | -1. 94743600 | 1. 85592200  |
| C          | 4. 07333600  | -0. 86577300 | 2. 37292700  |
| H          | 3. 93315200  | 1. 18198700  | 2. 97962600  |
| H          | 3. 87608800  | -2. 89542800 | 1. 72283800  |
| C          | -3. 03839800 | 0. 24085200  | -0. 37360600 |
| C          | -3. 38053300 | 1. 59493600  | -0. 55411400 |
| C          | -3. 74969200 | -0. 77803200 | -1. 05797200 |
| C          | -4. 42772000 | 1. 91612900  | -1. 42933500 |
| C          | -4. 78349000 | -0. 40227500 | -1. 91830200 |
| C          | -5. 14192900 | 0. 93865400  | -2. 11723400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.67944900 | 2.96305700  | -1.57942900 |
| H | -5.32970400 | -1.16823800 | -2.45998800 |
| C | 1.27897800  | -3.09862200 | 1.00655800  |
| C | 1.30135000  | 1.78714400  | 2.59704000  |
| C | -2.67834200 | 2.73101600  | 0.19282900  |
| C | -3.38453500 | -2.24906100 | -0.86560900 |
| H | -2.30057600 | -2.28210300 | -0.72233500 |
| H | 0.23815200  | -2.81646400 | 0.82570300  |
| H | 0.56714200  | 1.95127700  | 1.80207400  |
| H | -1.80168300 | 2.30253300  | 0.68824200  |
| C | 1.78331500  | -3.69990200 | -0.31505800 |
| C | 1.02587500  | -4.73224300 | -0.89658900 |
| C | 2.94056400  | -3.28672000 | -0.98654200 |
| C | 1.41673200  | -5.34102400 | -2.08813200 |
| H | 0.11071600  | -5.06269400 | -0.41144600 |
| C | 3.33839800  | -3.89488600 | -2.18252500 |
| H | 3.54050800  | -2.47742900 | -0.58949400 |
| C | 2.58331000  | -4.92730000 | -2.73708500 |
| H | 0.80861700  | -6.13593000 | -2.51118700 |
| H | 4.23939000  | -3.54567800 | -2.67732500 |
| H | 2.89314500  | -5.39949400 | -3.66490300 |
| C | 1.27246400  | -4.17545200 | 2.12312700  |
| H | 2.28552800  | -4.52868400 | 2.33770800  |
| H | 0.85367400  | -3.76850300 | 3.04895000  |
| H | 0.67321000  | -5.04168100 | 1.82945100  |
| C | 0.52618600  | 1.73435900  | 3.91933800  |
| C | 1.01384800  | 1.05440500  | 5.04465300  |
| C | -0.67212100 | 2.45277000  | 4.04759600  |
| C | 0.31917400  | 1.08365900  | 6.25654700  |
| H | 1.93978400  | 0.49184000  | 4.97102700  |
| C | -1.36910400 | 2.48509300  | 5.25705300  |
| H | -1.05917900 | 2.99936200  | 3.19102700  |
| C | -0.87600600 | 1.79698200  | 6.36798000  |
| H | 0.71403700  | 0.54633900  | 7.11448200  |
| H | -2.29679800 | 3.04600100  | 5.32990500  |
| H | -1.41692600 | 1.81685200  | 7.30963500  |
| C | 2.21899000  | 3.02999300  | 2.62655700  |
| H | 2.80334100  | 3.12766000  | 1.71080600  |
| H | 1.60424100  | 3.92832700  | 2.73549400  |
| H | 2.90499800  | 3.00562600  | 3.47875800  |
| C | -2.14768800 | 3.79439600  | -0.77390600 |
| C | -2.54913300 | 5.13506600  | -0.73346000 |
| C | -1.20380700 | 3.41741700  | -1.74453900 |
| C | -2.02618900 | 6.07093900  | -1.63356500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.27334800 | 5.46705300  | 0.00267300  |
| C | -0.68131500 | 4.34563000  | -2.64256600 |
| H | -0.88965500 | 2.37469500  | -1.80210800 |
| C | -1.09142200 | 5.68196800  | -2.59078300 |
| H | -2.35489600 | 7.10524700  | -1.58093800 |
| H | 0.04245900  | 4.02835500  | -3.38866700 |
| H | -0.68592200 | 6.40752500  | -3.28997800 |
| C | -3.59929100 | 3.29269200  | 1.29316500  |
| H | -3.90659500 | 2.49447400  | 1.97417200  |
| H | -3.09064000 | 4.06354400  | 1.88120100  |
| H | -4.50993000 | 3.73126600  | 0.87317500  |
| C | -4.01886400 | -2.87992200 | 0.37794700  |
| C | -5.32531200 | -2.57636100 | 0.78683300  |
| C | -3.30426400 | -3.84432600 | 1.10483100  |
| C | -5.89746400 | -3.21408700 | 1.89034800  |
| H | -5.89653400 | -1.82940800 | 0.24348200  |
| C | -3.87240500 | -4.48446300 | 2.20790300  |
| H | -2.29167100 | -4.09751500 | 0.79927500  |
| C | -5.17376300 | -4.17012300 | 2.60608100  |
| H | -6.91041800 | -2.96104600 | 2.19131600  |
| H | -3.29794500 | -5.22582900 | 2.75650600  |
| H | -5.61802300 | -4.66374600 | 3.46556300  |
| C | -3.69760400 | -3.12914200 | -2.09604900 |
| H | -3.27977500 | -4.12901600 | -1.94662500 |
| H | -4.77418200 | -3.24871800 | -2.25174500 |
| H | -3.26098100 | -2.70713700 | -3.00656400 |
| C | 5.54556600  | -0.97592400 | 2.69139900  |
| C | -6.26043600 | 1.30190900  | -3.06543800 |
| H | -6.50097400 | 2.36685600  | -3.00933400 |
| H | -5.98827300 | 1.07577500  | -4.10320100 |
| H | -7.17165100 | 0.73586300  | -2.84290300 |
| H | 5.84663100  | -2.01721400 | 2.83726300  |
| H | 6.14522900  | -0.56812700 | 1.87031200  |
| H | 5.80295800  | -0.41459200 | 3.59503800  |
| C | 5.08351100  | 0.78203000  | -0.98454200 |
| C | -1.19004400 | 0.32987200  | -4.17635500 |
| H | -1.23258000 | 1.42636700  | -4.16940600 |
| H | -1.25595600 | 0.02083700  | -5.23320300 |
| H | -2.08421100 | -0.04005000 | -3.66711600 |
| F | 2.86039600  | 3.60911500  | -0.61929000 |
| F | 5.12582300  | 2.61438400  | 0.51801900  |
| F | 6.20552600  | 0.28698700  | -0.43666400 |
| F | 5.02498700  | -1.03566800 | -2.46466000 |

**TS1(R)**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.10637200  | 2.19744800  | -0.09561200 |
| C  | 2.74940100  | 1.93677700  | -0.26051200 |
| C  | 2.26256200  | 1.00851600  | -1.17056600 |
| C  | 3.21062400  | 0.31594100  | -1.97229700 |
| C  | 4.56910200  | 0.57655500  | -1.80625400 |
| C  | 2.73687500  | -0.66781800 | -3.02414600 |
| H  | 2.26327900  | -1.52490600 | -2.53254100 |
| H  | 3.59707000  | -1.05651400 | -3.57542300 |
| C  | 1.73448700  | -0.05859100 | -4.03887400 |
| H  | 2.24078300  | 0.75957900  | -4.56556800 |
| H  | 1.50630800  | -0.82169100 | -4.79295500 |
| C  | 0.41672100  | 0.47675600  | -3.44936100 |
| C  | -0.57000800 | -0.41778500 | -2.92814400 |
| H  | -0.39429900 | -1.49127800 | -2.94325100 |
| H  | -1.61326100 | -0.12132700 | -2.99810500 |
| Ni | 0.38026500  | 0.32538200  | -1.34056200 |
| H  | 1.19706300  | 1.19241000  | -2.24349500 |
| C  | -0.47258400 | -0.24991600 | 0.25252500  |
| C  | -2.02103000 | -0.15210700 | 2.04726600  |
| C  | -1.11605900 | -1.36368700 | 2.24431600  |
| H  | -1.78852100 | 0.64058800  | 2.76650200  |
| H  | -3.08258800 | -0.39271300 | 2.11211800  |
| H  | -0.66289800 | -1.40172600 | 3.23454900  |
| H  | -1.64281900 | -2.30860900 | 2.05979300  |
| N  | -0.08418200 | -1.14558100 | 1.19950700  |
| N  | -1.65641900 | 0.28152300  | 0.67597900  |
| C  | 1.08422800  | -1.98374700 | 1.19902100  |
| C  | 2.22902200  | -1.56495700 | 1.92369700  |
| C  | 1.03458300  | -3.26660600 | 0.61300900  |
| C  | 3.30756100  | -2.44730800 | 2.02824000  |
| C  | 2.13904300  | -4.11755500 | 0.77302700  |
| C  | 3.28298200  | -3.72930700 | 1.46689500  |
| H  | 4.19593900  | -2.13779900 | 2.56887600  |
| H  | 2.09961900  | -5.11600600 | 0.34668800  |
| C  | -2.52956000 | 1.14608000  | -0.07532700 |
| C  | -2.40645400 | 2.54933000  | 0.00443700  |
| C  | -3.57717600 | 0.56290200  | -0.83602100 |
| C  | -3.32231700 | 3.34609800  | -0.69747000 |
| C  | -4.45085500 | 1.40681300  | -1.52688400 |
| C  | -4.34356600 | 2.80131400  | -1.47175700 |
| H  | -3.22081300 | 4.42603500  | -0.63819300 |
| H  | -5.24500000 | 0.97216300  | -2.12565400 |
| C  | -0.20143200 | -3.78782100 | -0.11266000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.29445500  | -0.18314400 | 2.57533100  |
| C | -1.36075900 | 3.24701400  | 0.87991200  |
| C | -3.78091200 | -0.95079700 | -0.88872400 |
| H | -2.79469800 | -1.40920400 | -0.77756600 |
| H | -0.96418600 | -3.00633700 | -0.05842700 |
| H | 1.79959500  | 0.51264600  | 1.89444200  |
| H | -0.54044900 | 2.54147500  | 1.04254700  |
| C | -0.02359600 | -4.09118400 | -1.60903900 |
| C | -1.17897400 | -4.34192500 | -2.37070500 |
| C | 1.21171600  | -4.14157300 | -2.26741100 |
| C | -1.10527100 | -4.64037700 | -3.73042200 |
| H | -2.15447400 | -4.29998600 | -1.89285900 |
| C | 1.29132200  | -4.44157400 | -3.63210200 |
| H | 2.12564300  | -3.94105700 | -1.72094200 |
| C | 0.13630500  | -4.69484500 | -4.37000700 |
| H | -2.01713600 | -4.82755600 | -4.29064600 |
| H | 2.26450600  | -4.47491500 | -4.11409600 |
| H | 0.19926600  | -4.92856500 | -5.42876900 |
| C | -0.76849200 | -5.03018700 | 0.62241300  |
| H | -0.07094000 | -5.87149900 | 0.57530800  |
| H | -0.95569200 | -4.80472600 | 1.67698000  |
| H | -1.70946300 | -5.35625400 | 0.16996300  |
| C | 1.55338800  | -0.09102600 | 3.91172000  |
| C | 1.58411200  | -1.12600700 | 4.85741500  |
| C | 0.87919900  | 1.09388900  | 4.24330500  |
| C | 0.95028700  | -0.98412000 | 6.09437100  |
| H | 2.09946400  | -2.05262000 | 4.62088100  |
| C | 0.24643300  | 1.23985700  | 5.47966400  |
| H | 0.85869800  | 1.90983200  | 3.52459900  |
| C | 0.27768700  | 0.19852400  | 6.41012800  |
| H | 0.98222900  | -1.79976800 | 6.81162900  |
| H | -0.27135200 | 2.16577400  | 5.71446600  |
| H | -0.21626900 | 0.30775800  | 7.37131100  |
| C | 3.73825900  | 0.33080400  | 2.77405100  |
| H | 4.33072100  | 0.20698300  | 1.86387300  |
| H | 3.71797700  | 1.39481900  | 3.02409100  |
| H | 4.24599200  | -0.19060000 | 3.59150900  |
| C | -0.75475900 | 4.46862500  | 0.17935000  |
| C | -0.82702300 | 5.76506500  | 0.70412900  |
| C | -0.08484700 | 4.29248600  | -1.04340300 |
| C | -0.25023600 | 6.84967600  | 0.03249600  |
| H | -1.33261800 | 5.94722700  | 1.64602000  |
| C | 0.48968100  | 5.36817600  | -1.71585900 |
| H | -0.01373200 | 3.29538500  | -1.46692700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.40957100  | 6.65744700  | -1.17931500 |
| H | -0.32123300 | 7.84461800  | 0.46358500  |
| H | 1.00334200  | 5.20190200  | -2.65911600 |
| H | 0.85769100  | 7.49823600  | -1.70113500 |
| C | -1.97620500 | 3.58111100  | 2.25453300  |
| H | -2.37922400 | 2.68190900  | 2.72521600  |
| H | -1.22822900 | 4.00924700  | 2.92952800  |
| H | -2.80131300 | 4.29446100  | 2.15907200  |
| C | -4.65730000 | -1.48655300 | 0.25173900  |
| C | -5.73501300 | -0.76091400 | 0.77916500  |
| C | -4.42375900 | -2.77765800 | 0.75100800  |
| C | -6.54915300 | -1.30707100 | 1.77479400  |
| H | -5.93558900 | 0.24206300  | 0.41568600  |
| C | -5.23447000 | -3.32715200 | 1.74561900  |
| H | -3.59750700 | -3.36134700 | 0.35257800  |
| C | -6.30288500 | -2.59144100 | 2.26317900  |
| H | -7.37639900 | -0.72405300 | 2.17020300  |
| H | -5.02941400 | -4.32740300 | 2.11694200  |
| H | -6.93419300 | -3.01362200 | 3.03960100  |
| C | -4.34980700 | -1.45093200 | -2.23670800 |
| H | -4.33746700 | -2.54457100 | -2.25673600 |
| H | -5.38756500 | -1.13802300 | -2.38434700 |
| H | -3.75436500 | -1.08662900 | -3.07897100 |
| C | 4.47159100  | -4.65201300 | 1.59766800  |
| C | -5.29702500 | 3.68114900  | -2.24532300 |
| H | -5.28065700 | 4.70971400  | -1.87480100 |
| H | -5.03131100 | 3.70999700  | -3.30917300 |
| H | -6.32516100 | 3.31044500  | -2.18082000 |
| H | 4.19398000  | -5.69184500 | 1.40385300  |
| H | 5.25925500  | -4.38255000 | 0.88342700  |
| H | 4.91224000  | -4.59618600 | 2.59809600  |
| C | 5.02741200  | 1.51148600  | -0.87940500 |
| C | -0.08208000 | 1.75973800  | -4.11213600 |
| H | 0.66445200  | 2.56127100  | -4.07752700 |
| H | -0.30383300 | 1.56791800  | -5.17013500 |
| H | -0.99779500 | 2.12366700  | -3.63834000 |
| F | 1.90390100  | 2.60332900  | 0.57294800  |
| F | 4.54030800  | 3.06881400  | 0.83489500  |
| F | 6.34390600  | 1.74361500  | -0.73487200 |
| F | 5.50142900  | -0.06462300 | -2.55051900 |

### IM3(R)

|   |            |            |            |
|---|------------|------------|------------|
| C | 0.39658700 | 0.12397200 | 0.55205100 |
| C | 1.72716100 | 0.50750600 | 2.48725200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.30256600  | 0.15301000  | 2.91657300  |
| H | 2.43825400  | -0.29019100 | 2.72647200  |
| H | 2.08466500  | 1.44374600  | 2.91789000  |
| H | 0.25837800  | -0.67425600 | 3.62523900  |
| H | -0.21381600 | 1.01726300  | 3.34396800  |
| N | -0.34265400 | -0.22895100 | 1.62666100  |
| N | 1.56667700  | 0.62669500  | 1.01907200  |
| C | -1.64716600 | -0.84290400 | 1.64818800  |
| C | -1.74724800 | -2.25789500 | 1.63074100  |
| C | -2.80062500 | -0.04611500 | 1.80391500  |
| C | -3.01867100 | -2.83095800 | 1.71950900  |
| C | -4.04756400 | -0.67859500 | 1.90305700  |
| C | -4.18189100 | -2.06327800 | 1.85167300  |
| H | -3.11518800 | -3.91081400 | 1.69003000  |
| H | -4.93561900 | -0.06203600 | 2.01231200  |
| C | 2.59598800  | 1.12496800  | 0.14689800  |
| C | 3.64807200  | 0.27957800  | -0.26691400 |
| C | 2.54901700  | 2.48365100  | -0.26594900 |
| C | 4.62154100  | 0.79987300  | -1.12962300 |
| C | 3.54673100  | 2.94541900  | -1.12582800 |
| C | 4.58643800  | 2.11946900  | -1.57584900 |
| H | 5.42141100  | 0.14772000  | -1.46864900 |
| H | 3.52310800  | 3.97599200  | -1.46363300 |
| C | -2.75124600 | 1.47532400  | 1.95904300  |
| C | -0.50777200 | -3.15082800 | 1.55391500  |
| C | 3.80255600  | -1.15525700 | 0.24936900  |
| C | 1.44904400  | 3.42086700  | 0.23503800  |
| H | 0.51697600  | 2.84719000  | 0.23113900  |
| H | -1.75789700 | 1.80633900  | 1.63403500  |
| H | 0.19126400  | -2.66858200 | 0.86788800  |
| H | 2.85457100  | -1.43802900 | 0.71446800  |
| C | -3.77394000 | 2.19591500  | 1.06855700  |
| C | -4.49532300 | 3.31475000  | 1.50885100  |
| C | -3.99046200 | 1.75439800  | -0.24657000 |
| C | -5.40171500 | 3.96672400  | 0.66631600  |
| H | -4.36236400 | 3.69060600  | 2.51716900  |
| C | -4.89869100 | 2.39652000  | -1.08853800 |
| H | -3.45032300 | 0.88761500  | -0.61262200 |
| C | -5.61069800 | 3.50974400  | -0.63411700 |
| H | -5.94817900 | 4.83017300  | 1.03587400  |
| H | -5.04855800 | 2.01856400  | -2.09551000 |
| H | -6.32071600 | 4.01092000  | -1.28569300 |
| C | -2.90222300 | 1.84124300  | 3.45372400  |
| H | -3.92055100 | 1.64281400  | 3.80255400  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -2. 22353100 | 1. 24714800  | 4. 06987800  |
| H | -2. 67879400 | 2. 89677200  | 3. 63580300  |
| C | 0. 21153100  | -3. 30292600 | 2. 89756100  |
| C | -0. 47673500 | -3. 36493200 | 4. 11786700  |
| C | 1. 60656800  | -3. 45626100 | 2. 91618700  |
| C | 0. 20950700  | -3. 56297600 | 5. 31895700  |
| H | -1. 55663400 | -3. 25024100 | 4. 13025800  |
| C | 2. 29589500  | -3. 65575500 | 4. 11385900  |
| H | 2. 15595200  | -3. 43152400 | 1. 97788600  |
| C | 1. 59842700  | -3. 70713700 | 5. 32303500  |
| H | -0. 34430900 | -3. 60463700 | 6. 25294300  |
| H | 3. 37634000  | -3. 77034100 | 4. 10171900  |
| H | 2. 13114700  | -3. 85881400 | 6. 25734600  |
| C | -0. 79496200 | -4. 55403300 | 0. 97270300  |
| H | -1. 32679600 | -4. 48138200 | 0. 02165900  |
| H | 0. 15088900  | -5. 07601300 | 0. 80013300  |
| H | -1. 38093200 | -5. 16832900 | 1. 66336200  |
| C | 4. 04659200  | -2. 16459300 | -0. 87532500 |
| C | 2. 95017000  | -2. 65406500 | -1. 60298700 |
| C | 5. 32509300  | -2. 62905600 | -1. 21495200 |
| C | 3. 12559600  | -3. 56840100 | -2. 64202500 |
| H | 1. 94646500  | -2. 31834200 | -1. 35783100 |
| C | 5. 50440900  | -3. 54333300 | -2. 25760600 |
| H | 6. 19523000  | -2. 28786400 | -0. 66324400 |
| C | 4. 40648200  | -4. 01552100 | -2. 97674900 |
| H | 2. 25913400  | -3. 93438900 | -3. 18584800 |
| H | 6. 50544000  | -3. 88848700 | -2. 50133900 |
| H | 4. 54518700  | -4. 72855200 | -3. 78430900 |
| C | 4. 88749400  | -1. 19635500 | 1. 34755800  |
| H | 4. 62423300  | -0. 53279900 | 2. 17588900  |
| H | 5. 00244800  | -2. 21075200 | 1. 74224200  |
| H | 5. 85851200  | -0. 86468100 | 0. 96835800  |
| C | 1. 67650600  | 3. 88865000  | 1. 67588200  |
| C | 2. 95549200  | 4. 17933800  | 2. 17141000  |
| C | 0. 57415400  | 4. 09881100  | 2. 51799000  |
| C | 3. 12771300  | 4. 65606600  | 3. 47341600  |
| H | 3. 82387000  | 4. 02491900  | 1. 53753400  |
| C | 0. 74225900  | 4. 57532100  | 3. 81955700  |
| H | -0. 42704400 | 3. 89371400  | 2. 14607100  |
| C | 2. 02256400  | 4. 85345800  | 4. 30376800  |
| H | 4. 12805900  | 4. 87184500  | 3. 83846300  |
| H | -0. 12604800 | 4. 72733800  | 4. 45469800  |
| H | 2. 15708100  | 5. 22058900  | 5. 31704600  |
| C | 1. 21596100  | 4. 65188000  | -0. 66719200 |



|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 0.33378700  | 5.19589200  | -0.31813200 |
| H  | 2.05976100  | 5.34789800  | -0.63401200 |
| H  | 1.04699100  | 4.35849700  | -1.70750400 |
| C  | -5.53918000 | -2.72192400 | 1.91672600  |
| C  | 5.62942000  | 2.65170000  | -2.52933800 |
| H  | 6.49994300  | 1.99237500  | -2.57876800 |
| H  | 5.22265100  | 2.74015500  | -3.54379100 |
| H  | 5.97016300  | 3.64846600  | -2.23106900 |
| H  | -5.90991300 | -2.95406900 | 0.91078900  |
| H  | -5.50055600 | -3.66440200 | 2.47174800  |
| H  | -6.27667700 | -2.07156600 | 2.39536700  |
| C  | -2.65293000 | -2.46765100 | -2.41298500 |
| C  | -1.46046600 | -1.85478100 | -2.04906500 |
| C  | -1.19154900 | -0.50611100 | -2.25076300 |
| C  | -2.15298900 | 0.25507900  | -2.95172800 |
| C  | -3.35558300 | -0.36544800 | -3.30960500 |
| C  | -1.97548700 | 1.70839400  | -3.37026200 |
| H  | -2.52709700 | 1.84105500  | -4.30745300 |
| H  | -2.48011100 | 2.35892100  | -2.64392100 |
| C  | -0.53712200 | 2.21172000  | -3.58365100 |
| H  | -0.08442900 | 2.48791800  | -2.62281500 |
| H  | -0.60864500 | 3.13920800  | -4.16760300 |
| C  | 0.39269600  | 1.19674500  | -4.28615900 |
| C  | 1.07383000  | 0.29258300  | -3.25219700 |
| H  | 1.36348100  | -0.67535800 | -3.67857500 |
| H  | 1.99578300  | 0.78793400  | -2.87644300 |
| Ni | 0.39429700  | 0.11040500  | -1.48260000 |
| F  | -2.87324800 | -3.77466100 | -2.16445700 |
| F  | -0.52490400 | -2.65818400 | -1.46016100 |
| F  | -4.32640700 | 0.34500500  | -3.94392200 |
| C  | -3.62689900 | -1.70415600 | -3.04606900 |
| F  | -4.79951000 | -2.25707300 | -3.40884000 |
| C  | 1.42520600  | 1.90613600  | -5.18048300 |
| H  | -0.23008700 | 0.57170100  | -4.94206300 |
| H  | 2.04564400  | 2.59197900  | -4.58946900 |
| H  | 0.93944500  | 2.49224500  | -5.97039600 |
| H  | 2.09590300  | 1.18422200  | -5.66015300 |

**TS2(R)**

|   |            |            |            |
|---|------------|------------|------------|
| C | 0.44149300 | 0.33273800 | 0.50862900 |
| C | 1.78693200 | 1.30948200 | 2.21414100 |
| C | 0.42360900 | 0.93402200 | 2.80552600 |
| H | 2.59618900 | 0.70041900 | 2.63014600 |
| H | 2.03585900 | 2.36314200 | 2.35219500 |
| H | 0.49957800 | 0.26989900 | 3.66787300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.14927200 | 1.81987600  | 3.09250500  |
| N | -0.24519800 | 0.23790900  | 1.67403100  |
| N | 1.59551000  | 1.00130500  | 0.77773400  |
| C | -1.51818900 | -0.40301500 | 1.88391900  |
| C | -1.57199500 | -1.80402900 | 2.10667100  |
| C | -2.69020200 | 0.37587400  | 1.96363900  |
| C | -2.81321900 | -2.38347300 | 2.37902700  |
| C | -3.90603900 | -0.25880500 | 2.25568900  |
| C | -3.99286500 | -1.63235000 | 2.46023500  |
| H | -2.87276800 | -3.45441500 | 2.53982400  |
| H | -4.80866100 | 0.34440200  | 2.30569200  |
| C | 2.60458400  | 1.30374400  | -0.20126300 |
| C | 3.72708200  | 0.46270400  | -0.33905600 |
| C | 2.47658200  | 2.47368500  | -0.99314300 |
| C | 4.69678900  | 0.78685200  | -1.29745700 |
| C | 3.47357100  | 2.74808800  | -1.93209300 |
| C | 4.58879800  | 1.91639100  | -2.10529000 |
| H | 5.55237600  | 0.12756500  | -1.41877100 |
| H | 3.39002200  | 3.63414800  | -2.55259000 |
| C | -2.69307600 | 1.89587200  | 1.79936700  |
| C | -0.31032500 | -2.66621100 | 2.07638300  |
| C | 3.95141500  | -0.76497600 | 0.54855100  |
| C | 1.28448000  | 3.41496600  | -0.81656800 |
| H | 0.40063200  | 2.78225600  | -0.68480800 |
| H | -1.71456600 | 2.18370100  | 1.39904700  |
| H | 0.29574700  | -2.31092200 | 1.23825300  |
| H | 3.04078000  | -0.91442200 | 1.13311700  |
| C | -3.74556200 | 2.37211600  | 0.78734400  |
| C | -4.48935600 | 3.54546200  | 0.97817700  |
| C | -3.97253800 | 1.63834100  | -0.38876800 |
| C | -5.42796300 | 3.96821000  | 0.03116800  |
| H | -4.35051800 | 4.14231900  | 1.87264500  |
| C | -4.91521300 | 2.05012200  | -1.33114600 |
| H | -3.41600300 | 0.72231800  | -0.55945500 |
| C | -5.64924300 | 3.22131900  | -1.12486300 |
| H | -5.99132900 | 4.88044000  | 0.20784500  |
| H | -5.07928200 | 1.44509000  | -2.21781400 |
| H | -6.38642500 | 3.54304300  | -1.85488400 |
| C | -2.84474000 | 2.56855900  | 3.18284600  |
| H | -3.85351900 | 2.42341100  | 3.58215600  |
| H | -2.14240500 | 2.13788500  | 3.90063800  |
| H | -2.64852200 | 3.64366700  | 3.13200900  |
| C | 0.54103700  | -2.53567100 | 3.34347700  |
| C | -0.02236500 | -2.31097200 | 4.60764800  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 1. 93001700  | -2. 72152900 | 3. 26152400  |
| C | 0. 77873400  | -2. 26013800 | 5. 75195100  |
| H | -1. 09535200 | -2. 17005200 | 4. 69832500  |
| C | 2. 73331800  | -2. 67254100 | 4. 40229800  |
| H | 2. 38361700  | -2. 92059000 | 2. 29354500  |
| C | 2. 16013100  | -2. 43731600 | 5. 65439800  |
| H | 0. 31997900  | -2. 08206500 | 6. 72081000  |
| H | 3. 80623400  | -2. 81941000 | 4. 31254200  |
| H | 2. 78259600  | -2. 39577200 | 6. 54357200  |
| C | -0. 58664100 | -4. 16396200 | 1. 81423900  |
| H | -1. 19641600 | -4. 30705100 | 0. 91960000  |
| H | 0. 36330300  | -4. 68523000 | 1. 66527400  |
| H | -1. 08615900 | -4. 63902000 | 2. 66438700  |
| C | 4. 14389100  | -2. 04474900 | -0. 27025600 |
| C | 3. 01667000  | -2. 66082100 | -0. 83849700 |
| C | 5. 39504800  | -2. 64189600 | -0. 47529000 |
| C | 3. 13298600  | -3. 83095200 | -1. 58801100 |
| H | 2. 03442500  | -2. 21563200 | -0. 69808000 |
| C | 5. 51655000  | -3. 81257900 | -1. 23117700 |
| H | 6. 28775400  | -2. 20423300 | -0. 04009900 |
| C | 4. 38790800  | -4. 41230600 | -1. 79009300 |
| H | 2. 23950500  | -4. 28699800 | -2. 00510400 |
| H | 6. 49752300  | -4. 25703600 | -1. 37570200 |
| H | 4. 48312800  | -5. 32488400 | -2. 37152100 |
| C | 5. 09629600  | -0. 49456000 | 1. 54588500  |
| H | 4. 86486700  | 0. 37671900  | 2. 16530800  |
| H | 5. 24930300  | -1. 35407500 | 2. 20601600  |
| H | 6. 04077900  | -0. 28350900 | 1. 03552500  |
| C | 1. 39219800  | 4. 29758500  | 0. 43075800  |
| C | 2. 61993300  | 4. 79545100  | 0. 88949600  |
| C | 0. 22448900  | 4. 68601300  | 1. 10540600  |
| C | 2. 67943800  | 5. 64885800  | 1. 99441500  |
| H | 3. 53709900  | 4. 50917800  | 0. 38309000  |
| C | 0. 28004900  | 5. 53916100  | 2. 20915800  |
| H | -0. 73920300 | 4. 32393200  | 0. 75464300  |
| C | 1. 51060300  | 6. 02252800  | 2. 66048600  |
| H | 3. 64209500  | 6. 02086900  | 2. 33437600  |
| H | -0. 63731300 | 5. 82580900  | 2. 71605300  |
| H | 1. 55744500  | 6. 68359700  | 3. 52100000  |
| C | 1. 00826100  | 4. 30969700  | -2. 04428400 |
| H | 0. 07096800  | 4. 85322400  | -1. 89535000 |
| H | 1. 79557600  | 5. 05545900  | -2. 19155600 |
| H | 0. 91718500  | 3. 71568800  | -2. 95869900 |
| C | -5. 31577600 | -2. 30420700 | 2. 74206600  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 5.63069300  | 2.23644500  | -3.15116200 |
| H  | 6.55087700  | 1.66998800  | -2.98488200 |
| H  | 5.26805300  | 1.99030100  | -4.15648400 |
| H  | 5.88094900  | 3.30236700  | -3.15198300 |
| H  | -5.67892600 | -2.84316900 | 1.85866200  |
| H  | -5.22746100 | -3.03681300 | 3.55104500  |
| H  | -6.08184600 | -1.57630400 | 3.02272700  |
| C  | -2.59552300 | -3.24494200 | -1.83484100 |
| C  | -1.38125400 | -2.58266500 | -1.75670800 |
| C  | -1.19353400 | -1.26385700 | -2.19468900 |
| C  | -2.28218100 | -0.64381900 | -2.86249800 |
| C  | -3.49835700 | -1.32304700 | -2.93723400 |
| C  | -2.16116100 | 0.70422500  | -3.55009700 |
| H  | -2.80383100 | 0.68153900  | -4.43699800 |
| H  | -2.57053500 | 1.49436300  | -2.90853700 |
| C  | -0.72801700 | 1.07302200  | -3.97476000 |
| H  | -0.20529300 | 1.57414700  | -3.14990600 |
| H  | -0.78585900 | 1.79588100  | -4.79775200 |
| C  | 0.10464200  | -0.15199700 | -4.39075400 |
| C  | 0.51775900  | -0.94128000 | -3.14263300 |
| H  | 0.73743000  | -1.98926900 | -3.35181500 |
| H  | 1.45619400  | -0.49858500 | -2.72842500 |
| Ni | 0.14586000  | -0.34092900 | -1.27707600 |
| F  | -2.74003200 | -4.48633100 | -1.33026700 |
| F  | -0.34080700 | -3.26114100 | -1.19400300 |
| F  | -4.56476800 | -0.73302400 | -3.53695000 |
| C  | -3.68199800 | -2.60401500 | -2.42627000 |
| F  | -4.87318000 | -3.22353200 | -2.51531500 |
| C  | 1.33781700  | 0.25191100  | -5.21436000 |
| H  | -0.52468600 | -0.79586000 | -5.02134600 |
| H  | 1.97314700  | 0.94429200  | -4.64902700 |
| H  | 1.04301000  | 0.74864700  | -6.14598900 |
| H  | 1.94591500  | -0.62109500 | -5.47584200 |

IM3(R)

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -0.02564000 | -0.33776000 | 0.73134100 |
| C | 0.47288500  | -0.46300000 | 3.04869300 |
| C | -0.60865200 | -1.50693400 | 2.70906700 |
| H | 1.38058000  | -0.93132300 | 3.43862400 |
| H | 0.13098000  | 0.28795500  | 3.76334000 |
| H | -0.28282400 | -2.52953700 | 2.90232300 |
| H | -1.53823500 | -1.32825000 | 3.25565300 |
| N | -0.81243400 | -1.29825900 | 1.25695100 |
| N | 0.73164700  | 0.16270100  | 1.73317100 |
| C | -1.81862200 | -1.97130400 | 0.49373600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.45194300 | -3.02291200 | -0.37534100 |
| C | -3.14953800 | -1.54898400 | 0.59426400  |
| C | -2.45266900 | -3.63193000 | -1.12748300 |
| C | -4.12160900 | -2.18567300 | -0.18696300 |
| C | -3.79244800 | -3.22388700 | -1.05342800 |
| H | -2.19254200 | -4.43200100 | -1.81112200 |
| H | -5.15012900 | -1.83923300 | -0.13027700 |
| C | 1.69075400  | 1.19998800  | 1.51437600  |
| C | 3.05315600  | 0.87914400  | 1.45373200  |
| C | 1.24911200  | 2.53160600  | 1.33083300  |
| C | 3.97855500  | 1.90230500  | 1.21017600  |
| C | 2.20678200  | 3.51774700  | 1.10555100  |
| C | 3.57734400  | 3.22425400  | 1.03943800  |
| H | 5.03238200  | 1.64869300  | 1.13401600  |
| H | 1.88953900  | 4.54519200  | 0.96401500  |
| C | -3.55642000 | -0.41127300 | 1.51626300  |
| C | 0.00698100  | -3.44229700 | -0.47760700 |
| C | 3.54565100  | -0.55120600 | 1.63304700  |
| C | -0.23605700 | 2.85530100  | 1.38721600  |
| H | -0.74511800 | 2.09880400  | 0.77947900  |
| H | -2.64618700 | -0.02282400 | 1.97857700  |
| H | 0.57413800  | -2.52561700 | -0.66660800 |
| H | 2.66466300  | -1.18991400 | 1.71188200  |
| C | -4.13170500 | 0.76166300  | 0.73128200  |
| C | -5.34774300 | 1.36909400  | 1.05698100  |
| C | -3.36611900 | 1.31043700  | -0.31170900 |
| C | -5.78506500 | 2.50761300  | 0.37163700  |
| H | -5.96099600 | 0.96593300  | 1.85499600  |
| C | -3.79445100 | 2.44949000  | -0.98865900 |
| H | -2.41841900 | 0.84582700  | -0.58022200 |
| C | -5.00856600 | 3.05457800  | -0.64710000 |
| H | -6.73249100 | 2.96498300  | 0.64186000  |
| H | -3.19343700 | 2.85838500  | -1.79127700 |
| H | -5.34417500 | 3.94141300  | -1.17626700 |
| C | -4.45287600 | -0.92355300 | 2.65266400  |
| H | -5.41403900 | -1.28886800 | 2.27823900  |
| H | -3.96185800 | -1.75428400 | 3.16717400  |
| H | -4.64623500 | -0.13720200 | 3.38833000  |
| C | 0.51422000  | -4.02523800 | 0.83340000  |
| C | -0.29092200 | -4.84797200 | 1.63033100  |
| C | 1.81889500  | -3.75129200 | 1.25997300  |
| C | 0.18635700  | -5.35848300 | 2.83919000  |
| H | -1.30562100 | -5.06776500 | 1.31219800  |
| C | 2.29727800  | -4.24989400 | 2.47218100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.46310200  | -3.14266500 | 0.63477400  |
| C | 1.47848100  | -5.05092400 | 3.27163800  |
| H | -0.45531800 | -5.98834400 | 3.44865400  |
| H | 3.30830600  | -4.01182700 | 2.79040100  |
| H | 1.84472200  | -5.43591400 | 4.21858400  |
| C | 0.31468700  | -4.39246200 | -1.64467400 |
| H | 0.00134200  | -3.94973300 | -2.59221500 |
| H | 1.39260800  | -4.57152400 | -1.68758100 |
| H | -0.17794900 | -5.36210100 | -1.52028000 |
| C | 4.29246700  | -1.02712500 | 0.39349000  |
| C | 3.54901100  | -1.30716100 | -0.76291300 |
| C | 5.67946600  | -1.20086300 | 0.35337700  |
| C | 4.17100400  | -1.75754300 | -1.92511600 |
| H | 2.47236400  | -1.15417000 | -0.75394400 |
| C | 6.30870300  | -1.64296700 | -0.81439500 |
| H | 6.27940400  | -0.99873700 | 1.23427200  |
| C | 5.55784000  | -1.92595300 | -1.95521400 |
| H | 3.56750100  | -1.96980800 | -2.80080800 |
| H | 7.38727000  | -1.77094900 | -0.82685500 |
| H | 6.04731300  | -2.27628100 | -2.85901800 |
| C | 4.33577300  | -0.69550500 | 2.94230600  |
| H | 3.70480900  | -0.42264100 | 3.79298100  |
| H | 4.67492600  | -1.72652900 | 3.08144700  |
| H | 5.21217300  | -0.04123100 | 2.96513100  |
| C | -0.79619100 | 2.74103000  | 2.80116100  |
| C | 0.00196100  | 2.91369000  | 3.93784200  |
| C | -2.16300600 | 2.48792800  | 2.97627400  |
| C | -0.54719400 | 2.80790700  | 5.21831300  |
| H | 1.06209500  | 3.11461200  | 3.82089200  |
| C | -2.71381800 | 2.37651300  | 4.25221000  |
| H | -2.79861900 | 2.37713200  | 2.10504800  |
| C | -1.90526800 | 2.52996700  | 5.38120700  |
| H | 0.08971900  | 2.93873300  | 6.08843200  |
| H | -3.77495400 | 2.17164400  | 4.36205900  |
| H | -2.33013000 | 2.43937800  | 6.37635200  |
| C | -0.61100400 | 4.21861300  | 0.78241400  |
| H | -1.69948900 | 4.30873500  | 0.74242200  |
| H | -0.22877300 | 5.04937400  | 1.38329600  |
| H | -0.22527900 | 4.31818100  | -0.23607300 |
| C | -4.83490800 | -3.88200700 | -1.92239000 |
| C | 4.57633200  | 4.32280400  | 0.77450600  |
| H | 5.59749000  | 3.93450900  | 0.74633000  |
| H | 4.37559300  | 4.81322100  | -0.18434200 |
| H | 4.52840800  | 5.09643300  | 1.54890000  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -4.66446000 | -3.64604700 | -2.97917400 |
| H  | -4.80282200 | -4.97264100 | -1.82671800 |
| H  | -5.84194900 | -3.54605300 | -1.66232100 |
| C  | -1.06201000 | -0.80635300 | -3.36571400 |
| C  | 0.24292000  | -0.51441600 | -2.88209200 |
| C  | 0.71826600  | 0.84299200  | -2.85732900 |
| C  | -0.22327500 | 1.88562400  | -3.15046000 |
| C  | -1.50109500 | 1.54458900  | -3.54664600 |
| C  | 0.18881200  | 3.34085600  | -3.12883900 |
| H  | 0.14277500  | 3.73560700  | -4.15273900 |
| H  | -0.54519100 | 3.91711200  | -2.55464500 |
| C  | 1.59821800  | 3.54103400  | -2.56888100 |
| H  | 1.59930200  | 3.38114400  | -1.48405600 |
| H  | 1.91634700  | 4.57517100  | -2.74251200 |
| C  | 2.58268900  | 2.55526700  | -3.20707600 |
| C  | 2.20881700  | 1.13200700  | -2.77777200 |
| H  | 2.75188500  | 0.39355400  | -3.37612400 |
| H  | 2.55396100  | 0.98617900  | -1.74656700 |
| Ni | 0.13442500  | 0.21595900  | -1.05962400 |
| F  | -1.43793800 | -2.08735700 | -3.52837100 |
| F  | 1.15174000  | -1.54685100 | -3.01675500 |
| F  | -2.39342000 | 2.52117300  | -3.85438600 |
| C  | -1.93834700 | 0.21266500  | -3.65497300 |
| F  | -3.20488000 | -0.05115700 | -4.02253000 |
| C  | 4.03391400  | 2.85498600  | -2.82697600 |
| H  | 2.47895400  | 2.63196400  | -4.29985100 |
| H  | 4.16200300  | 2.79224600  | -1.74119900 |
| H  | 4.33129600  | 3.85864600  | -3.14897300 |
| H  | 4.72034400  | 2.13414800  | -3.28412600 |

**2(R)<sup>C-H</sup><sub>endo</sub>**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.98056600 | -0.76661900 | 0.03023600  |
| C | -0.73806100 | -1.36931600 | -0.13207900 |
| C | 0.44170400  | -0.63081100 | -0.23203900 |
| C | 0.36360400  | 0.77297100  | -0.17211500 |
| C | -0.88756100 | 1.36727700  | -0.00636300 |
| C | 1.59760300  | 1.64827500  | -0.25158400 |
| H | 1.79616800  | 2.06506300  | 0.74482800  |
| H | 1.39082100  | 2.51147800  | -0.89289400 |
| C | 2.83085500  | 0.88941200  | -0.76095900 |
| H | 2.74609500  | 0.74690700  | -1.84596100 |
| H | 3.72615200  | 1.49826300  | -0.59239900 |
| C | 2.98666600  | -0.48837800 | -0.09165200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.75934900  | -1.35488400 | -0.43214800 |
| H | 1.82193000  | -1.67681000 | -1.48082800 |
| H | 1.76091500  | -2.27490400 | 0.16208200  |
| C | 3.21996100  | -0.38986500 | 1.42403500  |
| H | 3.86373400  | -0.97898500 | -0.53192700 |
| H | 2.35002600  | 0.02092200  | 1.94745600  |
| H | 3.42048300  | -1.37877200 | 1.84975700  |
| H | 4.07878700  | 0.25214100  | 1.64820100  |
| C | -2.05663300 | 0.62158600  | 0.09263800  |
| F | -3.09514800 | -1.50549800 | 0.12558200  |
| F | -3.24420500 | 1.22393800  | 0.24764600  |
| F | -0.98658000 | 2.71126600  | 0.06119800  |
| F | -0.69369500 | -2.71672700 | -0.19177600 |

### IM5

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.51464600 | -1.11074800 | -3.57481100 |
| C  | -0.17067100 | -0.86884200 | -3.41568400 |
| C  | 0.60675200  | -1.56081200 | -2.44945500 |
| C  | -0.01184000 | -2.59108100 | -1.65054500 |
| C  | -1.41000400 | -2.79402100 | -1.84744400 |
| H  | 1.68697100  | -1.52584200 | -2.56878000 |
| C  | 0.80933200  | -3.68686200 | -0.99089000 |
| H  | 0.20110600  | -4.18152900 | -0.22845000 |
| H  | 1.65706900  | -3.23575800 | -0.46622700 |
| C  | 1.37416900  | -4.73844700 | -1.98628200 |
| H  | 2.00569300  | -4.22105300 | -2.71712400 |
| H  | 2.03256500  | -5.40615500 | -1.41185800 |
| C  | 0.34332600  | -5.57447400 | -2.71421500 |
| C  | 0.16398300  | -5.46087300 | -4.03597300 |
| H  | 0.74170500  | -4.75897600 | -4.63172300 |
| H  | -0.56439100 | -6.06809100 | -4.56718300 |
| Ni | 0.10801200  | -0.83858100 | -0.65311200 |
| C  | 0.19523200  | 0.57884800  | 0.61754100  |
| C  | -0.01006500 | 1.77315100  | 2.66442700  |
| C  | 0.78240300  | 2.63135500  | 1.66551800  |
| H  | -0.89891800 | 2.28718700  | 3.03715200  |
| H  | 0.59062300  | 1.45825700  | 3.52186400  |
| H  | 0.25603800  | 3.54639200  | 1.38014100  |
| H  | 1.76902500  | 2.90541700  | 2.04753400  |
| N  | 0.90545700  | 1.72945400  | 0.49512000  |
| N  | -0.38455000 | 0.59412000  | 1.84568600  |
| C  | 1.62985500  | 2.12722500  | -0.68060600 |
| C  | 0.94203700  | 2.70384500  | -1.77831100 |
| C  | 3.03029800  | 1.97796500  | -0.71147000 |
| C  | 1.68714100  | 3.08329300  | -2.89747800 |



|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 3. 72795000  | 2. 38123700  | -1. 85748000 |
| C | 3. 07809000  | 2. 92858500  | -2. 96148900 |
| H | 1. 17527800  | 3. 51247300  | -3. 75255500 |
| H | 4. 80654800  | 2. 24786700  | -1. 88712600 |
| C | -1. 26508300 | -0. 42625500 | 2. 34419500  |
| C | -2. 65493400 | -0. 19288000 | 2. 35300200  |
| C | -0. 73474100 | -1. 63969800 | 2. 85124700  |
| C | -3. 50414800 | -1. 19088300 | 2. 84878300  |
| C | -1. 62806500 | -2. 60054000 | 3. 33144800  |
| C | -3. 01514400 | -2. 40007700 | 3. 33695700  |
| H | -4. 57729800 | -1. 01725100 | 2. 83619300  |
| H | -1. 24246100 | -3. 53872100 | 3. 71624800  |
| C | 3. 82268800  | 1. 42516900  | 0. 47631900  |
| C | -0. 56877500 | 2. 93046000  | -1. 73806200 |
| C | -3. 27234700 | 1. 12494200  | 1. 87745800  |
| C | 0. 77367800  | -1. 88873400 | 2. 87909800  |
| H | 1. 16750700  | -1. 53128200 | 1. 92101900  |
| H | 3. 09651700  | 1. 05389600  | 1. 20496700  |
| H | -1. 00017800 | 2. 08828700  | -1. 18914100 |
| H | -2. 47025800 | 1. 71717500  | 1. 42941400  |
| C | 4. 67693400  | 0. 22163600  | 0. 06994400  |
| C | 6. 07690000  | 0. 24655900  | 0. 04594900  |
| C | 4. 02918000  | -0. 97081600 | -0. 29723000 |
| C | 6. 80944100  | -0. 88249600 | -0. 33733200 |
| H | 6. 61222300  | 1. 14651400  | 0. 32963700  |
| C | 4. 75653500  | -2. 09786600 | -0. 67687600 |
| H | 2. 94044700  | -1. 00289700 | -0. 28945500 |
| C | 6. 15428400  | -2. 05812300 | -0. 69998200 |
| H | 7. 89504500  | -0. 83797700 | -0. 34841500 |
| H | 4. 23457500  | -3. 00944900 | -0. 95551200 |
| H | 6. 72309500  | -2. 93494100 | -0. 99568800 |
| C | 4. 62113700  | 2. 55250000  | 1. 15949200  |
| H | 5. 35192600  | 3. 00295600  | 0. 48077200  |
| H | 3. 94917200  | 3. 35185200  | 1. 48457100  |
| H | 5. 15525100  | 2. 17890400  | 2. 03907800  |
| C | -0. 96726200 | 4. 20698800  | -0. 98850800 |
| C | -0. 16300500 | 5. 35523700  | -0. 97469600 |
| C | -2. 21092700 | 4. 26145200  | -0. 33911800 |
| C | -0. 58480700 | 6. 51889300  | -0. 32577600 |
| H | 0. 80352100  | 5. 33907400  | -1. 46909200 |
| C | -2. 63507200 | 5. 42201200  | 0. 31041200  |
| H | -2. 85788300 | 3. 38768400  | -0. 35253500 |
| C | -1. 82097500 | 6. 55740400  | 0. 32152800  |
| H | 0. 05675100  | 7. 39598400  | -0. 32635600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.60128500 | 5.43820200  | 0.80736100  |
| H | -2.14701300 | 7.46117400  | 0.82826600  |
| C | -1.23677300 | 2.92771600  | -3.13154500 |
| H | -0.96755000 | 2.03326800  | -3.69827500 |
| H | -2.32401700 | 2.94608500  | -3.01285700 |
| H | -0.96103800 | 3.80957700  | -3.71827500 |
| C | -4.30488500 | 0.91084400  | 0.76636700  |
| C | -3.86083600 | 0.48741800  | -0.49851600 |
| C | -5.67572000 | 1.13956400  | 0.94133000  |
| C | -4.75344400 | 0.30828600  | -1.55501200 |
| H | -2.80137400 | 0.29013400  | -0.65029900 |
| C | -6.57551300 | 0.95304900  | -0.11370800 |
| H | -6.05647200 | 1.47257000  | 1.90105800  |
| C | -6.11899100 | 0.54069700  | -1.36451000 |
| H | -4.38432700 | -0.01837500 | -2.52143600 |
| H | -7.63434300 | 1.13692700  | 0.04705600  |
| H | -6.81717200 | 0.40154000  | -2.18487100 |
| C | -3.81339500 | 1.92591000  | 3.07839500  |
| H | -3.01655600 | 2.11341500  | 3.80384900  |
| H | -4.21405800 | 2.89223500  | 2.75612200  |
| H | -4.60565000 | 1.38569300  | 3.60569100  |
| C | 1.49438100  | -1.10952000 | 3.98179900  |
| C | 0.91352800  | -0.88752900 | 5.23845400  |
| C | 2.80456500  | -0.65578300 | 3.76544200  |
| C | 1.61771400  | -0.22329300 | 6.24594400  |
| H | -0.09986700 | -1.22969300 | 5.42748000  |
| C | 3.51129000  | 0.00817600  | 4.77017400  |
| H | 3.27754500  | -0.83196500 | 2.80205200  |
| C | 2.91836300  | 0.22957300  | 6.01563800  |
| H | 1.14727100  | -0.05884300 | 7.21155400  |
| H | 4.52411400  | 0.35236500  | 4.57925700  |
| H | 3.46453500  | 0.74864200  | 6.79801400  |
| C | 1.15866000  | -3.38001100 | 2.98318000  |
| H | 2.24110800  | -3.48546800 | 2.86660700  |
| H | 0.89478600  | -3.80349900 | 3.95721400  |
| H | 0.67084600  | -3.97271200 | 2.20341200  |
| C | 3.84084900  | 3.32527700  | -4.20350600 |
| C | -3.94712600 | -3.47794800 | 3.83838000  |
| H | -4.10262800 | -4.25029000 | 3.07513200  |
| H | -3.54097500 | -3.97717100 | 4.72392500  |
| H | -4.92827900 | -3.06956900 | 4.09593600  |
| H | 4.90872500  | 3.43913400  | -3.99746200 |
| H | 3.73547400  | 2.56672300  | -4.98878800 |
| H | 3.46966600  | 4.26878000  | -4.61649100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.14279300 | -2.08950000 | -2.77544400 |
| C | -0.44900800 | -6.55736700 | -1.88538500 |
| H | 0.21783700  | -7.21914000 | -1.31788700 |
| H | -1.08431500 | -6.04138000 | -1.15772300 |
| H | -1.09488600 | -7.17822300 | -2.51209000 |
| F | 0.42275400  | 0.05256400  | -4.20570300 |
| F | -2.25961800 | -0.40544500 | -4.44781100 |
| F | -3.46256100 | -2.30639300 | -2.93025200 |
| F | -2.04682500 | -3.74668100 | -1.12844200 |

### TS3

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -4.00522000 | 2.10842100  | 2.20648600  |
| C  | -2.80770600 | 1.53443800  | 1.80696600  |
| C  | -2.17263300 | 1.81845100  | 0.59197900  |
| C  | -2.78253400 | 2.80348800  | -0.23718400 |
| C  | -3.95819200 | 3.41441900  | 0.19701900  |
| H  | -0.70434000 | 1.97365200  | 0.73613700  |
| C  | -2.15869000 | 3.19534800  | -1.56332200 |
| H  | -1.31880800 | 2.51596200  | -1.73613500 |
| H  | -1.73293100 | 4.20539400  | -1.48501400 |
| C  | -3.10917500 | 3.19018900  | -2.79349100 |
| H  | -3.77018800 | 4.05700600  | -2.73975900 |
| H  | -2.47836400 | 3.32338400  | -3.68390400 |
| C  | -3.94300200 | 1.93703400  | -2.95355700 |
| C  | -5.27464300 | 1.96743200  | -2.82210000 |
| H  | -5.80079700 | 2.88790600  | -2.58510300 |
| H  | -5.87973900 | 1.07202400  | -2.94032300 |
| Ni | -0.72966000 | 0.63906300  | 0.16296300  |
| C  | 0.80862800  | -0.52000700 | 0.05266200  |
| C  | 2.10717000  | -2.46805500 | -0.34746100 |
| C  | 2.92033000  | -1.49909400 | 0.52031400  |
| H  | 1.82263600  | -3.37022800 | 0.20425900  |
| H  | 2.62718300  | -2.76524700 | -1.25966700 |
| H  | 3.26298700  | -1.94710800 | 1.45450700  |
| H  | 3.78684100  | -1.10163300 | -0.01721900 |
| N  | 1.94200800  | -0.41527800 | 0.78974600  |
| N  | 0.90162000  | -1.66499500 | -0.66781600 |
| C  | 2.25952900  | 0.66576200  | 1.68516700  |
| C  | 1.77687800  | 0.63405700  | 3.01846100  |
| C  | 3.08224600  | 1.72005000  | 1.24637300  |
| C  | 2.11649200  | 1.68848300  | 3.86799900  |
| C  | 3.39384600  | 2.75199100  | 2.14285900  |
| C  | 2.92070700  | 2.75903200  | 3.45173300  |
| H  | 1.74486800  | 1.68896600  | 4.88727400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.01234000  | 3.57542700  | 1.79502100  |
| C | -0.07119300 | -2.11958900 | -1.62311100 |
| C | -1.05167800 | -3.05779500 | -1.24345600 |
| C | 0.00933800  | -1.65774300 | -2.96192400 |
| C | -1.96018900 | -3.50718100 | -2.21132000 |
| C | -0.91740600 | -2.14553700 | -3.88570800 |
| C | -1.91204500 | -3.06733000 | -3.53206400 |
| H | -2.72976400 | -4.21556800 | -1.91713500 |
| H | -0.87519200 | -1.80049000 | -4.91365100 |
| C | 3.68867900  | 1.76600800  | -0.15811000 |
| C | 0.91067900  | -0.52368800 | 3.51476100  |
| C | -1.12116900 | -3.64864700 | 0.16831100  |
| C | 1.09332200  | -0.66744400 | -3.38915600 |
| H | 1.23329800  | 0.02804200  | -2.55599000 |
| H | 3.20646100  | 0.97992400  | -0.74672900 |
| H | 0.19929000  | -0.74806200 | 2.71449500  |
| H | -0.42375900 | -3.08255500 | 0.79023000  |
| C | 3.38029100  | 3.08508800  | -0.87353800 |
| C | 4.37507000  | 3.98043200  | -1.28649900 |
| C | 2.04056800  | 3.41092900  | -1.14785900 |
| C | 4.04467800  | 5.16614800  | -1.95233300 |
| H | 5.42052900  | 3.76206300  | -1.09697600 |
| C | 1.70947800  | 4.58989900  | -1.81306000 |
| H | 1.25237500  | 2.73379000  | -0.82548900 |
| C | 2.71246100  | 5.47583900  | -2.21926700 |
| H | 4.83517500  | 5.84436200  | -2.26188700 |
| H | 0.66683200  | 4.81850100  | -2.01568500 |
| H | 2.45539900  | 6.39517200  | -2.73758200 |
| C | 5.19306900  | 1.43433000  | -0.09327400 |
| H | 5.74461800  | 2.17893600  | 0.48896400  |
| H | 5.35022200  | 0.46605500  | 0.38949900  |
| H | 5.63300900  | 1.38966500  | -1.09474200 |
| C | 1.71058600  | -1.80184100 | 3.77923800  |
| C | 3.00736000  | -1.77431800 | 4.31212400  |
| C | 1.11379500  | -3.05108900 | 3.55030300  |
| C | 3.69060200  | -2.95962400 | 4.59640100  |
| H | 3.48840900  | -0.81872000 | 4.50008300  |
| C | 1.79299600  | -4.23772600 | 3.83340200  |
| H | 0.10053300  | -3.09210000 | 3.15758700  |
| C | 3.08784700  | -4.19616700 | 4.35582000  |
| H | 4.69595300  | -2.91518700 | 5.00638000  |
| H | 1.31066200  | -5.19310600 | 3.64568500  |
| H | 3.62045500  | -5.11717200 | 4.57464500  |
| C | 0.06714000  | -0.18375500 | 4.76180500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.53988600 | 0.70961600  | 4.59409800  |
| H | -0.60747000 | -1.01632700 | 4.98069400  |
| H | 0.68997100  | -0.02899300 | 5.64834600  |
| C | -2.49992600 | -3.47449100 | 0.80929700  |
| C | -2.80122900 | -2.26333900 | 1.45128500  |
| C | -3.48132600 | -4.47553200 | 0.79563600  |
| C | -4.04032200 | -2.05212900 | 2.05745500  |
| H | -2.05469900 | -1.47430200 | 1.48508000  |
| C | -4.72713900 | -4.26642200 | 1.39482700  |
| H | -3.27964400 | -5.43330400 | 0.32623800  |
| C | -5.01187300 | -3.05571600 | 2.02744200  |
| H | -4.23662600 | -1.10930800 | 2.55912500  |
| H | -5.47200700 | -5.05720300 | 1.37193700  |
| H | -5.97764200 | -2.89786100 | 2.49881100  |
| C | -0.63633300 | -5.11385800 | 0.15365600  |
| H | 0.39022500  | -5.17370100 | -0.21938900 |
| H | -0.66241300 | -5.54205900 | 1.16074100  |
| H | -1.25132200 | -5.74030600 | -0.49912000 |
| C | 2.45078500  | -1.32996100 | -3.64915000 |
| C | 2.56755800  | -2.62984800 | -4.16073800 |
| C | 3.62657900  | -0.59402600 | -3.43371900 |
| C | 3.82151500  | -3.18099800 | -4.43857300 |
| H | 1.67284000  | -3.21905700 | -4.33811900 |
| C | 4.88065800  | -1.14091200 | -3.71089000 |
| H | 3.55650900  | 0.42314800  | -3.05541700 |
| C | 4.98321900  | -2.44061100 | -4.21290500 |
| H | 3.88810500  | -4.19177500 | -4.83169700 |
| H | 5.77655700  | -0.55228400 | -3.53368800 |
| H | 5.95758600  | -2.87041500 | -4.42631300 |
| C | 0.70470000  | 0.19137500  | -4.61220000 |
| H | 1.46502200  | 0.96058800  | -4.77474200 |
| H | 0.64449900  | -0.40326900 | -5.52875400 |
| H | -0.25711600 | 0.68833400  | -4.45585300 |
| C | 3.24910500  | 3.88598600  | 4.40243500  |
| C | -2.91194500 | -3.55040400 | -4.55592500 |
| H | -3.66610800 | -2.78144100 | -4.76272900 |
| H | -2.42568000 | -3.78736200 | -5.50786600 |
| H | -3.43816000 | -4.44393100 | -4.20962800 |
| H | 3.96816400  | 4.58251000  | 3.96322900  |
| H | 2.35005100  | 4.45550900  | 4.66557200  |
| H | 3.67260600  | 3.50644100  | 5.33891200  |
| C | -4.58649000 | 3.07344700  | 1.39242600  |
| C | -3.20210900 | 0.66469300  | -3.27391200 |
| H | -2.64957400 | 0.76228200  | -4.21760300 |

|            |             |             |             |
|------------|-------------|-------------|-------------|
| H          | -2.46088300 | 0.42739900  | -2.50114600 |
| H          | -3.88032400 | -0.18829000 | -3.36281700 |
| F          | -2.26096900 | 0.62893600  | 2.66771600  |
| F          | -4.60423100 | 1.73730000  | 3.35306700  |
| F          | -5.73396100 | 3.66789200  | 1.75712600  |
| F          | -4.55366200 | 4.38054900  | -0.54409100 |
| <b>IM6</b> |             |             |             |
| C          | 3.82729300  | 1.95617200  | -2.64260700 |
| C          | 2.76870100  | 1.29582000  | -2.03050700 |
| C          | 2.16589500  | 1.70157200  | -0.84457900 |
| C          | 2.66971900  | 2.88758100  | -0.25010300 |
| C          | 3.70677600  | 3.57681400  | -0.88194600 |
| H          | -0.10676500 | 1.55294300  | -0.96147600 |
| C          | 2.08702100  | 3.42388000  | 1.04539400  |
| H          | 1.35367200  | 2.69057700  | 1.39462600  |
| H          | 1.52714200  | 4.34830100  | 0.84554900  |
| C          | 3.10629400  | 3.74113600  | 2.17559200  |
| H          | 3.64771600  | 4.65503900  | 1.92427300  |
| H          | 2.52357700  | 3.95394300  | 3.08350400  |
| C          | 4.10161400  | 2.63932800  | 2.46877000  |
| C          | 5.40793800  | 2.79976700  | 2.22594400  |
| H          | 5.79585600  | 3.72014500  | 1.79832100  |
| H          | 6.12914700  | 2.01442300  | 2.43843200  |
| Ni         | 0.68312300  | 0.60649900  | -0.28036400 |
| C          | -0.82043000 | -0.56146300 | 0.05269000  |
| C          | -2.01409300 | -2.41305500 | 0.93250700  |
| C          | -2.86561100 | -1.73736400 | -0.15373800 |
| H          | -1.71591000 | -3.42707500 | 0.64959700  |
| H          | -2.51055700 | -2.45274000 | 1.90403700  |
| H          | -3.12675000 | -2.41226000 | -0.97079700 |
| H          | -3.78557300 | -1.30854000 | 0.25282700  |
| N          | -1.97148900 | -0.65782900 | -0.64677200 |
| N          | -0.82410500 | -1.52958900 | 0.99618300  |
| C          | -2.36786200 | 0.17838100  | -1.74959700 |
| C          | -1.87630000 | -0.09805600 | -3.05007300 |
| C          | -3.27498700 | 1.23203600  | -1.53122200 |
| C          | -2.29831900 | 0.71934800  | -4.09996400 |
| C          | -3.66734400 | 2.01805500  | -2.62338300 |
| C          | -3.19163300 | 1.78316400  | -3.91038100 |
| H          | -1.92310700 | 0.53309800  | -5.10072100 |
| H          | -4.35129000 | 2.84522700  | -2.45170000 |
| C          | 0.19771800  | -1.71166600 | 1.99156700  |
| C          | 1.18938200  | -2.69668000 | 1.80875700  |
| C          | 0.15460200  | -0.93495700 | 3.17836200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.14477200  | -2.87889900 | 2.81768400  |
| C | 1.12867900  | -1.16647200 | 4.15177900  |
| C | 2.13327700  | -2.13032100 | 3.99212500  |
| H | 2.92331500  | -3.62271700 | 2.67262600  |
| H | 1.11622800  | -0.58075500 | 5.06506000  |
| C | -3.87742700 | 1.53619700  | -0.15697300 |
| C | -0.91529100 | -1.25977700 | -3.29945300 |
| C | 1.23261900  | -3.60897500 | 0.57819900  |
| C | -0.93506400 | 0.11394200  | 3.40130400  |
| H | -1.13632600 | 0.57777900  | 2.43105200  |
| H | -3.34776800 | 0.92015100  | 0.57529300  |
| H | -0.21174800 | -1.27119400 | -2.46173500 |
| H | 0.49822400  | -3.22873500 | -0.13639400 |
| C | -3.64088500 | 2.99173800  | 0.26025400  |
| C | -4.67701800 | 3.92304700  | 0.40611100  |
| C | -2.32654300 | 3.41653500  | 0.52081900  |
| C | -4.41030900 | 5.23981800  | 0.79716000  |
| H | -5.70512400 | 3.63114100  | 0.21990300  |
| C | -2.05878800 | 4.72698600  | 0.91305700  |
| H | -1.50608900 | 2.71341100  | 0.39936800  |
| C | -3.10213000 | 5.64732400  | 1.05297000  |
| H | -5.23137900 | 5.94365400  | 0.90256100  |
| H | -1.03413800 | 5.03054100  | 1.10954800  |
| H | -2.89508100 | 6.66895200  | 1.35834700  |
| C | -5.36038300 | 1.11608000  | -0.12118600 |
| H | -5.95585900 | 1.67103900  | -0.85246500 |
| H | -5.46393700 | 0.05443800  | -0.36218800 |
| H | -5.79282700 | 1.28337700  | 0.87031800  |
| C | -1.61207200 | -2.62351500 | -3.31884300 |
| C | -2.91094900 | -2.79430900 | -3.81873800 |
| C | -0.91472800 | -3.76057800 | -2.88186400 |
| C | -3.49819400 | -4.06140900 | -3.87093800 |
| H | -3.46957400 | -1.92905900 | -4.16332200 |
| C | -1.49796800 | -5.02793500 | -2.93262100 |
| H | 0.10116400  | -3.65189000 | -2.50920400 |
| C | -2.79585700 | -5.18303400 | -3.42575300 |
| H | -4.50691700 | -4.17018600 | -4.26000300 |
| H | -0.93866100 | -5.89300400 | -2.58697800 |
| H | -3.25369500 | -6.16726600 | -3.46389300 |
| C | -0.06025400 | -1.10053700 | -4.57484900 |
| H | 0.47498500  | -0.14747400 | -4.57168700 |
| H | 0.67980800  | -1.90450600 | -4.61697000 |
| H | -0.66444300 | -1.16775200 | -5.48473100 |
| C | 2.58815300  | -3.55413600 | -0.13146500 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2. 84682700  | -2. 50232100 | -1. 02368200 |
| C | 3. 59436600  | -4. 50979400 | 0. 06782700  |
| C | 4. 06910000  | -2. 39605600 | -1. 68787400 |
| H | 2. 08311300  | -1. 75438700 | -1. 21468200 |
| C | 4. 82251300  | -4. 40678100 | -0. 59270000 |
| H | 3. 42755600  | -5. 35043400 | 0. 73409600  |
| C | 5. 06617600  | -3. 35026300 | -1. 47098800 |
| H | 4. 22847600  | -1. 57146400 | -2. 37580100 |
| H | 5. 58673800  | -5. 16002400 | -0. 42167000 |
| H | 6. 01941300  | -3. 27448600 | -1. 98604800 |
| C | 0. 80050900  | -5. 04001800 | 0. 96074100  |
| H | -0. 21354900 | -5. 03880400 | 1. 37102600  |
| H | 0. 81598200  | -5. 69660300 | 0. 08519900  |
| H | 1. 45393500  | -5. 47278200 | 1. 72384100  |
| C | -2. 26079500 | -0. 48047700 | 3. 89035500  |
| C | -2. 32387600 | -1. 63414700 | 4. 68412000  |
| C | -3. 45990700 | 0. 18502500  | 3. 58951500  |
| C | -3. 54958000 | -2. 11298300 | 5. 15570400  |
| H | -1. 41032300 | -2. 16616800 | 4. 93180700  |
| C | -4. 68514200 | -0. 28963800 | 4. 05994300  |
| H | -3. 43003400 | 1. 09084600  | 2. 98847000  |
| C | -4. 73482600 | -1. 44469700 | 4. 84446100  |
| H | -3. 57538400 | -3. 01062900 | 5. 76739300  |
| H | -5. 59998700 | 0. 24198600  | 3. 81311200  |
| H | -5. 68701100 | -1. 81850800 | 5. 20954800  |
| C | -0. 50805900 | 1. 25996000  | 4. 34517900  |
| H | -1. 27449400 | 2. 03993500  | 4. 34119200  |
| H | -0. 39669700 | 0. 92024300  | 5. 37915900  |
| H | 0. 43680900  | 1. 70685500  | 4. 02156800  |
| C | -3. 60702800 | 2. 65167800  | -5. 07412000 |
| C | 3. 18399100  | -2. 32813800 | 5. 05872500  |
| H | 3. 92087400  | -1. 51616200 | 5. 03808200  |
| H | 2. 74008300  | -2. 33405400 | 6. 05951300  |
| H | 3. 72415700  | -3. 26819000 | 4. 91855400  |
| H | -3. 96134600 | 2. 04687400  | -5. 91594400 |
| H | -4. 40618100 | 3. 34231800  | -4. 79225000 |
| H | -2. 76378400 | 3. 24869400  | -5. 44084300 |
| C | 4. 29851600  | 3. 12463600  | -2. 05835700 |
| C | 3. 55044500  | 1. 36283500  | 3. 05040900  |
| H | 3. 03353400  | 1. 55599000  | 3. 99970000  |
| H | 2. 81142000  | 0. 90569400  | 2. 38206900  |
| H | 4. 33920800  | 0. 62777900  | 3. 23398900  |
| F | 2. 32141000  | 0. 17198100  | -2. 67966300 |
| F | 4. 39092800  | 1. 49084500  | -3. 77463300 |



|            |             |             |             |
|------------|-------------|-------------|-------------|
| F          | 5.31219600  | 3.80635900  | -2.62150600 |
| F          | 4.19129500  | 4.73747700  | -0.36918400 |
| <b>IM7</b> |             |             |             |
| C          | 3.80300400  | 1.73791100  | 1.06316200  |
| C          | 2.54818700  | 1.15898400  | 0.89624400  |
| C          | 1.79275300  | 0.55754000  | 1.89529100  |
| C          | 2.47006700  | 0.44435900  | 3.14234200  |
| C          | 3.75666900  | 0.96603900  | 3.30761700  |
| H          | -1.63481800 | -0.09088100 | 1.47688600  |
| C          | 1.89597900  | -0.21273600 | 4.39017300  |
| H          | 1.76120500  | 0.54802400  | 5.17226600  |
| H          | 2.65124100  | -0.89754700 | 4.79260600  |
| C          | 0.59423100  | -0.99014400 | 4.22999100  |
| H          | 0.71799500  | -1.78776800 | 3.48281500  |
| H          | 0.38476300  | -1.50972600 | 5.17590900  |
| C          | -0.63532900 | -0.18482000 | 3.87294500  |
| C          | -0.60550400 | 1.15046400  | 3.58332900  |
| H          | 0.29667300  | 1.74213600  | 3.66426600  |
| H          | -1.53516500 | 1.69468600  | 3.44722800  |
| Ni         | -0.20012700 | 0.17620800  | 1.65573500  |
| C          | -0.41349200 | -0.01491100 | -0.21720000 |
| C          | -0.92351600 | 0.63879400  | -2.41243000 |
| C          | -0.47016500 | -0.81804200 | -2.42918700 |
| H          | -1.84391200 | 0.80415400  | -2.97063100 |
| H          | -0.15439500 | 1.31824100  | -2.79774000 |
| H          | -1.29395600 | -1.51871600 | -2.60409500 |
| H          | 0.30384400  | -0.99516400 | -3.17153200 |
| N          | 0.05022300  | -0.98873500 | -1.04710300 |
| N          | -1.11865400 | 0.87912500  | -0.96563300 |
| C          | 0.72624000  | -2.18942900 | -0.60978000 |
| C          | 0.02003700  | -3.14105600 | 0.17247700  |
| C          | 2.06856400  | -2.44762000 | -0.98858100 |
| C          | 0.73004600  | -4.21035400 | 0.72780800  |
| C          | 2.72317000  | -3.53801500 | -0.40188600 |
| C          | 2.09353500  | -4.40179000 | 0.49259400  |
| H          | 0.20542900  | -4.93211300 | 1.34384700  |
| H          | 3.76369400  | -3.71463100 | -0.64952400 |
| C          | -1.97963900 | 1.94167900  | -0.49543700 |
| C          | -3.37735200 | 1.72048300  | -0.44307200 |
| C          | -1.45647500 | 3.21573300  | -0.16649700 |
| C          | -4.20930000 | 2.75000800  | 0.01209900  |
| C          | -2.33520500 | 4.20310100  | 0.29368900  |
| C          | -3.71191900 | 3.99174400  | 0.40416500  |
| H          | -5.27898400 | 2.56529900  | 0.06662500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.93601100 | 5.17548500  | 0.56410200  |
| C | 2.77040400  | -1.69762000 | -2.13494400 |
| C | -1.50470700 | -3.11600300 | 0.29057700  |
| C | -4.04973200 | 0.43789800  | -0.94309000 |
| C | 0.01719500  | 3.54596700  | -0.35613200 |
| H | 0.56522000  | 2.61448000  | -0.25424800 |
| H | 2.32506500  | -0.70122900 | -2.19857300 |
| H | -1.81793100 | -2.07949200 | 0.43438800  |
| H | -3.27581900 | -0.33048900 | -1.03044200 |
| C | 4.27827700  | -1.48851000 | -1.96459900 |
| C | 5.22637400  | -2.48684400 | -2.24733800 |
| C | 4.75490000  | -0.23737900 | -1.55445300 |
| C | 6.59353300  | -2.24923600 | -2.08785800 |
| H | 4.90881400  | -3.46117300 | -2.60502900 |
| C | 6.11987400  | 0.00626300  | -1.39158500 |
| H | 4.04752000  | 0.55947900  | -1.37010200 |
| C | 7.04753600  | -1.00275600 | -1.65271500 |
| H | 7.30375500  | -3.04081200 | -2.31081000 |
| H | 6.44776800  | 0.98684300  | -1.05969800 |
| H | 8.11093600  | -0.81909600 | -1.52841300 |
| C | 2.48466600  | -2.45195800 | -3.46061700 |
| H | 1.41476800  | -2.60506000 | -3.62045700 |
| H | 2.88928400  | -1.89747100 | -4.31331000 |
| H | 2.94312400  | -3.44442800 | -3.45252700 |
| C | -2.18795300 | -3.63365100 | -0.98595800 |
| C | -1.55966900 | -4.50706600 | -1.88521900 |
| C | -3.52115500 | -3.27187400 | -1.23965100 |
| C | -2.23763400 | -4.99264700 | -3.00723800 |
| H | -0.53221400 | -4.81023500 | -1.71199200 |
| C | -4.20033900 | -3.75452100 | -2.35931500 |
| H | -4.03629500 | -2.61091400 | -0.54829900 |
| C | -3.55919000 | -4.61721800 | -3.25183000 |
| H | -1.72782200 | -5.66639200 | -3.69058700 |
| H | -5.23088100 | -3.45615800 | -2.53185900 |
| H | -4.08412100 | -4.99275000 | -4.12548300 |
| C | -2.05344900 | -3.90974800 | 1.49752900  |
| H | -1.54392800 | -3.63027800 | 2.42423600  |
| H | -3.12056900 | -3.70424400 | 1.61772300  |
| H | -1.94408900 | -4.98965600 | 1.35960400  |
| C | -5.09334000 | -0.09789500 | 0.04539000  |
| C | -4.67626000 | -0.50336700 | 1.32498900  |
| C | -6.45304400 | -0.22226400 | -0.27026100 |
| C | -5.58196600 | -1.01474600 | 2.25291000  |
| H | -3.62547800 | -0.40978400 | 1.58620900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -7.36616900 | -0.73026700 | 0.66096000  |
| H | -6.81861600 | 0.07439500  | -1.24706800 |
| C | -6.93651600 | -1.12919200 | 1.92506400  |
| H | -5.23133400 | -1.32443600 | 3.23374900  |
| H | -8.41506900 | -0.81353600 | 0.38993800  |
| H | -7.64480200 | -1.52624300 | 2.64649400  |
| C | -4.63016900 | 0.67036800  | -2.35433300 |
| H | -5.03712500 | -0.25676800 | -2.76988700 |
| H | -5.42552600 | 1.42178200  | -2.33848200 |
| H | -3.86132800 | 1.03640100  | -3.03838800 |
| C | 0.34265000  | 4.08741800  | -1.75571600 |
| C | -0.57194500 | 4.81789400  | -2.52673800 |
| C | 1.63543600  | 3.88935800  | -2.27101300 |
| C | -0.20809300 | 5.33627000  | -3.77283500 |
| H | -1.57903300 | 4.98132600  | -2.15598300 |
| C | 2.00038300  | 4.40675400  | -3.51456300 |
| H | 2.35880000  | 3.32661100  | -1.68841500 |
| C | 1.07880500  | 5.13363300  | -4.27274200 |
| H | -0.93528600 | 5.89829500  | -4.35288000 |
| H | 3.00533600  | 4.23897800  | -3.89247700 |
| H | 1.36079000  | 5.53493500  | -5.24203600 |
| C | 0.57956700  | 4.50514900  | 0.71772400  |
| H | 1.66577800  | 4.57763800  | 0.61155900  |
| H | 0.17720400  | 5.51826100  | 0.62229400  |
| H | 0.35848300  | 4.13773500  | 1.72499200  |
| C | 2.85074600  | -5.52415200 | 1.16045300  |
| C | -4.62593900 | 5.06969400  | 0.93619700  |
| H | -4.25714500 | 6.06796900  | 0.68197800  |
| H | -5.63978800 | 4.96676100  | 0.53867200  |
| H | -4.69807800 | 5.01911400  | 2.02977400  |
| H | 3.69097600  | -5.86196000 | 0.54682000  |
| H | 3.26230700  | -5.19957800 | 2.12428100  |
| H | 2.20228100  | -6.38323900 | 1.35774000  |
| C | 4.43275400  | 1.63037000  | 2.29252600  |
| C | -1.94740600 | -0.89925000 | 4.09499800  |
| H | -2.06356900 | -1.09856600 | 5.16918400  |
| H | -2.79592800 | -0.29835000 | 3.76387700  |
| H | -1.98088900 | -1.86477900 | 3.58468800  |
| F | 2.07344700  | 1.25115000  | -0.39507900 |
| F | 4.41730700  | 2.38991500  | 0.04798000  |
| F | 5.65687200  | 2.15057000  | 2.49053100  |
| F | 4.39030600  | 0.85140000  | 4.50259100  |

**TS4(R)**

|   |            |             |            |
|---|------------|-------------|------------|
| C | 3.71670200 | -0.44035000 | 2.57775300 |
|---|------------|-------------|------------|

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.47358800  | -0.00606400 | 2.12539600  |
| C  | 1.30148000  | -0.72619900 | 2.27384400  |
| C  | 1.39149800  | -1.96505100 | 2.96676000  |
| C  | 2.64863500  | -2.42320500 | 3.37356700  |
| H  | -1.95654400 | -0.63752200 | 1.50276300  |
| C  | 0.21510500  | -2.81829700 | 3.45914200  |
| H  | 0.20621500  | -2.74327100 | 4.55589300  |
| H  | 0.45210000  | -3.87040100 | 3.26381400  |
| C  | -1.23039700 | -2.59093500 | 2.96259100  |
| H  | -1.33237300 | -2.94906800 | 1.93309600  |
| H  | -1.87138800 | -3.25287200 | 3.56331700  |
| C  | -1.81014000 | -1.17324400 | 3.04245100  |
| C  | -0.98656700 | -0.16814900 | 3.60613300  |
| H  | -0.13997800 | -0.41495800 | 4.22892800  |
| H  | -1.43045800 | 0.80989400  | 3.79033700  |
| Ni | -0.48652700 | -0.29173100 | 1.64759800  |
| C  | -0.43430700 | 0.14590000  | -0.26944900 |
| C  | -1.07157500 | 1.45035000  | -2.13635100 |
| C  | -0.28737800 | 0.24148100  | -2.61870900 |
| H  | -2.00346100 | 1.59077300  | -2.68079400 |
| H  | -0.49135100 | 2.37871500  | -2.18309400 |
| H  | -0.93217400 | -0.53020100 | -3.05365400 |
| H  | 0.48088700  | 0.50025500  | -3.34081700 |
| N  | 0.29175200  | -0.26760600 | -1.34606800 |
| N  | -1.31703600 | 1.08144100  | -0.72328400 |
| C  | 1.37927800  | -1.21510800 | -1.36067800 |
| C  | 1.13845600  | -2.58140200 | -1.07221400 |
| C  | 2.67402400  | -0.79101900 | -1.75156100 |
| C  | 2.22846100  | -3.45549600 | -1.02589600 |
| C  | 3.72130500  | -1.72119700 | -1.71536900 |
| C  | 3.53294200  | -3.04284800 | -1.31701900 |
| H  | 2.06167800  | -4.49862700 | -0.78031400 |
| H  | 4.71514500  | -1.39144300 | -2.00438100 |
| C  | -2.23483100 | 1.83634400  | 0.08922800  |
| C  | -3.62477100 | 1.65815400  | -0.08747100 |
| C  | -1.74634300 | 2.79227000  | 1.01827800  |
| C  | -4.50436400 | 2.38408100  | 0.72674100  |
| C  | -2.67163600 | 3.48123200  | 1.80661700  |
| C  | -4.05324600 | 3.28372800  | 1.68988200  |
| H  | -5.57326800 | 2.23028600  | 0.60566300  |
| H  | -2.31266100 | 4.20431200  | 2.53158500  |
| C  | 2.95306300  | 0.57392100  | -2.39184500 |
| C  | -0.28377800 | -3.12729000 | -0.94178500 |
| C  | -4.22356400 | 0.77035900  | -1.18732900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.25475500 | 3.11449800  | 1.11745500  |
| H | 0.29289100  | 2.17459100  | 1.03022000  |
| H | 2.12980600  | 1.24598100  | -2.12563800 |
| H | -0.86491600 | -2.41253000 | -0.35236700 |
| H | -3.41947600 | 0.13893900  | -1.57625000 |
| C | 4.23807800  | 1.27932400  | -1.93080000 |
| C | 4.92186400  | 2.16420700  | -2.78256500 |
| C | 4.73399300  | 1.12003700  | -0.62980400 |
| C | 6.05510200  | 2.85711100  | -2.34965500 |
| H | 4.57826900  | 2.32302100  | -3.79844300 |
| C | 5.86721400  | 1.80837000  | -0.19307300 |
| H | 4.23586100  | 0.44294100  | 0.04813000  |
| C | 6.53561600  | 2.68172300  | -1.05144000 |
| H | 6.56286800  | 3.53127300  | -3.03416500 |
| H | 6.21832100  | 1.65589800  | 0.82224500  |
| H | 7.41867900  | 3.21720200  | -0.71464800 |
| C | 2.94438000  | 0.37912600  | -3.93332300 |
| H | 2.12866200  | -0.27615100 | -4.24701800 |
| H | 2.83217300  | 1.32856700  | -4.46449900 |
| H | 3.87759200  | -0.08839800 | -4.26208700 |
| C | -0.97113800 | -3.25092600 | -2.30912400 |
| C | -0.27111300 | -3.62220300 | -3.46651000 |
| C | -2.35581000 | -3.05097200 | -2.41046900 |
| C | -0.93374500 | -3.77938200 | -4.68623000 |
| H | 0.80150300  | -3.78326200 | -3.41641200 |
| C | -3.02189700 | -3.20503900 | -3.62814400 |
| H | -2.92307100 | -2.77644100 | -1.52600900 |
| C | -2.31133900 | -3.56874600 | -4.77401000 |
| H | -0.36970300 | -4.06517100 | -5.56994500 |
| H | -4.09452200 | -3.03924900 | -3.67857000 |
| H | -2.82506200 | -3.68697300 | -5.72371200 |
| C | -0.37212400 | -4.48710700 | -0.21583200 |
| H | 0.13771100  | -4.45998200 | 0.75190100  |
| H | -1.42192700 | -4.74376100 | -0.04611000 |
| H | 0.06351000  | -5.29463700 | -0.81174100 |
| C | -5.29966300 | -0.18921400 | -0.67109500 |
| C | -4.90659200 | -1.37579000 | -0.03308300 |
| C | -6.67301100 | 0.04549800  | -0.82689500 |
| C | -5.84541200 | -2.29815300 | 0.42929200  |
| H | -3.84682200 | -1.56933200 | 0.10784200  |
| C | -7.61897300 | -0.87130700 | -0.35742100 |
| H | -7.02108000 | 0.94299500  | -1.32712100 |
| C | -7.21084300 | -2.04799100 | 0.26977500  |
| H | -5.51127000 | -3.21297400 | 0.91111500  |

|               |             |             |             |
|---------------|-------------|-------------|-------------|
| H             | -8.67706100 | -0.66412200 | -0.49146800 |
| H             | -7.94544300 | -2.76393200 | 0.62658500  |
| C             | -4.73356900 | 1.65416400  | -2.34733700 |
| H             | -5.14018600 | 1.03976900  | -3.15677400 |
| H             | -5.51467900 | 2.34332300  | -2.01361000 |
| H             | -3.92831700 | 2.27022400  | -2.75559800 |
| C             | 0.22469900  | 4.01970700  | -0.02220800 |
| C             | -0.55235400 | 5.07770200  | -0.51504700 |
| C             | 1.50726300  | 3.82884100  | -0.55986800 |
| C             | -0.06395700 | 5.91796800  | -1.51865700 |
| H             | -1.54903700 | 5.24349400  | -0.11628800 |
| C             | 1.99778000  | 4.66667600  | -1.56427200 |
| H             | 2.12600600  | 3.01937600  | -0.18315900 |
| C             | 1.21192700  | 5.71496300  | -2.04897100 |
| H             | -0.68359700 | 6.73107000  | -1.88746300 |
| H             | 2.99233000  | 4.49435900  | -1.96608000 |
| H             | 1.58966100  | 6.36688100  | -2.83159300 |
| C             | 0.17163000  | 3.72154000  | 2.47087300  |
| H             | 1.26292200  | 3.77515400  | 2.50953700  |
| H             | -0.21293900 | 4.73661500  | 2.61186300  |
| H             | -0.16709600 | 3.10103600  | 3.30659100  |
| C             | 4.69279300  | -4.00418000 | -1.21750800 |
| C             | -5.01722000 | 4.02753700  | 2.58360500  |
| H             | -5.01952800 | 3.60762500  | 3.59685000  |
| H             | -4.74304100 | 5.08365700  | 2.67511200  |
| H             | -6.04023400 | 3.97247100  | 2.20164600  |
| H             | 5.51547400  | -3.70799000 | -1.87466000 |
| H             | 5.08722000  | -4.03587500 | -0.19430800 |
| H             | 4.39278600  | -5.02328100 | -1.48027600 |
| C             | 3.81108700  | -1.68311100 | 3.18848100  |
| C             | -3.32140700 | -1.10221700 | 3.21623900  |
| H             | -3.56892300 | -1.45018100 | 4.22803600  |
| H             | -3.68796500 | -0.07851400 | 3.10766600  |
| H             | -3.85445300 | -1.73607300 | 2.50488500  |
| F             | 2.45466000  | 1.22730200  | 1.53047300  |
| F             | 4.82970800  | 0.31266300  | 2.43405000  |
| F             | 4.99992600  | -2.14378600 | 3.62193500  |
| F             | 2.77038900  | -3.60833800 | 4.02566000  |
| <b>IM2(S)</b> |             |             |             |
| C             | 5.31018400  | 0.34057200  | -0.72827400 |
| C             | 4.49883900  | -0.67170100 | -1.22784400 |
| C             | 3.46664600  | -0.40173400 | -2.11546800 |
| C             | 3.22525600  | 0.90748000  | -2.55280000 |
| C             | 4.04821600  | 1.91224700  | -2.04002600 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | 2. 17937900  | 1. 28145300  | -3. 58617900 |
| H  | 1. 48070100  | 1. 99825700  | -3. 14038500 |
| H  | 2. 69763500  | 1. 84048000  | -4. 37553400 |
| C  | 1. 40340100  | 0. 11729700  | -4. 21934100 |
| H  | 2. 08524400  | -0. 72915500 | -4. 37297400 |
| H  | 1. 12195500  | 0. 42988600  | -5. 23759200 |
| C  | 0. 13153300  | -0. 37117700 | -3. 52014300 |
| C  | -0. 86850100 | 0. 54205500  | -3. 11789200 |
| H  | -0. 69268600 | 1. 61831800  | -3. 15433900 |
| H  | -1. 92250700 | 0. 26457200  | -3. 15473800 |
| Ni | -0. 13896100 | -0. 22384900 | -1. 50031500 |
| H  | 2. 85652400  | -1. 22579100 | -2. 46277000 |
| C  | 5. 07696900  | 1. 64983800  | -1. 13989500 |
| C  | -0. 28467300 | -1. 75520000 | -3. 99640200 |
| H  | 0. 45458500  | -2. 52072900 | -3. 73100900 |
| H  | -0. 38919300 | -1. 78293400 | -5. 09430600 |
| H  | -1. 24442300 | -2. 05874900 | -3. 56808700 |
| F  | 4. 73815300  | -1. 93687200 | -0. 82316400 |
| F  | 6. 29556400  | 0. 07263000  | 0. 14395100  |
| F  | 5. 84168100  | 2. 64520300  | -0. 66982400 |
| F  | 3. 86232400  | 3. 19551700  | -2. 42427100 |
| C  | -0. 81517700 | -0. 20570000 | 0. 29782900  |
| C  | -2. 40851900 | 0. 02747700  | 2. 05619900  |
| C  | -1. 22743000 | -0. 80260800 | 2. 56617100  |
| H  | -2. 45558600 | 1. 01011400  | 2. 53974000  |
| H  | -3. 36959900 | -0. 47260100 | 2. 18626100  |
| H  | -0. 79058300 | -0. 40664700 | 3. 48438500  |
| H  | -1. 50275200 | -1. 85133400 | 2. 73277100  |
| N  | -0. 26627000 | -0. 70294400 | 1. 44053300  |
| N  | -2. 08510500 | 0. 17573800  | 0. 61680100  |
| C  | 1. 09426300  | -1. 12010900 | 1. 62625100  |
| C  | 2. 04674300  | -0. 17032000 | 2. 07490600  |
| C  | 1. 44785000  | -2. 47601900 | 1. 47205900  |
| C  | 3. 34815800  | -0. 60747100 | 2. 33411300  |
| C  | 2. 76028900  | -2. 86288800 | 1. 78103300  |
| C  | 3. 72572500  | -1. 94919400 | 2. 19924300  |
| H  | 4. 09606700  | 0. 10982500  | 2. 65771500  |
| H  | 3. 03915300  | -3. 90788300 | 1. 67978800  |
| C  | -3. 01494300 | 0. 79937800  | -0. 28395200 |
| C  | -3. 09776500 | 2. 20353300  | -0. 35275700 |
| C  | -3. 87823800 | -0. 01138400 | -1. 06228700 |
| C  | -4. 03013500 | 2. 78093200  | -1. 22577700 |
| C  | -4. 79205400 | 0. 61529400  | -1. 91204400 |
| C  | -4. 88261100 | 2. 01046800  | -2. 01284400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.08129100 | 3.86427000  | -1.29551900 |
| H | -5.45139100 | 0.00865400  | -2.52454000 |
| C | 0.43803900  | -3.53004700 | 1.03364300  |
| C | 1.66341100  | 1.29236000  | 2.29138900  |
| C | -2.24256000 | 3.11960800  | 0.52872900  |
| C | -3.79933100 | -1.53536500 | -0.97717800 |
| H | -2.73681800 | -1.78549000 | -0.89400000 |
| H | -0.53251500 | -3.03305600 | 0.94928900  |
| H | 0.87228000  | 1.52124600  | 1.57193200  |
| H | -1.52234000 | 2.48275900  | 1.04709200  |
| C | 0.70624200  | -4.16755300 | -0.33907800 |
| C | -0.30247900 | -4.96896600 | -0.90289200 |
| C | 1.89832700  | -4.01688200 | -1.06028300 |
| C | -0.12528800 | -5.60823300 | -2.12909700 |
| H | -1.24274800 | -5.09858100 | -0.37234000 |
| C | 2.08118300  | -4.65988500 | -2.28992900 |
| H | 2.69716500  | -3.39636200 | -0.67301300 |
| C | 1.07509600  | -5.46038000 | -2.82929600 |
| H | -0.92398300 | -6.22157700 | -2.53698700 |
| H | 3.01960800  | -4.53122200 | -2.82260800 |
| H | 1.22023200  | -5.96008400 | -3.78264100 |
| C | 0.29221900  | -4.62507700 | 2.12072700  |
| H | 1.21803700  | -5.19551700 | 2.23988300  |
| H | 0.04302500  | -4.17689500 | 3.08776900  |
| H | -0.50020400 | -5.33111000 | 1.85731000  |
| C | 1.08907800  | 1.57660000  | 3.68493300  |
| C | 1.47674000  | 0.86092300  | 4.82626700  |
| C | 0.18154200  | 2.63600700  | 3.84459700  |
| C | 0.96867800  | 1.19041900  | 6.08606800  |
| H | 2.17540800  | 0.03559400  | 4.73064800  |
| C | -0.32723400 | 2.96846400  | 5.10080900  |
| H | -0.12032200 | 3.21329100  | 2.97400500  |
| C | 0.06401900  | 2.24358100  | 6.22924100  |
| H | 1.28160000  | 0.61979100  | 6.95621600  |
| H | -1.02997300 | 3.79150100  | 5.19716800  |
| H | -0.33242500 | 2.49701000  | 7.20818300  |
| C | 2.81535000  | 2.28048100  | 2.00285100  |
| H | 3.24601900  | 2.10292700  | 1.01360200  |
| H | 2.43546900  | 3.30564200  | 2.03088800  |
| H | 3.61395300  | 2.20975300  | 2.74716900  |
| C | -1.41355500 | 4.12135600  | -0.27945500 |
| C | -1.83023200 | 5.43877500  | -0.51574300 |
| C | -0.16976000 | 3.72029600  | -0.79403300 |
| C | -1.03471400 | 6.32390100  | -1.24979400 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.77656600 | 5.79167600  | -0.11810800 |
| C | 0.63326600  | 4.60376600  | -1.51690400 |
| H | 0.16658000  | 2.69886900  | -0.63136100 |
| C | 0.20031300  | 5.91187800  | -1.75059100 |
| H | -1.38019100 | 7.34003800  | -1.41967900 |
| H | 1.60024800  | 4.27385500  | -1.88571400 |
| H | 0.82301500  | 6.60342700  | -2.31089400 |
| C | -3.12221700 | 3.79034600  | 1.60555400  |
| H | -3.60788700 | 3.03317200  | 2.22800200  |
| H | -2.52221300 | 4.43667800  | 2.25431700  |
| H | -3.91642100 | 4.39823000  | 1.16236700  |
| C | -4.49546500 | -2.10334100 | 0.26213900  |
| C | -5.72244900 | -1.60221800 | 0.72081000  |
| C | -3.93357800 | -3.19737600 | 0.93623300  |
| C | -6.36406700 | -2.17466700 | 1.82170100  |
| H | -6.17451300 | -0.75223900 | 0.21765100  |
| C | -4.57115400 | -3.77320900 | 2.03710600  |
| H | -2.98618200 | -3.60285600 | 0.59004400  |
| C | -5.79084200 | -3.26161600 | 2.48559100  |
| H | -7.31272000 | -1.76835800 | 2.16183200  |
| H | -4.11405400 | -4.61825400 | 2.54465800  |
| H | -6.28848700 | -3.70418500 | 3.34363600  |
| C | -4.32427600 | -2.25819000 | -2.23605400 |
| H | -5.40754000 | -2.15160600 | -2.35070000 |
| H | -3.84097000 | -1.87655900 | -3.14090400 |
| H | -4.11033800 | -3.32820100 | -2.15856300 |
| C | 5.14811500  | -2.37537800 | 2.47261200  |
| C | -5.86678700 | 2.64981500  | -2.96405200 |
| H | -5.95669100 | 3.72436900  | -2.78343900 |
| H | -5.55391300 | 2.51367500  | -4.00632500 |
| H | -6.86259100 | 2.20401700  | -2.86763300 |
| H | 5.24245600  | -3.46433500 | 2.49801800  |
| H | 5.81456800  | -1.99700100 | 1.69055400  |
| H | 5.50791300  | -1.97892200 | 3.42802900  |

### TS1(S)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.60455000 | -0.84070800 | -1.17084800 |
| C | -3.35564100 | -0.24132600 | -1.31459000 |
| C | -2.18766000 | -0.96898800 | -1.48586800 |
| C | -2.30892100 | -2.37467000 | -1.64146700 |
| C | -3.55785000 | -2.97797700 | -1.51080700 |
| C | -1.09734600 | -3.16786200 | -2.08334800 |
| H | -0.32144900 | -3.13549400 | -1.31102200 |
| H | -1.36413600 | -4.21916600 | -2.21472900 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.50869000 | -2.63055200 | -3.41934100 |
| H  | -1.27626500 | -2.74047700 | -4.19485900 |
| H  | 0.32877500  | -3.27526500 | -3.71044400 |
| C  | -0.03093100 | -1.16003300 | -3.39593000 |
| C  | 1.21318500  | -0.83782800 | -2.74276200 |
| H  | 1.81244600  | -1.64337100 | -2.32599600 |
| H  | 1.79605700  | -0.01181500 | -3.14548800 |
| Ni | -0.19130600 | -0.34213600 | -1.44054200 |
| H  | -1.16326000 | -0.71179800 | -2.57080600 |
| C  | -4.70473800 | -2.22556100 | -1.25859900 |
| C  | -0.40037200 | -0.35827600 | -4.64518900 |
| H  | -1.48329700 | -0.33358100 | -4.81339300 |
| H  | 0.05915500  | -0.81273600 | -5.53204500 |
| H  | -0.04149900 | 0.67258000  | -4.57307000 |
| F  | -3.32881800 | 1.11265100  | -1.29850300 |
| F  | -5.71474400 | -0.10572800 | -0.95340200 |
| F  | -5.90233400 | -2.82522900 | -1.13373300 |
| F  | -3.71063600 | -4.31741200 | -1.65051800 |
| C  | 0.60575700  | 0.26580900  | 0.21103000  |
| C  | 0.92287200  | 1.40311200  | 2.27839900  |
| C  | 2.16831300  | 0.57455700  | 1.98214200  |
| H  | 1.11552900  | 2.47848700  | 2.19850400  |
| H  | 0.49031400  | 1.19475100  | 3.25776900  |
| H  | 3.08781000  | 1.16113000  | 2.00010300  |
| H  | 2.27761600  | -0.27108800 | 2.67139100  |
| N  | 1.89595000  | 0.07785000  | 0.60953200  |
| N  | -0.00140200 | 0.97456600  | 1.20077600  |
| C  | 3.00007200  | -0.49548800 | -0.11112300 |
| C  | 3.78281200  | 0.33828000  | -0.94778500 |
| C  | 3.38605400  | -1.82832600 | 0.14012500  |
| C  | 4.92758400  | -0.20214500 | -1.53915400 |
| C  | 4.56681800  | -2.30369600 | -0.45093700 |
| C  | 5.34338600  | -1.51696300 | -1.29961200 |
| H  | 5.52966000  | 0.41832700  | -2.19547400 |
| H  | 4.89020700  | -3.31855400 | -0.23847400 |
| C  | -1.38057500 | 1.37283600  | 1.28799900  |
| C  | -1.76884800 | 2.66089800  | 0.87452000  |
| C  | -2.31126300 | 0.49803400  | 1.89958900  |
| C  | -3.10809600 | 3.04036600  | 1.02894600  |
| C  | -3.63614000 | 0.92210100  | 2.01602200  |
| C  | -4.05926900 | 2.18211300  | 1.57338400  |
| H  | -3.41730900 | 4.02203300  | 0.67932700  |
| H  | -4.37189300 | 0.25457000  | 2.45331100  |
| C  | 2.60123700  | -2.73874000 | 1.07854300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.40520700  | 1.79839200  | -1.19250400 |
| C | -0.77778400 | 3.67582700  | 0.29694700  |
| C | -1.87596500 | -0.86221800 | 2.44209900  |
| H | -1.07451300 | -1.22440400 | 1.79251100  |
| H | 1.77924500  | -2.14786100 | 1.49161700  |
| H | 2.31422300  | 1.85552600  | -1.14731300 |
| H | 0.17376300  | 3.15608400  | 0.15703800  |
| C | 1.94674000  | -3.97011700 | 0.43099100  |
| C | 0.96494700  | -4.65192600 | 1.17200500  |
| C | 2.27991900  | -4.48061700 | -0.83070500 |
| C | 0.35279600  | -5.80537300 | 0.68414300  |
| H | 0.67714800  | -4.27508900 | 2.15052400  |
| C | 1.67022900  | -5.63951600 | -1.32361900 |
| H | 3.01526500  | -3.97501800 | -1.44537400 |
| C | 0.70841800  | -6.31000100 | -0.56959600 |
| H | -0.40252600 | -6.30813300 | 1.28158300  |
| H | 1.95177100  | -6.01364600 | -2.30413900 |
| H | 0.23624100  | -7.20953200 | -0.95351400 |
| C | 3.48862700  | -3.17855200 | 2.27195500  |
| H | 4.31561900  | -3.81259100 | 1.93910700  |
| H | 3.91290400  | -2.30758300 | 2.78157400  |
| H | 2.90469800  | -3.75062300 | 2.99853800  |
| C | 3.94772000  | 2.75892800  | -0.12733200 |
| C | 5.15716100  | 2.53819600  | 0.54675700  |
| C | 3.24629900  | 3.94452700  | 0.14409200  |
| C | 5.64544200  | 3.46899100  | 1.46819900  |
| H | 5.72051800  | 1.62987200  | 0.35637100  |
| C | 3.73137800  | 4.87681500  | 1.06258100  |
| H | 2.31490600  | 4.14414600  | -0.38045000 |
| C | 4.93496600  | 4.64108100  | 1.73152300  |
| H | 6.58367400  | 3.27446900  | 1.98059700  |
| H | 3.16872400  | 5.78595500  | 1.25570500  |
| H | 5.31380300  | 5.36291900  | 2.44921300  |
| C | 3.81442400  | 2.31251300  | -2.59168600 |
| H | 3.45726900  | 1.64353800  | -3.38065900 |
| H | 3.38106900  | 3.30253900  | -2.75960800 |
| H | 4.89933000  | 2.41396700  | -2.68989000 |
| C | -1.20134800 | 4.16870500  | -1.08949500 |
| C | -1.76111200 | 5.43393400  | -1.31111800 |
| C | -1.02309900 | 3.32126200  | -2.19511500 |
| C | -2.13827300 | 5.83847400  | -2.59588100 |
| H | -1.90302700 | 6.12094400  | -0.48320800 |
| C | -1.39489000 | 3.72232500  | -3.47742000 |
| H | -0.59277400 | 2.33335900  | -2.04243900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.95730400 | 4.98553200  | -3.68385700 |
| H | -2.57009900 | 6.82482700  | -2.74207200 |
| H | -1.24655800 | 3.04851800  | -4.31695300 |
| H | -2.24751200 | 5.30015000  | -4.68224000 |
| C | -0.53636000 | 4.81624300  | 1.30666700  |
| H | -0.14104500 | 4.41825300  | 2.24552600  |
| H | 0.18087300  | 5.54424900  | 0.91391500  |
| H | -1.46234200 | 5.34658100  | 1.54754000  |
| C | -1.29953200 | -0.78028500 | 3.86057200  |
| C | -1.82471700 | 0.08099700  | 4.83499700  |
| C | -0.24905600 | -1.63328100 | 4.23187700  |
| C | -1.31349800 | 0.09081400  | 6.13507600  |
| H | -2.63426200 | 0.75553100  | 4.57311800  |
| C | 0.26518000  | -1.62759000 | 5.53000900  |
| H | 0.16703900  | -2.31396700 | 3.49332400  |
| C | -0.26590100 | -0.76200000 | 6.48872200  |
| H | -1.73498800 | 0.76908400  | 6.87197400  |
| H | 1.08067600  | -2.29677400 | 5.79037200  |
| H | 0.13286400  | -0.75146800 | 7.49897100  |
| C | -2.98799600 | -1.93258700 | 2.40154400  |
| H | -3.79351100 | -1.71592800 | 3.10964800  |
| H | -3.41587600 | -2.01301600 | 1.39893900  |
| H | -2.56959800 | -2.90536000 | 2.67679500  |
| C | 6.58893700  | -2.06567000 | -1.95485900 |
| C | -5.51799000 | 2.56407200  | 1.64339400  |
| H | -5.66204900 | 3.63752300  | 1.49337700  |
| H | -6.08034800 | 2.03741100  | 0.86300900  |
| H | -5.96207900 | 2.28839800  | 2.60564800  |
| H | 6.95307500  | -2.95717900 | -1.43681400 |
| H | 6.39475600  | -2.34679200 | -2.99723300 |
| H | 7.39412200  | -1.32423600 | -1.96663100 |

### IM3(S)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.14697800 | -2.17367700 | -1.94508000 |
| C | -2.09683700 | -1.26686000 | -1.82206600 |
| C | -0.76920000 | -1.65837200 | -1.74313500 |
| C | -0.47966200 | -3.03309300 | -1.88639700 |
| C | -1.52964500 | -3.94034400 | -2.01691400 |
| C | 0.95601900  | -3.49886400 | -1.95405800 |
| H | 1.02656300  | -4.56537100 | -1.72004600 |
| H | 1.51408400  | -2.96074300 | -1.18239300 |
| C | 1.60805200  | -3.23439300 | -3.33124800 |
| H | 2.69953300  | -3.28945300 | -3.20908200 |
| H | 1.33508900  | -4.04507200 | -4.01958600 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.23842400  | -1.89129700 | -3.99664600 |
| C  | 1.35310900  | -0.69296600 | -3.05508000 |
| H  | 1.07922800  | 0.22944300  | -3.59514500 |
| H  | 2.39873900  | -0.58048700 | -2.69802800 |
| Ni | 0.53424200  | -0.36348500 | -1.36612200 |
| C  | 0.25612900  | 0.47153300  | 0.45523800  |
| C  | 0.97485500  | 2.03088900  | 2.09672600  |
| C  | -0.18959200 | 1.20506800  | 2.65930300  |
| H  | 1.86095300  | 1.98932900  | 2.73323300  |
| H  | 0.71181700  | 3.08060100  | 1.93331200  |
| H  | 0.11722600  | 0.53792800  | 3.46858800  |
| H  | -1.00439600 | 1.83322300  | 3.01744600  |
| N  | -0.61662100 | 0.39801100  | 1.48146100  |
| N  | 1.21968300  | 1.36120400  | 0.79794900  |
| C  | -1.76654000 | -0.47048300 | 1.53209100  |
| C  | -1.58646200 | -1.86602600 | 1.70525400  |
| C  | -3.06247200 | 0.07986900  | 1.42363000  |
| C  | -2.71674000 | -2.68569700 | 1.66569900  |
| C  | -4.15613200 | -0.79362300 | 1.38196400  |
| C  | -4.00477300 | -2.17579800 | 1.46715600  |
| H  | -2.59859600 | -3.75841200 | 1.77048100  |
| H  | -5.15141500 | -0.37851100 | 1.25397000  |
| C  | 2.26027800  | 1.76351800  | -0.11030400 |
| C  | 3.57319100  | 1.28064600  | 0.08237000  |
| C  | 1.96778500  | 2.65752500  | -1.17383500 |
| C  | 4.56638600  | 1.65068400  | -0.83110200 |
| C  | 2.99817800  | 2.98260500  | -2.06152800 |
| C  | 4.29858500  | 2.48463500  | -1.91667600 |
| H  | 5.57219800  | 1.26235800  | -0.69366300 |
| H  | 2.79032000  | 3.65061800  | -2.89100600 |
| C  | -3.32978700 | 1.59213700  | 1.45322900  |
| C  | -0.20074000 | -2.46832600 | 1.94816200  |
| C  | 3.96328100  | 0.42339900  | 1.28857200  |
| C  | 0.59119900  | 3.30700800  | -1.31730600 |
| H  | -0.14778700 | 2.58754100  | -0.95517000 |
| H  | -2.38759600 | 2.09795900  | 1.22333200  |
| H  | 0.47838600  | -2.01008300 | 1.22246600  |
| H  | 3.03628000  | 0.08379400  | 1.76052000  |
| C  | -4.33848100 | 2.07600800  | 0.40706100  |
| C  | -5.70896000 | 2.20746900  | 0.67743400  |
| C  | -3.88728000 | 2.43610100  | -0.87172300 |
| C  | -6.59636000 | 2.66968100  | -0.29847100 |
| H  | -6.09905800 | 1.95874200  | 1.65895700  |
| C  | -4.76753100 | 2.90345800  | -1.84783800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.83369200 | 2.33487000  | -1.10894700 |
| C | -6.13018400 | 3.02072600  | -1.56551800 |
| H | -7.65289500 | 2.76022900  | -0.06168400 |
| H | -4.38761300 | 3.17638100  | -2.82843500 |
| H | -6.81873500 | 3.38472800  | -2.32257200 |
| C | -3.74919700 | 2.00176900  | 2.88522300  |
| H | -4.66817100 | 1.49338300  | 3.19009600  |
| H | -2.98368100 | 1.72675800  | 3.61549200  |
| H | -3.91659300 | 3.08161300  | 2.94913200  |
| C | 0.34933000  | -2.15851300 | 3.34380400  |
| C | -0.48104800 | -2.07678200 | 4.47059000  |
| C | 1.73367200  | -2.01918000 | 3.52763000  |
| C | 0.05458400  | -1.84806000 | 5.74069100  |
| H | -1.55513100 | -2.18513100 | 4.35162000  |
| C | 2.27245900  | -1.79003600 | 4.79535700  |
| H | 2.39652500  | -2.10051900 | 2.66932800  |
| C | 1.43295800  | -1.69968500 | 5.90831000  |
| H | -0.60786300 | -1.78503600 | 6.59973500  |
| H | 3.34746700  | -1.68292700 | 4.91234900  |
| H | 1.84883900  | -1.51849700 | 6.89524700  |
| C | -0.12594600 | -3.99370200 | 1.71869800  |
| H | -0.49584800 | -4.26811100 | 0.72747700  |
| H | 0.91475500  | -4.32031800 | 1.79920400  |
| H | -0.69760800 | -4.54552100 | 2.47153800  |
| C | 4.72567600  | -0.83806800 | 0.87406100  |
| C | 4.05530100  | -1.81310800 | 0.11668700  |
| C | 6.06076200  | -1.07839800 | 1.22238000  |
| C | 4.69308000  | -2.98790600 | -0.27775400 |
| H | 3.02224500  | -1.63822800 | -0.17337300 |
| C | 6.70644400  | -2.25433100 | 0.82426300  |
| H | 6.61184200  | -0.35361600 | 1.81189200  |
| C | 6.02720600  | -3.21340100 | 0.07479700  |
| H | 4.14922900  | -3.72758800 | -0.85858900 |
| H | 7.74307800  | -2.41685700 | 1.10614300  |
| H | 6.52807100  | -4.12723200 | -0.23113000 |
| C | 4.71427700  | 1.28718700  | 2.32201600  |
| H | 4.10517900  | 2.14448800  | 2.62143200  |
| H | 4.94984600  | 0.70768300  | 3.22011400  |
| H | 5.64896200  | 1.68363600  | 1.91352300  |
| C | 0.44068500  | 4.56851600  | -0.45564200 |
| C | 1.50785500  | 5.44145800  | -0.20140200 |
| C | -0.82335800 | 4.90050500  | 0.05761700  |
| C | 1.31827600  | 6.60762900  | 0.54451300  |
| H | 2.49670100  | 5.20785900  | -0.58355800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.01595600 | 6.06478600  | 0.80311700  |
| H | -1.66926200 | 4.24571500  | -0.13594500 |
| C | 0.05681100  | 6.92415000  | 1.05130900  |
| H | 2.16096900  | 7.26789000  | 0.73041500  |
| H | -2.00371800 | 6.29798400  | 1.19088600  |
| H | -0.08908400 | 7.82911300  | 1.63395200  |
| C | 0.20480100  | 3.62245200  | -2.77935700 |
| H | -0.83505100 | 3.95937700  | -2.81735100 |
| H | 0.81910200  | 4.42140500  | -3.20480600 |
| H | 0.30132400  | 2.73364800  | -3.41072900 |
| C | -5.18305300 | -3.10437800 | 1.29946900  |
| C | 5.37438900  | 2.83390900  | -2.91706500 |
| H | 6.37290300  | 2.72313400  | -2.48542000 |
| H | 5.32060100  | 2.17657800  | -3.79342000 |
| H | 5.26703800  | 3.86174300  | -3.27687100 |
| H | -6.12455200 | -2.61444900 | 1.56387300  |
| H | -5.26077200 | -3.42622300 | 0.25363100  |
| H | -5.07808900 | -4.00498700 | 1.91222000  |
| F | -4.43082400 | -1.76424300 | -1.94721400 |
| F | -2.43033500 | 0.05039100  | -1.75233400 |
| F | -1.28532600 | -5.27105300 | -2.12203000 |
| C | -2.86080300 | -3.52926800 | -2.03170300 |
| F | -3.86426100 | -4.42687400 | -2.11084900 |
| C | 2.08122300  | -1.69918300 | -5.27157600 |
| H | 0.18876200  | -1.96076600 | -4.31318900 |
| H | 3.14607400  | -1.60043200 | -5.02577200 |
| H | 1.97515700  | -2.55006000 | -5.95628200 |
| H | 1.77937700  | -0.79504000 | -5.81199100 |

**TS2(S)**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.55046700  | -4.15128200 | -2.06237600 |
| C | -0.12389700 | -2.94833900 | -1.88943000 |
| C | 0.46968800  | -1.70597800 | -2.13488700 |
| C | 1.78778700  | -1.71164900 | -2.66908100 |
| C | 2.45134700  | -2.91987800 | -2.83990400 |
| C | 2.37250300  | -0.40047000 | -3.13367200 |
| H | 3.41587000  | -0.53072200 | -3.42962000 |
| H | 2.36079500  | 0.29394000  | -2.28687700 |
| C | 1.54873600  | 0.21386000  | -4.30619700 |
| H | 1.46285700  | 1.29705400  | -4.15174800 |
| H | 2.09286700  | 0.07796800  | -5.24808700 |
| C | 0.14081500  | -0.38706400 | -4.48189500 |
| C | -0.64994100 | -0.44769500 | -3.16881200 |
| H | -1.56836700 | -1.03083200 | -3.27984500 |
| H | -0.93969800 | 0.59800600  | -2.87646900 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Ni | -0.21958200 | -0.18094300 | -1.26790000 |
| C  | -0.14370700 | 0.45564700  | 0.55905100  |
| C  | 0.28407500  | 1.91569000  | 2.38675600  |
| C  | -0.71394100 | 0.84096000  | 2.83470100  |
| H  | 1.17000300  | 1.94466500  | 3.02292900  |
| H  | -0.15349100 | 2.91795700  | 2.35681200  |
| H  | -0.30873100 | 0.18022400  | 3.60484700  |
| H  | -1.64852200 | 1.26870200  | 3.20373500  |
| N  | -0.94822200 | 0.07860000  | 1.58280600  |
| N  | 0.62978400  | 1.47724300  | 1.01172400  |
| C  | -1.93543400 | -0.96822900 | 1.55235200  |
| C  | -1.54864100 | -2.31684500 | 1.75799100  |
| C  | -3.29366300 | -0.62872900 | 1.39519600  |
| C  | -2.54777000 | -3.29170700 | 1.78232600  |
| C  | -4.25312700 | -1.64990800 | 1.42138900  |
| C  | -3.90424100 | -2.98365900 | 1.61365100  |
| H  | -2.27063000 | -4.33033800 | 1.92730500  |
| H  | -5.29816600 | -1.38788700 | 1.27640800  |
| C  | 1.59325500  | 2.20279300  | 0.22907800  |
| C  | 2.96864300  | 2.00616900  | 0.47265200  |
| C  | 1.16168500  | 3.14988500  | -0.73491100 |
| C  | 3.89814200  | 2.72860500  | -0.28694000 |
| C  | 2.13373200  | 3.83610700  | -1.46796500 |
| C  | 3.50575800  | 3.63752500  | -1.26685900 |
| H  | 4.95749100  | 2.56119900  | -0.11007000 |
| H  | 1.82217200  | 4.55614300  | -2.21767500 |
| C  | -3.77525100 | 0.81529100  | 1.23463700  |
| C  | -0.08054100 | -2.70418000 | 1.94270700  |
| C  | 3.49230300  | 1.07808700  | 1.57426000  |
| C  | -0.32134800 | 3.45270600  | -0.94801000 |
| H  | -0.86302800 | 2.50837600  | -0.83335600 |
| H  | -2.88861500 | 1.44581900  | 1.11982200  |
| H  | 0.49555200  | -2.10915800 | 1.22701900  |
| H  | 2.64979800  | 0.47164500  | 1.91986900  |
| C  | -4.59799400 | 0.99665800  | -0.04567100 |
| C  | -5.93862900 | 1.40206600  | -0.04605200 |
| C  | -3.97964800 | 0.76004800  | -1.28548900 |
| C  | -6.64037500 | 1.56426600  | -1.24617100 |
| H  | -6.45093500 | 1.59847500  | 0.88967700  |
| C  | -4.67403500 | 0.92306900  | -2.48244600 |
| H  | -2.94115300 | 0.43638700  | -1.30609600 |
| C  | -6.01305400 | 1.32648100  | -2.46794200 |
| H  | -7.68015100 | 1.87859200  | -1.21942900 |
| H  | -4.17039200 | 0.73367600  | -3.42665700 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -6.55803400 | 1.45320500  | -3.39894200 |
| C | -4.50441100 | 1.28363900  | 2.50929400  |
| H | -5.41070800 | 0.69936400  | 2.69621000  |
| H | -3.85963100 | 1.16618100  | 3.38461300  |
| H | -4.78579900 | 2.33894700  | 2.43640400  |
| C | 0.46474700  | -2.38160800 | 3.33635600  |
| C | -0.31511600 | -2.52333400 | 4.49287500  |
| C | 1.80692100  | -1.99930300 | 3.48295400  |
| C | 0.22714500  | -2.27974900 | 5.75726900  |
| H | -1.35661500 | -2.81829800 | 4.40279000  |
| C | 2.35250000  | -1.75567600 | 4.74520900  |
| H | 2.43335600  | -1.90008000 | 2.59941700  |
| C | 1.56235800  | -1.89241000 | 5.88909700  |
| H | -0.39635000 | -2.39253800 | 6.64008300  |
| H | 3.39443200  | -1.46018900 | 4.83329400  |
| H | 1.98298800  | -1.70090300 | 6.87206700  |
| C | 0.21264200  | -4.18746900 | 1.62527900  |
| H | -0.17840200 | -4.47414800 | 0.64653900  |
| H | 1.29399700  | -4.35208200 | 1.62634300  |
| H | -0.21592100 | -4.85528000 | 2.37935600  |
| C | 4.54449900  | 0.09853700  | 1.04512800  |
| C | 4.15135200  | -0.89376200 | 0.13113300  |
| C | 5.89144800  | 0.14485100  | 1.42820700  |
| C | 5.07386900  | -1.79916500 | -0.39271500 |
| H | 3.11136100  | -0.94795900 | -0.18066100 |
| C | 6.81865500  | -0.76580500 | 0.91032200  |
| H | 6.23357100  | 0.89038300  | 2.13779600  |
| C | 6.41528900  | -1.73755400 | -0.00360900 |
| H | 4.75274900  | -2.53898800 | -1.11847500 |
| H | 7.85740800  | -0.70886000 | 1.22415800  |
| H | 7.13566800  | -2.44139200 | -0.41043500 |
| C | 3.98717800  | 1.91303500  | 2.77348900  |
| H | 3.19151200  | 2.56122800  | 3.14982300  |
| H | 4.31487200  | 1.26644600  | 3.59361200  |
| H | 4.82189300  | 2.56325900  | 2.49428500  |
| C | -0.89608400 | 4.42122000  | 0.09197200  |
| C | -0.12534200 | 5.42163600  | 0.70017900  |
| C | -2.26217900 | 4.35069000  | 0.40924100  |
| C | -0.70101300 | 6.32045600  | 1.60262100  |
| H | 0.93332000  | 5.49686900  | 0.47141200  |
| C | -2.84002100 | 5.24725700  | 1.30945000  |
| H | -2.88071400 | 3.59019300  | -0.06175300 |
| C | -2.05937600 | 6.23664400  | 1.91260000  |
| H | -0.08380400 | 7.08660300  | 2.06391100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.89941500 | 5.17237000  | 1.53913800  |
| H | -2.50544500 | 6.93394100  | 2.61586400  |
| C | -0.65238400 | 3.96759800  | -2.36573900 |
| H | -1.73752100 | 4.02269600  | -2.49068600 |
| H | -0.25473400 | 4.97153600  | -2.54215800 |
| H | -0.25235900 | 3.29614700  | -3.13217100 |
| C | -4.94663900 | -4.07671300 | 1.62227500  |
| C | 4.52357400  | 4.37761800  | -2.10213400 |
| H | 4.66861100  | 3.88605600  | -3.07202800 |
| H | 4.20345100  | 5.40431300  | -2.30571200 |
| H | 5.49715300  | 4.41466700  | -1.60557200 |
| H | -5.95824200 | -3.66396500 | 1.66269100  |
| H | -4.87550700 | -4.69574800 | 0.72000500  |
| H | -4.81675500 | -4.74498600 | 2.48030000  |
| F | -0.04135800 | -5.32003100 | -1.74440500 |
| F | -1.40284800 | -3.02071200 | -1.43743000 |
| F | 3.72196400  | -2.95180400 | -3.31808900 |
| C | 1.86049100  | -4.14405300 | -2.52798600 |
| F | 2.53305200  | -5.29786300 | -2.69190600 |
| C | -0.64718200 | 0.37516800  | -5.56020500 |
| H | 0.26187300  | -1.41873500 | -4.83748900 |
| H | -0.80178400 | 1.42163500  | -5.27176700 |
| H | -0.10983400 | 0.36757000  | -6.51551600 |
| H | -1.63131300 | -0.07664000 | -5.72549000 |

**2(S)<sup>C-H</sup><sub>endo</sub>**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.99226300  | -0.90892500 | 0.00702600  |
| C | 0.68536000  | -1.38334400 | 0.02747700  |
| C | -0.41757700 | -0.52911000 | 0.02056500  |
| C | -0.19398700 | 0.85956900  | -0.00022900 |
| C | 1.12071200  | 1.32507300  | -0.02316000 |
| C | -1.33870800 | 1.85218800  | -0.02131400 |
| H | -1.42011000 | 2.27188300  | -1.03380000 |
| H | -1.09954600 | 2.69807900  | 0.63159700  |
| C | -2.67618600 | 1.21778300  | 0.37868900  |
| H | -2.69545000 | 1.04008000  | 1.46297200  |
| H | -3.48974600 | 1.91854500  | 0.15978900  |
| C | -2.90633200 | -0.11397300 | -0.35037800 |
| C | -1.81396100 | -1.11625600 | 0.05616400  |
| H | -1.85162100 | -2.00394200 | -0.58463500 |
| H | -2.01952600 | -1.47672600 | 1.07520600  |
| F | 3.03012900  | -1.75757000 | 0.01153700  |
| F | 0.49888700  | -2.71951200 | 0.05292100  |
| F | 1.36130200  | 2.65249900  | -0.04988900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.21324100  | 0.46489000  | -0.01760300 |
| F | 3.46478100  | 0.94504700  | -0.03608800 |
| C | -4.30224400 | -0.68585200 | -0.08478900 |
| H | -2.80965200 | 0.07350000  | -1.43029500 |
| H | -4.45545100 | -0.86333300 | 0.98661300  |
| H | -5.08167000 | 0.00455100  | -0.42401100 |
| H | -4.44860200 | -1.63907800 | -0.60445100 |

**IM7'**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.80314400 | 1.73790100  | 1.06294700  |
| C  | -2.54830900 | 1.15899500  | 0.89610700  |
| C  | -1.79288900 | 0.55763900  | 1.89521800  |
| C  | -2.47022900 | 0.44454800  | 3.14226300  |
| C  | -3.75684300 | 0.96621700  | 3.30746600  |
| H  | 1.63468000  | -0.09086400 | 1.47693000  |
| C  | -1.89616400 | -0.21244700 | 4.39015700  |
| H  | -1.76136400 | 0.54838200  | 5.17217900  |
| H  | -2.65144900 | -0.89719500 | 4.79265100  |
| C  | -0.59444000 | -0.98990800 | 4.23004800  |
| H  | -0.71821000 | -1.78756900 | 3.48291000  |
| H  | -0.38501000 | -1.50944600 | 5.17599900  |
| C  | 0.63515200  | -0.18464100 | 3.87298900  |
| C  | 0.60537800  | 1.15062400  | 3.58328100  |
| H  | -0.29678800 | 1.74232300  | 3.66413700  |
| H  | 1.53506100  | 1.69480300  | 3.44716600  |
| Ni | 0.19999800  | 0.17627000  | 1.65572800  |
| C  | 0.41347700  | -0.01489700 | -0.21719300 |
| C  | 0.92356100  | 0.63874300  | -2.41242900 |
| C  | 0.47024000  | -0.81810700 | -2.42915200 |
| H  | 1.84398500  | 0.80409600  | -2.97058600 |
| H  | 0.15444900  | 1.31815700  | -2.79781500 |
| H  | 1.29404100  | -1.51877500 | -2.60404100 |
| H  | -0.30376000 | -0.99525500 | -3.17150200 |
| N  | -0.05016600 | -0.98877600 | -1.04707500 |
| N  | 1.11861500  | 0.87914900  | -0.96563600 |
| C  | -0.72607300 | -2.18952100 | -0.60971900 |
| C  | -0.01977600 | -3.14108700 | 0.17252400  |
| C  | -2.06838600 | -2.44782000 | -0.98849300 |
| C  | -0.72968700 | -4.21044600 | 0.72786200  |
| C  | -2.72289100 | -3.53826700 | -0.40178500 |
| C  | -2.09316400 | -4.40199300 | 0.49267800  |
| H  | -0.20499800 | -4.93216700 | 1.34388400  |
| H  | -3.76340600 | -3.71497000 | -0.64939200 |
| C  | 1.97955800  | 1.94173800  | -0.49543800 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 3. 37726100  | 1. 72059000  | -0. 44300800 |
| C | 1. 45633500  | 3. 21579900  | -0. 16656200 |
| C | 4. 20916100  | 2. 75016700  | 0. 01217200  |
| C | 2. 33500400  | 4. 20320500  | 0. 29361900  |
| C | 3. 71173400  | 3. 99189200  | 0. 40416300  |
| H | 5. 27884600  | 2. 56548800  | 0. 06676100  |
| H | 1. 93576900  | 5. 17558900  | 0. 56397700  |
| C | -2. 77030000 | -1. 69786600 | -2. 13484100 |
| C | 1. 50497000  | -3. 11592300 | 0. 29059000  |
| C | 4. 04971900  | 0. 43802400  | -0. 94296600 |
| C | -0. 01734000 | 3. 54596700  | -0. 35628500 |
| H | -0. 56533600 | 2. 61446700  | -0. 25436100 |
| H | -2. 32501600 | -0. 70145200 | -2. 19847000 |
| H | 1. 81812200  | -2. 07938100 | 0. 43433000  |
| H | 3. 27583900  | -0. 33039300 | -1. 03035300 |
| C | -4. 27818100 | -1. 48882700 | -1. 96446800 |
| C | -5. 22623800 | -2. 48722700 | -2. 24711200 |
| C | -4. 75485700 | -0. 23769000 | -1. 55440600 |
| C | -6. 59340300 | -2. 24967500 | -2. 08760600 |
| H | -4. 90864600 | -3. 46156500 | -2. 60474800 |
| C | -6. 11983600 | 0. 00589700  | -1. 39151200 |
| H | -4. 04751300 | 0. 55921900  | -1. 37014400 |
| C | -7. 04745500 | -1. 00318700 | -1. 65253700 |
| H | -7. 30359400 | -3. 04130100 | -2. 31048100 |
| H | -6. 44776600 | 0. 98648700  | -1. 05968900 |
| H | -8. 11086100 | -0. 81957300 | -1. 52821500 |
| C | -2. 48454200 | -2. 45217100 | -3. 46053100 |
| H | -1. 41463700 | -2. 60519800 | -3. 62039800 |
| H | -2. 88921600 | -1. 89769700 | -4. 31320600 |
| H | -2. 94293700 | -3. 44466900 | -3. 45244500 |
| C | 2. 18822900  | -3. 63360200 | -0. 98592900 |
| C | 1. 55997800  | -4. 50707900 | -1. 88515100 |
| C | 3. 52141200  | -3. 27176800 | -1. 23965100 |
| C | 2. 23795800  | -4. 99267500 | -3. 00715500 |
| H | 0. 53253700  | -4. 81028500 | -1. 71191100 |
| C | 4. 20060700  | -3. 75442800 | -2. 35929900 |
| H | 4. 03652400  | -2. 61074900 | -0. 54833400 |
| C | 3. 55949400  | -4. 61719600 | -3. 25177200 |
| H | 1. 72817000  | -5. 66647300 | -3. 69047200 |
| H | 5. 23113200  | -3. 45602100 | -2. 53186900 |
| H | 4. 08443800  | -4. 99274200 | -4. 12541000 |
| C | 2. 05379600  | -3. 90955300 | 1. 49758100  |
| H | 1. 54426600  | -3. 63007100 | 2. 42427900  |
| H | 3. 12090000  | -3. 70395700 | 1. 61774700  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 1. 94451700  | -4. 98947700 | 1. 35971700  |
| C | 5. 09329300  | -0. 09771400 | 0. 04557900  |
| C | 4. 67616700  | -0. 50315300 | 1. 32517200  |
| C | 6. 45300900  | -0. 22207800 | -0. 27001500 |
| C | 5. 58184300  | -1. 01449300 | 2. 25314400  |
| H | 3. 62537400  | -0. 40957700 | 1. 58634900  |
| C | 7. 36610500  | -0. 73004000 | 0. 66125800  |
| H | 6. 81861700  | 0. 07455000  | -1. 24681700 |
| C | 6. 93640800  | -1. 12893100 | 1. 92535700  |
| H | 5. 23117600  | -1. 32415900 | 3. 23397800  |
| H | 8. 41501600  | -0. 81330500 | 0. 39027800  |
| H | 7. 64466900  | -1. 52595000 | 2. 64682700  |
| C | 4. 63023200  | 0. 67049200  | -2. 35417800 |
| H | 5. 03725100  | -0. 25663500 | -2. 76969200 |
| H | 5. 42555900  | 1. 42193700  | -2. 33829400 |
| H | 3. 86141500  | 1. 03648100  | -3. 03828200 |
| C | -0. 34274900 | 4. 08730700  | -1. 75592400 |
| C | 0. 57186400  | 4. 81774800  | -2. 52695800 |
| C | -1. 63551100 | 3. 88919600  | -2. 27125500 |
| C | 0. 20805300  | 5. 33603200  | -3. 77310400 |
| H | 1. 57893500  | 4. 98122000  | -2. 15617400 |
| C | -2. 00041800 | 4. 40649900  | -3. 51485600 |
| H | -2. 35889200 | 3. 32648200  | -1. 68864600 |
| C | -1. 07882100 | 5. 13333800  | -4. 27304900 |
| H | 0. 93525900  | 5. 89803000  | -4. 35315900 |
| H | -3. 00535300 | 4. 23868200  | -3. 89279800 |
| H | -1. 36077500 | 5. 53457300  | -5. 24238100 |
| C | -0. 57980300 | 4. 50520600  | 0. 71747300  |
| H | -1. 66601500 | 4. 57761600  | 0. 61127400  |
| H | -0. 17750300 | 5. 51833500  | 0. 62196300  |
| H | -0. 35872000 | 4. 13789700  | 1. 72478000  |
| C | -2. 85026600 | -5. 52442400 | 1. 16054700  |
| C | 4. 62565700  | 5. 06995200  | 0. 93613900  |
| H | 4. 25837000  | 6. 06811200  | 0. 67926300  |
| H | 5. 64024200  | 4. 96530800  | 0. 54096500  |
| H | 4. 69536200  | 5. 02138800  | 2. 02996200  |
| H | -3. 69052600 | -5. 86224500 | 0. 54696400  |
| H | -3. 26176500 | -5. 19991200 | 2. 12442300  |
| H | -2. 20174000 | -6. 38348600 | 1. 35774600  |
| C | -4. 43291900 | 1. 63044600  | 2. 29230500  |
| C | 1. 94720000  | -0. 89909700 | 4. 09512700  |
| H | 2. 06332000  | -1. 09835600 | 5. 16932900  |
| H | 2. 79575100  | -0. 29824100 | 3. 76400400  |
| H | 1. 98067100  | -1. 86465600 | 3. 58487300  |

|               |             |             |             |
|---------------|-------------|-------------|-------------|
| F             | -2.07352900 | 1.25108200  | -0.39520700 |
| F             | -4.41744800 | 2.38979900  | 0.04769500  |
| F             | -5.65705800 | 2.15063000  | 2.49023600  |
| F             | -4.39050600 | 0.85166300  | 4.50243800  |
| <b>TS4(S)</b> |             |             |             |
| C             | -3.99807000 | 1.67797700  | 1.59788900  |
| C             | -2.67024200 | 1.43971900  | 1.25476500  |
| C             | -1.80415700 | 0.61935900  | 1.95889100  |
| C             | -2.37643500 | -0.07459400 | 3.06374400  |
| C             | -3.72873000 | 0.10837000  | 3.36870300  |
| H             | 1.37838200  | -0.47160000 | 2.01965700  |
| C             | -1.62776000 | -0.98299900 | 4.04247400  |
| H             | -1.61677300 | -0.49249900 | 5.02585200  |
| H             | -2.23362900 | -1.88373600 | 4.19309100  |
| C             | -0.19957900 | -1.45897300 | 3.71910000  |
| H             | -0.22838700 | -2.10682700 | 2.83545300  |
| H             | 0.11888900  | -2.10371100 | 4.55021000  |
| C             | 0.87379700  | -0.37763700 | 3.51074200  |
| C             | 0.42855600  | 0.97171500  | 3.54132500  |
| H             | -0.50459200 | 1.24967900  | 4.00749100  |
| H             | 1.18397400  | 1.75731600  | 3.50935300  |
| Ni            | 0.11963200  | 0.30659800  | 1.66001300  |
| C             | 0.41423300  | 0.07359100  | -0.24954300 |
| C             | 1.15750200  | 0.76205800  | -2.38014700 |
| C             | 0.41467800  | -0.56299700 | -2.52500900 |
| H             | 2.12799200  | 0.75847600  | -2.87489600 |
| H             | 0.57618700  | 1.60982300  | -2.75929000 |
| H             | 1.08149600  | -1.40246000 | -2.74813700 |
| H             | -0.35541000 | -0.51402600 | -3.29151000 |
| N             | -0.17577400 | -0.73690900 | -1.17134500 |
| N             | 1.29799200  | 0.87248700  | -0.91032500 |
| C             | -0.97285500 | -1.89311200 | -0.83365500 |
| C             | -0.37133700 | -2.97876600 | -0.14391800 |
| C             | -2.33185900 | -1.97146400 | -1.22647000 |
| C             | -1.19189300 | -4.01694200 | 0.30935300  |
| C             | -3.10035900 | -3.03915600 | -0.74638200 |
| C             | -2.56624900 | -4.04501300 | 0.05818200  |
| H             | -0.74941600 | -4.84331300 | 0.85531000  |
| H             | -4.15229600 | -3.08203200 | -1.00653800 |
| C             | 2.22756700  | 1.80604700  | -0.31713100 |
| C             | 3.59327800  | 1.45052200  | -0.21659300 |
| C             | 1.80090400  | 3.09391100  | 0.08938800  |
| C             | 4.48121100  | 2.34826600  | 0.38871400  |
| C             | 2.72906200  | 3.94504100  | 0.69830000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 4.06933100  | 3.58775200  | 0.87618300  |
| H | 5.52558200  | 2.06200600  | 0.48133800  |
| H | 2.40261000  | 4.92438600  | 1.03374400  |
| C | -2.93965500 | -1.03465000 | -2.28426700 |
| C | 1.14792000  | -3.12028700 | -0.02859500 |
| C | 4.17718500  | 0.17895100  | -0.84094900 |
| C | 0.38648100  | 3.57873600  | -0.19213000 |
| H | -0.25774900 | 2.70393900  | -0.17939100 |
| H | -2.39062500 | -0.08877700 | -2.24300800 |
| H | 1.56941000  | -2.12619800 | 0.13871200  |
| H | 3.34517600  | -0.49994700 | -1.05206300 |
| C | -4.41940800 | -0.69248200 | -2.08967400 |
| C | -5.45445700 | -1.54023400 | -2.52036100 |
| C | -4.77822900 | 0.52737800  | -1.50135300 |
| C | -6.79502800 | -1.19026500 | -2.34714700 |
| H | -5.22515900 | -2.48325500 | -3.00596100 |
| C | -6.11781400 | 0.88236600  | -1.32605800 |
| H | -4.00007900 | 1.21065200  | -1.18060500 |
| C | -7.13343200 | 0.02314200  | -1.74655600 |
| H | -7.57368600 | -1.86674400 | -2.68883100 |
| H | -6.35959700 | 1.82873500  | -0.85421500 |
| H | -8.17589200 | 0.29750700  | -1.61254900 |
| C | -2.71803900 | -1.66711500 | -3.68406700 |
| H | -1.66668600 | -1.90097700 | -3.86366700 |
| H | -3.06485000 | -0.99062100 | -4.47158600 |
| H | -3.26512200 | -2.60861200 | -3.77873600 |
| C | 1.77198000  | -3.66801400 | -1.32446500 |
| C | 1.04927500  | -4.42098700 | -2.26065200 |
| C | 3.13952600  | -3.45379400 | -1.56494500 |
| C | 1.67003800  | -4.93347800 | -3.40374600 |
| H | -0.00778200 | -4.60674300 | -2.10159000 |
| C | 3.76162600  | -3.96353700 | -2.70533200 |
| H | 3.72710700  | -2.88856900 | -0.84664800 |
| C | 3.02719300  | -4.70572300 | -3.63354600 |
| H | 1.08689800  | -5.51170600 | -4.11532900 |
| H | 4.82039200  | -3.78021500 | -2.86702900 |
| H | 3.50776900  | -5.10166500 | -4.52353600 |
| C | 1.61689600  | -3.99422900 | 1.15645400  |
| H | 1.17797400  | -3.65838300 | 2.09998900  |
| H | 2.70482400  | -3.93379000 | 1.24743500  |
| H | 1.36272200  | -5.04847100 | 1.01287500  |
| C | 5.12030100  | -0.56679900 | 0.10855900  |
| C | 4.59632000  | -1.12638400 | 1.28575500  |
| C | 6.48826700  | -0.73537700 | -0.14466400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 5.40670000  | -1.82684200 | 2.17787900  |
| H | 3.53931300  | -0.99933900 | 1.50146900  |
| C | 7.30576100  | -1.43571300 | 0.74936800  |
| H | 6.93369600  | -0.32500500 | -1.04406900 |
| C | 6.77031500  | -1.98473700 | 1.91288900  |
| H | 4.97613800  | -2.24824800 | 3.08185700  |
| H | 8.36343700  | -1.55033500 | 0.52885300  |
| H | 7.40436800  | -2.53004800 | 2.60585200  |
| C | 4.84407900  | 0.52781200  | -2.18900500 |
| H | 5.19482600  | -0.37487000 | -2.69891900 |
| H | 5.69641600  | 1.19944100  | -2.04890400 |
| H | 4.14355700  | 1.04069000  | -2.85179900 |
| C | 0.23992000  | 4.21411800  | -1.58191000 |
| C | 1.26866700  | 4.93447300  | -2.20491300 |
| C | -0.99466600 | 4.11473500  | -2.24548200 |
| C | 1.07162200  | 5.53583100  | -3.45097400 |
| H | 2.23535800  | 5.02156200  | -1.71861900 |
| C | -1.19381700 | 4.71398400  | -3.49027000 |
| H | -1.80573500 | 3.56601200  | -1.77557800 |
| C | -0.15930600 | 5.42801200  | -4.09984800 |
| H | 1.88491400  | 6.08750800  | -3.91493800 |
| H | -2.15724900 | 4.62090800  | -3.98420400 |
| H | -0.31104500 | 5.89322600  | -5.06969300 |
| C | -0.17153800 | 4.53539800  | 0.88383300  |
| H | -1.23575000 | 4.70491500  | 0.70018500  |
| H | 0.32420200  | 5.51097600  | 0.87082500  |
| H | -0.06290500 | 4.10256800  | 1.88337500  |
| C | -3.43869500 | -5.14365600 | 0.61625800  |
| C | 5.03636700  | 4.51699000  | 1.57034100  |
| H | 4.81345800  | 5.56507300  | 1.34816500  |
| H | 6.06899700  | 4.31512500  | 1.27180800  |
| H | 4.98152700  | 4.39864100  | 2.65961400  |
| H | -4.29748300 | -5.34123000 | -0.03184400 |
| H | -3.83269100 | -4.86777200 | 1.60227200  |
| H | -2.87938700 | -6.07600500 | 0.73958000  |
| C | -4.54697900 | 0.98529100  | 2.66528800  |
| C | 2.26021000  | -0.74807800 | 4.02626700  |
| H | 2.21807300  | -0.80191600 | 5.12179000  |
| H | 3.00742000  | 0.00000600  | 3.75090200  |
| H | 2.58665200  | -1.72562400 | 3.65837100  |
| F | -2.25261500 | 2.10348700  | 0.12636300  |
| F | -4.75257100 | 2.55781200  | 0.90503500  |
| F | -5.83324600 | 1.16662400  | 3.01622300  |
| F | -4.28846200 | -0.54934100 | 4.41618800  |



**IM2'**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 6.91089100  | -1.84566200 | -1.46334500 |
| C  | 6.21377400  | -0.84750100 | -0.78847800 |
| C  | 4.96088800  | -1.09124400 | -0.24684900 |
| C  | 4.34956400  | -2.34672500 | -0.37008300 |
| C  | 5.07013500  | -3.34282900 | -1.03079000 |
| C  | 2.99132900  | -2.62426000 | 0.24095100  |
| H  | 2.66059600  | -1.72608400 | 0.77086800  |
| H  | 3.11651400  | -3.40795400 | 0.99891000  |
| C  | 1.87989900  | -3.08790800 | -0.72307700 |
| H  | 2.26096100  | -3.93294700 | -1.31362200 |
| H  | 1.07294600  | -3.51239800 | -0.10824400 |
| C  | 1.25846800  | -2.07555600 | -1.67646400 |
| C  | 1.75063800  | -0.78715400 | -1.92245400 |
| H  | 2.64224200  | -0.41123700 | -1.42831100 |
| H  | 1.49605700  | -0.27706800 | -2.85220700 |
| Ni | 0.21177400  | -0.62351100 | -0.71137200 |
| H  | 4.45546300  | -0.29040300 | 0.28076400  |
| C  | -1.05324900 | 0.41818700  | 0.26748300  |
| C  | -2.43724600 | 2.25684000  | 0.86769100  |
| C  | -2.72519800 | 1.09132700  | 1.82107800  |
| H  | -2.16747100 | 3.16952600  | 1.40181200  |
| H  | -3.27922300 | 2.48000400  | 0.20494000  |
| H  | -2.40550000 | 1.29552000  | 2.84692600  |
| H  | -3.78267500 | 0.82019000  | 1.83695200  |
| N  | -1.90403600 | -0.00043600 | 1.24321100  |
| N  | -1.29311500 | 1.74465700  | 0.07464100  |
| C  | -1.96295900 | -1.33013700 | 1.78492300  |
| C  | -0.96945400 | -1.77968500 | 2.69433100  |
| C  | -3.05183100 | -2.16026700 | 1.45069200  |
| C  | -1.09175100 | -3.06715800 | 3.22164100  |
| C  | -3.12426300 | -3.44238300 | 2.01269600  |
| C  | -2.15813600 | -3.91642400 | 2.89517400  |
| H  | -0.33860900 | -3.43113300 | 3.91239600  |
| H  | -3.95488800 | -4.08745200 | 1.73743100  |
| C  | -0.69004900 | 2.56189000  | -0.94390600 |
| C  | 0.25029100  | 3.54351800  | -0.57042400 |
| C  | -1.08803000 | 2.43018400  | -2.29953000 |
| C  | 0.79859200  | 4.36964100  | -1.56088700 |
| C  | -0.49959700 | 3.27263800  | -3.24621500 |
| C  | 0.44511200  | 4.24833400  | -2.90218300 |
| H  | 1.53210800  | 5.11692000  | -1.26883500 |
| H  | -0.78639000 | 3.17779000  | -4.28853900 |
| C  | -4.18269700 | -1.70868100 | 0.52171500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.20556100  | -0.88416900 | 3.08952000  |
| C | 0.65799900  | 3.77906400  | 0.88385500  |
| C | -2.15074600 | 1.41871400  | -2.72383600 |
| H | -2.02727000 | 0.54350400  | -2.07851200 |
| H | -3.88829800 | -0.74835800 | 0.08903600  |
| H | 0.55736400  | -0.40956700 | 2.16600000  |
| H | 0.27775800  | 2.93453700  | 1.46835300  |
| C | -4.35929100 | -2.66823700 | -0.65889200 |
| C | -5.48522600 | -3.48528100 | -0.82100400 |
| C | -3.35090200 | -2.72934900 | -1.63607100 |
| C | -5.60117600 | -4.33941300 | -1.92320900 |
| H | -6.28748200 | -3.45998600 | -0.09141400 |
| C | -3.46601000 | -3.57555300 | -2.73825500 |
| H | -2.46507900 | -2.10781300 | -1.52326900 |
| C | -4.59474200 | -4.38760200 | -2.88636100 |
| H | -6.48455500 | -4.96370600 | -2.02605200 |
| H | -2.67490400 | -3.60065400 | -3.48224300 |
| H | -4.68679500 | -5.04734600 | -3.74426900 |
| C | -5.47793600 | -1.47555000 | 1.32452000  |
| H | -5.82643200 | -2.39294800 | 1.80855400  |
| H | -5.31190700 | -0.73972600 | 2.11623200  |
| H | -6.27865200 | -1.10397000 | 0.67724400  |
| C | -0.17641200 | 0.23698900  | 4.05799200  |
| C | -1.13135000 | 0.05838200  | 5.06893600  |
| C | 0.49916500  | 1.46495400  | 3.99141100  |
| C | -1.41033800 | 1.08124700  | 5.97926300  |
| H | -1.66521000 | -0.88491800 | 5.14077200  |
| C | 0.22398400  | 2.48887800  | 4.90000300  |
| H | 1.25485500  | 1.61683600  | 3.22439300  |
| C | -0.73615900 | 2.30149800  | 5.89736300  |
| H | -2.15632600 | 0.92285500  | 6.75336600  |
| H | 0.76159800  | 3.43035900  | 4.82793500  |
| H | -0.95492200 | 3.09680400  | 6.60407900  |
| C | 1.40609600  | -1.65624600 | 3.67847100  |
| H | 1.72087500  | -2.47164900 | 3.02074000  |
| H | 2.25105400  | -0.97339700 | 3.80562600  |
| H | 1.17730200  | -2.07488400 | 4.66359400  |
| C | 2.18150800  | 3.79341700  | 1.06753200  |
| C | 2.96957100  | 2.79794100  | 0.46156400  |
| C | 2.83326600  | 4.75980800  | 1.84653200  |
| C | 4.35576800  | 2.78091500  | 0.61811000  |
| H | 2.48877100  | 2.04062500  | -0.15240800 |
| C | 4.22180600  | 4.73901600  | 2.01408400  |
| H | 2.26491200  | 5.54677200  | 2.32934700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 4.98926500  | 3.75287500  | 1.39841600  |
| H | 4.95194300  | 2.02154400  | 0.12144500  |
| H | 4.69875000  | 5.50288600  | 2.62211400  |
| H | 6.06874400  | 3.74057800  | 1.51808500  |
| C | -0.02998700 | 5.05367900  | 1.41860000  |
| H | -1.10216400 | 5.02844000  | 1.20840400  |
| H | 0.09405000  | 5.15207500  | 2.50135800  |
| H | 0.37422500  | 5.95304700  | 0.94298400  |
| C | -3.58457000 | 1.92633400  | -2.53270000 |
| C | -3.92653600 | 3.28358400  | -2.61366200 |
| C | -4.61520600 | 0.99508600  | -2.32526300 |
| C | -5.25552800 | 3.69724700  | -2.48473500 |
| H | -3.14895800 | 4.02421900  | -2.77319500 |
| C | -5.94313700 | 1.40477500  | -2.19692700 |
| H | -4.37423000 | -0.06378800 | -2.27256800 |
| C | -6.26922700 | 2.76118500  | -2.27443500 |
| H | -5.49642300 | 4.75497900  | -2.54854200 |
| H | -6.72164200 | 0.66396600  | -2.03591300 |
| H | -7.30132700 | 3.08405300  | -2.17220300 |
| C | -1.97343600 | 0.90840400  | -4.17147900 |
| H | -2.67102200 | 0.08676600  | -4.35756500 |
| H | -2.18350600 | 1.68542700  | -4.91274800 |
| H | -0.95597400 | 0.53883200  | -4.33440600 |
| C | -2.23780400 | -5.30827600 | 3.47686300  |
| C | 1.06879700  | 5.12498400  | -3.96241900 |
| H | 0.32314900  | 5.46682000  | -4.68762400 |
| H | 1.54626600  | 6.00512800  | -3.52308800 |
| H | 1.83686200  | 4.57899300  | -4.52385800 |
| H | -2.05540500 | -5.30029000 | 4.55675200  |
| H | -3.21812000 | -5.75904700 | 3.30075000  |
| H | -1.48438500 | -5.96751700 | 3.02910100  |
| C | 6.32909700  | -3.10456700 | -1.57927200 |
| C | 0.35581800  | -2.74285600 | -2.70049900 |
| H | 0.93860200  | -3.41028300 | -3.35452100 |
| H | -0.40940300 | -3.36418800 | -2.21991500 |
| H | -0.15063800 | -2.01126700 | -3.33638600 |
| F | 4.56877400  | -4.59043000 | -1.14959300 |
| F | 6.98688300  | -4.08566200 | -2.21190600 |
| F | 8.11986100  | -1.61001600 | -1.99101800 |
| F | 6.78221100  | 0.37006100  | -0.67521600 |

**TS1'**

|   |            |            |             |
|---|------------|------------|-------------|
| C | 4.90196200 | 1.26550000 | -0.51503400 |
| C | 3.51962700 | 1.44391000 | -0.50127700 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | 2. 63117900  | 0. 54772000  | -1. 07116800 |
| C  | 3. 16770900  | -0. 62026700 | -1. 68785100 |
| C  | 4. 55060100  | -0. 79696900 | -1. 69788500 |
| C  | 2. 27031700  | -1. 73964700 | -2. 20941400 |
| H  | 1. 72327900  | -2. 12598000 | -1. 34252000 |
| H  | 2. 90948300  | -2. 55530400 | -2. 56017200 |
| C  | 1. 23085900  | -1. 47258200 | -3. 33398100 |
| H  | 1. 77227600  | -1. 29657700 | -4. 27639400 |
| H  | 0. 68965100  | -2. 41496700 | -3. 46480400 |
| C  | 0. 21587200  | -0. 33215200 | -3. 15471100 |
| C  | 0. 75608800  | 0. 97733400  | -3. 30614000 |
| H  | 1. 71373200  | 1. 09112000  | -3. 82176800 |
| H  | 0. 07037600  | 1. 80707200  | -3. 47750400 |
| Ni | 0. 59802600  | 0. 43610700  | -1. 26983200 |
| H  | 1. 62015300  | 1. 19033700  | -2. 08963500 |
| C  | -0. 49618300 | -0. 06949600 | 0. 19544500  |
| C  | -1. 95075500 | 0. 46692300  | 1. 99451800  |
| C  | -1. 41798900 | -0. 94593300 | 2. 20390200  |
| H  | -1. 49736700 | 1. 16873600  | 2. 70193800  |
| H  | -3. 03561400 | 0. 53521700  | 2. 07300300  |
| H  | -0. 96687200 | -1. 08820800 | 3. 18627700  |
| H  | -2. 19338200 | -1. 70761300 | 2. 05716200  |
| N  | -0. 38883500 | -1. 04560900 | 1. 13905700  |
| N  | -1. 49497000 | 0. 76837800  | 0. 61477900  |
| C  | 0. 52996000  | -2. 15050800 | 1. 16987800  |
| C  | 1. 79297200  | -1. 98203300 | 1. 79149800  |
| C  | 0. 11562700  | -3. 42170500 | 0. 71466400  |
| C  | 2. 63171300  | -3. 09425200 | 1. 90033400  |
| C  | 0. 98465000  | -4. 50931100 | 0. 89118600  |
| C  | 2. 24781500  | -4. 36677800 | 1. 46184700  |
| H  | 3. 60992600  | -2. 97880800 | 2. 35489800  |
| H  | 0. 66277000  | -5. 49751500 | 0. 57566500  |
| C  | -2. 13323200 | 1. 81065000  | -0. 14824800 |
| C  | -1. 64133600 | 3. 13717600  | -0. 13254500 |
| C  | -3. 33282000 | 1. 50405600  | -0. 84306800 |
| C  | -2. 35240100 | 4. 12438500  | -0. 82586400 |
| C  | -3. 99084300 | 2. 53116400  | -1. 52928100 |
| C  | -3. 52436000 | 3. 84803800  | -1. 52908300 |
| H  | -1. 96821800 | 5. 14026500  | -0. 81785400 |
| H  | -4. 89864200 | 2. 30449100  | -2. 07862700 |
| C  | -1. 27190300 | -3. 66649000 | 0. 12876900  |
| C  | 2. 22305500  | -0. 62679600 | 2. 35370000  |
| C  | -0. 40365200 | 3. 56399400  | 0. 66852500  |
| C  | -3. 93386300 | 0. 09740900  | -0. 83688200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.10190300 | -0.60832700 | -0.75563400 |
| H | -1.79419600 | -2.70611900 | 0.11957100  |
| H | 1.88154800  | 0.13186400  | 1.64444500  |
| H | 0.24732000  | 2.68834900  | 0.76715200  |
| C | -1.32658000 | -4.18179300 | -1.31868800 |
| C | -2.57447400 | -4.16655600 | -1.96774900 |
| C | -0.23071600 | -4.68350900 | -2.03216200 |
| C | -2.72742900 | -4.64633600 | -3.26767600 |
| H | -3.44347700 | -3.77309000 | -1.44602300 |
| C | -0.37937500 | -5.16881000 | -3.33658500 |
| H | 0.75397900  | -4.69000300 | -1.58073200 |
| C | -1.62607700 | -5.15692000 | -3.95978500 |
| H | -3.70537800 | -4.61914300 | -3.74014300 |
| H | 0.48956300  | -5.55357600 | -3.86329900 |
| H | -1.73943800 | -5.53386400 | -4.97198800 |
| C | -2.07453300 | -4.61520900 | 1.05788500  |
| H | -1.62345900 | -5.61134100 | 1.08759600  |
| H | -2.10175400 | -4.22616400 | 2.08046900  |
| H | -3.10414500 | -4.72862400 | 0.70654400  |
| C | 1.58780100  | -0.30503100 | 3.70898800  |
| C | 1.42599800  | -1.27760800 | 4.70674900  |
| C | 1.22148100  | 1.01647400  | 4.00488200  |
| C | 0.90648100  | -0.94053400 | 5.95902400  |
| H | 1.70266500  | -2.30764300 | 4.50047100  |
| C | 0.70274200  | 1.35753900  | 5.25599200  |
| H | 1.35232500  | 1.78603100  | 3.24785800  |
| C | 0.54109900  | 0.37816100  | 6.23860600  |
| H | 0.78734600  | -1.71045900 | 6.71653000  |
| H | 0.42474400  | 2.38759300  | 5.46167500  |
| H | 0.13565700  | 0.63980700  | 7.21172200  |
| C | 3.75415800  | -0.46760300 | 2.47233000  |
| H | 4.25197100  | -0.72309200 | 1.53354400  |
| H | 3.99451500  | 0.57153500  | 2.71412900  |
| H | 4.16896100  | -1.09155400 | 3.27021600  |
| C | 0.41077200  | 4.63771300  | -0.06372600 |
| C | 0.98563500  | 4.33118800  | -1.30796600 |
| C | 0.61317700  | 5.92537600  | 0.44938700  |
| C | 1.72999100  | 5.27216100  | -2.01521600 |
| H | 0.84524900  | 3.33758700  | -1.72013000 |
| C | 1.36160100  | 6.87484000  | -0.25621500 |
| H | 0.19186100  | 6.20599200  | 1.40826100  |
| C | 1.92189200  | 6.55443300  | -1.49092200 |
| H | 2.16552300  | 5.00457700  | -2.97425000 |
| H | 1.50285600  | 7.86577800  | 0.16669200  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 2. 50327800  | 7. 29052400  | -2. 03875000 |
| C | -0. 82967300 | 4. 00173000  | 2. 08520900  |
| H | -1. 37709300 | 3. 20440200  | 2. 59023400  |
| H | 0. 04072600  | 4. 25547900  | 2. 69867900  |
| H | -1. 49024600 | 4. 87394800  | 2. 04823200  |
| C | -4. 86547200 | -0. 16797700 | 0. 35442300  |
| C | -5. 66247900 | 0. 83289800  | 0. 92814000  |
| C | -4. 98707700 | -1. 47490700 | 0. 85240400  |
| C | -6. 54564300 | 0. 53704800  | 1. 96992700  |
| H | -5. 58664100 | 1. 85298000  | 0. 56480200  |
| C | -5. 86815800 | -1. 77490900 | 1. 89235800  |
| H | -4. 38527600 | -2. 26869500 | 0. 41642300  |
| C | -6. 65216600 | -0. 76656600 | 2. 45752900  |
| H | -7. 14998000 | 1. 33020400  | 2. 40146100  |
| H | -5. 93967900 | -2. 79420000 | 2. 26155600  |
| H | -7. 33665200 | -0. 99449900 | 3. 26936900  |
| C | -4. 69277100 | -0. 25577700 | -2. 13788800 |
| H | -4. 95299500 | -1. 31816400 | -2. 13247500 |
| H | -5. 62812800 | 0. 30409700  | -2. 22710500 |
| H | -4. 08320300 | -0. 05729700 | -3. 02311100 |
| C | 3. 18378400  | -5. 54450100 | 1. 59621300  |
| C | -4. 27671200 | 4. 94433400  | -2. 24606200 |
| H | -4. 86441600 | 5. 54535100  | -1. 54115000 |
| H | -3. 59256900 | 5. 62777200  | -2. 75857300 |
| H | -4. 96978800 | 4. 53576700  | -2. 98667300 |
| H | 3. 72278700  | -5. 51998400 | 2. 54850700  |
| H | 2. 64432900  | -6. 49364700 | 1. 53266200  |
| H | 3. 93753700  | -5. 53990900 | 0. 79932900  |
| C | 5. 42210700  | 0. 13363900  | -1. 12778400 |
| C | -1. 20956700 | -0. 62418900 | -3. 56043200 |
| H | -1. 25572700 | -0. 92056200 | -4. 62102600 |
| H | -1. 64085500 | -1. 44679300 | -2. 98277100 |
| H | -1. 84249600 | 0. 25882800  | -3. 43634300 |
| F | 5. 11683700  | -1. 89558600 | -2. 25655900 |
| F | 6. 75214900  | -0. 06796500 | -1. 16342700 |
| F | 5. 73174300  | 2. 15671200  | 0. 06016100  |
| F | 3. 05846200  | 2. 56057800  | 0. 12604100  |

### IM3'

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 4. 83290000 | -1. 55284000 | -0. 15551600 |
| C | 3. 51418800 | -1. 11750100 | -0. 17497700 |
| C | 2. 68749400 | -1. 13697100 | -1. 29230300 |
| C | 3. 26810900 | -1. 61826600 | -2. 48245500 |
| C | 4. 59334800 | -2. 05619800 | -2. 48415900 |
| C | 2. 47905800 | -1. 67606600 | -3. 77187200 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 2.20424000  | -2.71835100 | -3.98540600 |
| H  | 3.11935400  | -1.37163800 | -4.60803600 |
| C  | 1.22455300  | -0.80406000 | -3.74810700 |
| H  | 1.51420900  | 0.25449400  | -3.71924200 |
| H  | 0.70774600  | -0.95029800 | -4.71218700 |
| C  | 0.20865400  | -1.07804100 | -2.63042500 |
| C  | -1.04166000 | -0.23851900 | -2.88734800 |
| H  | -1.48674100 | -0.51131000 | -3.85885700 |
| H  | -1.80787300 | -0.39970400 | -2.12676400 |
| Ni | 0.90956300  | -0.52590700 | -0.89797700 |
| H  | -0.80648300 | 0.82987200  | -2.92355200 |
| C  | -0.62271500 | 0.13679600  | 0.25914700  |
| C  | -1.52049900 | 1.57460700  | 1.92445000  |
| C  | -2.09500400 | 0.17172700  | 2.12843300  |
| H  | -0.84214500 | 1.85712200  | 2.73424500  |
| H  | -2.28840900 | 2.34238300  | 1.82418500  |
| H  | -1.88602300 | -0.23309600 | 3.11973600  |
| H  | -3.17551100 | 0.13235200  | 1.95653000  |
| N  | -1.37711800 | -0.61961700 | 1.09271000  |
| N  | -0.75035200 | 1.42755400  | 0.65930800  |
| C  | -1.54217600 | -2.05232000 | 1.08158600  |
| C  | -0.57215300 | -2.87126600 | 1.71215600  |
| C  | -2.73230400 | -2.61399100 | 0.56673600  |
| C  | -0.80247200 | -4.24798400 | 1.77219800  |
| C  | -2.92557900 | -3.99767100 | 0.69740600  |
| C  | -1.97261400 | -4.83315200 | 1.27669400  |
| H  | -0.05981200 | -4.88825300 | 2.23625500  |
| H  | -3.85153100 | -4.43429000 | 0.33472700  |
| C  | -0.33329300 | 2.60576600  | -0.06410600 |
| C  | 0.92694700  | 3.19609800  | 0.17347400  |
| C  | -1.25726300 | 3.22140900  | -0.94900400 |
| C  | 1.25321100  | 4.37618600  | -0.50853000 |
| C  | -0.86424600 | 4.38382700  | -1.61921400 |
| C  | 0.38481700  | 4.97896500  | -1.41555300 |
| H  | 2.22564500  | 4.82501800  | -0.32888900 |
| H  | -1.55330300 | 4.85095300  | -2.31547900 |
| C  | -3.85004400 | -1.77044900 | -0.04209700 |
| C  | 0.68057000  | -2.27094900 | 2.34466700  |
| C  | 1.92801800  | 2.65201500  | 1.19636600  |
| C  | -2.67373400 | 2.68173100  | -1.14790300 |
| H  | -2.64285300 | 1.60603400  | -0.95658900 |
| H  | -3.52538900 | -0.72691900 | -0.00996600 |
| H  | 1.00687400  | -1.45358700 | 1.70041200  |
| H  | 1.71159700  | 1.58832200  | 1.34105000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.19649800 | -2.04655600 | -1.51583800 |
| C | -5.01323500 | -1.11188100 | -2.17738000 |
| C | -3.76719200 | -3.16268700 | -2.24416000 |
| C | -5.39184400 | -1.28553300 | -3.50745300 |
| H | -5.35915800 | -0.23019400 | -1.64381600 |
| C | -4.14467300 | -3.34228100 | -3.57932300 |
| H | -3.12020200 | -3.89760400 | -1.78138300 |
| C | -4.95911800 | -2.40856400 | -4.21753500 |
| H | -6.02158500 | -0.54288200 | -3.98938600 |
| H | -3.79309400 | -4.21758300 | -4.11843800 |
| H | -5.24993100 | -2.54886200 | -5.25449000 |
| C | -5.12747600 | -1.87838700 | 0.83184900  |
| H | -5.53477100 | -2.89332000 | 0.80917000  |
| H | -4.90940600 | -1.62606600 | 1.87432000  |
| H | -5.90618900 | -1.20087600 | 0.47048900  |
| C | 0.42553900  | -1.66329700 | 3.72742300  |
| C | -0.46813300 | -2.23220900 | 4.64583600  |
| C | 1.15289400  | -0.52945300 | 4.12216800  |
| C | -0.63584800 | -1.67985000 | 5.91846500  |
| H | -1.04203000 | -3.10974000 | 4.36260300  |
| C | 0.98828200  | 0.02400800  | 5.39330100  |
| H | 1.86376400  | -0.08805400 | 3.42823100  |
| C | 0.08954700  | -0.54838900 | 6.29682600  |
| H | -1.33544100 | -2.13552500 | 6.61394300  |
| H | 1.56174400  | 0.90222400  | 5.67701300  |
| H | -0.04277700 | -0.11793500 | 7.28525900  |
| C | 1.87266200  | -3.24910800 | 2.41819900  |
| H | 2.06953600  | -3.70124000 | 1.44108400  |
| H | 2.76806400  | -2.70285400 | 2.72403600  |
| H | 1.70743100  | -4.04877800 | 3.14677700  |
| C | 3.37415200  | 2.74506900  | 0.69172500  |
| C | 3.70113400  | 2.20441600  | -0.56300400 |
| C | 4.40233600  | 3.33835800  | 1.43591200  |
| C | 5.00382600  | 2.25111200  | -1.05480800 |
| H | 2.92434700  | 1.73330900  | -1.15742000 |
| C | 5.71219900  | 3.38895900  | 0.94538700  |
| H | 4.19729500  | 3.76909200  | 2.40964100  |
| C | 6.01940000  | 2.84721400  | -0.30124100 |
| H | 5.22675100  | 1.81766100  | -2.02588000 |
| H | 6.48940800  | 3.85545400  | 1.54457000  |
| H | 7.03588800  | 2.88549700  | -0.68226600 |
| C | 1.71776300  | 3.35901400  | 2.55223900  |
| H | 0.67399400  | 3.29549500  | 2.86616200  |
| H | 2.33148400  | 2.90455900  | 3.33604700  |



|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 1. 97440900  | 4. 42127200  | 2. 48687700  |
| C | -3. 69326700 | 3. 28045100  | -0. 16682900 |
| C | -3. 62377600 | 4. 60675500  | 0. 28329000  |
| C | -4. 77945500 | 2. 49775000  | 0. 25591400  |
| C | -4. 60609900 | 5. 13044400  | 1. 12772100  |
| H | -2. 79195000 | 5. 23454700  | -0. 01934700 |
| C | -5. 76308800 | 3. 01656000  | 1. 09931300  |
| H | -4. 85548600 | 1. 46759000  | -0. 08233700 |
| C | -5. 67948200 | 4. 33904700  | 1. 54002200  |
| H | -4. 52827500 | 6. 16019200  | 1. 46543400  |
| H | -6. 59134200 | 2. 38728600  | 1. 41297900  |
| H | -6. 44071600 | 4. 74667600  | 2. 19874800  |
| C | -3. 20077800 | 2. 85400100  | -2. 59182700 |
| H | -4. 14370500 | 2. 31142200  | -2. 70472600 |
| H | -3. 39922400 | 3. 90251400  | -2. 83189400 |
| H | -2. 48930600 | 2. 45872400  | -3. 32214500 |
| C | -2. 18589700 | -6. 32583400 | 1. 35889600  |
| C | 0. 78195800  | 6. 22536300  | -2. 17010500 |
| H | 1. 57345200  | 6. 77188200  | -1. 64984100 |
| H | 1. 15901300  | 5. 97526000  | -3. 16941500 |
| H | -0. 06935300 | 6. 89962700  | -2. 30546200 |
| H | -1. 65711100 | -6. 84260200 | 0. 54861700  |
| H | -1. 80669200 | -6. 73251700 | 2. 30152400  |
| H | -3. 24531500 | -6. 58414700 | 1. 27610800  |
| C | 5. 38352000  | -2. 03409300 | -1. 33891400 |
| C | -0. 14105500 | -2. 56030800 | -2. 50364700 |
| H | -0. 58925900 | -2. 92856100 | -3. 44240800 |
| H | 0. 73456800  | -3. 17855900 | -2. 28910200 |
| H | -0. 87384900 | -2. 72756900 | -1. 71136700 |
| F | 5. 15772200  | -2. 52488600 | -3. 62508000 |
| F | 6. 65982700  | -2. 46065200 | -1. 37142200 |
| F | 5. 57809100  | -1. 50559800 | 0. 96577400  |
| F | 3. 02874700  | -0. 61241100 | 1. 01356400  |

**TS2'**

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -2. 55423300 | -3. 23759700 | -1. 43260500 |
| C | -1. 33358700 | -2. 61281100 | -1. 63115900 |
| C | -3. 64708800 | -1. 37595800 | -2. 46958400 |
| C | 0. 50396500  | 0. 34837000  | 0. 37768500  |
| C | 1. 78183700  | 1. 40248100  | 2. 09410400  |
| C | 0. 40970700  | 1. 01946800  | 2. 65848100  |
| H | 2. 59107000  | 0. 82888600  | 2. 55800600  |
| H | 2. 00422500  | 2. 46614200  | 2. 20054400  |
| H | 0. 47413100  | 0. 38339400  | 3. 54239200  |
| H | -0. 18344400 | 1. 90394200  | 2. 90531100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -0.21391900 | 0.27989600  | 1.53071600  |
| N | 1.64415400  | 1.03835000  | 0.66519200  |
| C | -1.47770500 | -0.38884100 | 1.69937300  |
| C | -1.50061100 | -1.78944500 | 1.92638300  |
| C | -2.67599000 | 0.35535600  | 1.70368600  |
| C | -2.74157400 | -2.41793100 | 2.05290000  |
| C | -3.89113400 | -0.32658200 | 1.85786900  |
| C | -3.94930500 | -1.71110200 | 1.99690000  |
| H | -2.78074200 | -3.49304200 | 2.18830000  |
| H | -4.81518000 | 0.24480500  | 1.83836700  |
| C | 2.68410400  | 1.34186500  | -0.27733300 |
| C | 3.83825000  | 0.53603400  | -0.33673000 |
| C | 2.55756900  | 2.48449600  | -1.10914500 |
| C | 4.84718500  | 0.87184900  | -1.25012700 |
| C | 3.59464200  | 2.77325100  | -1.99849400 |
| C | 4.74741600  | 1.98011600  | -2.08762400 |
| H | 5.72868700  | 0.23896700  | -1.31215000 |
| H | 3.51224800  | 3.63859400  | -2.64808900 |
| C | -2.69606300 | 1.88383900  | 1.64068400  |
| C | -0.20570900 | -2.59382300 | 2.05976600  |
| C | 4.04842500  | -0.66984100 | 0.58434100  |
| C | 1.31467300  | 3.37171600  | -1.03588800 |
| H | 0.45931800  | 2.69905000  | -0.91368500 |
| H | -1.71118400 | 2.20865600  | 1.28691600  |
| H | 0.46200400  | -2.25806700 | 1.26102300  |
| H | 3.12003600  | -0.81804800 | 1.14014300  |
| C | -3.72404500 | 2.45149000  | 0.65145800  |
| C | -4.39604000 | 3.65992500  | 0.89138800  |
| C | -3.99270400 | 1.78673800  | -0.55559000 |
| C | -5.30245000 | 4.18117600  | -0.03711200 |
| H | -4.22618500 | 4.20942400  | 1.81070000  |
| C | -4.90589700 | 2.29626300  | -1.47946100 |
| H | -3.49564700 | 0.84638600  | -0.76594700 |
| C | -5.56604000 | 3.50064700  | -1.22518800 |
| H | -5.80852500 | 5.11816000  | 0.17913900  |
| H | -5.10798300 | 1.73631600  | -2.38731000 |
| H | -6.27980800 | 3.89867700  | -1.94076700 |
| C | -2.88481300 | 2.44038400  | 3.07249300  |
| H | -3.90900600 | 2.27483100  | 3.42159300  |
| H | -2.21298800 | 1.93971900  | 3.77364200  |
| H | -2.67418000 | 3.51273900  | 3.12171300  |
| C | 0.51275600  | -2.34735500 | 3.38983800  |
| C | -0.18525400 | -2.11529200 | 4.58379500  |
| C | 1.91235600  | -2.43231800 | 3.44695300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.49531000  | -1.95701600 | 5.79392500  |
| H | -1.26923100 | -2.05145600 | 4.56569100  |
| C | 2.59625200  | -2.27493100 | 4.65417700  |
| H | 2.47008500  | -2.63739200 | 2.53634800  |
| C | 1.88909800  | -2.03208500 | 5.83417600  |
| H | -0.06631200 | -1.77476000 | 6.70617500  |
| H | 3.68063000  | -2.34230300 | 4.67231500  |
| H | 2.41818300  | -1.90593000 | 6.77438900  |
| C | -0.38723100 | -4.11663300 | 1.87743800  |
| H | -0.89602100 | -4.34915500 | 0.94097700  |
| H | 0.59515200  | -4.59761100 | 1.86318800  |
| H | -0.95096200 | -4.55710100 | 2.70596400  |
| C | 4.27993300  | -1.96518700 | -0.19850500 |
| C | 3.17144200  | -2.63457400 | -0.74279700 |
| C | 5.54953400  | -2.52618300 | -0.39179800 |
| C | 3.32457800  | -3.82156100 | -1.45924800 |
| H | 2.17601200  | -2.21720500 | -0.61061400 |
| C | 5.70753300  | -3.71366100 | -1.11378200 |
| H | 6.42843000  | -2.04692500 | 0.02766300  |
| C | 4.59748000  | -4.36647300 | -1.65006700 |
| H | 2.44620000  | -4.31987600 | -1.85983600 |
| H | 6.70219600  | -4.12957800 | -1.24930800 |
| H | 4.72085500  | -5.29207500 | -2.20496600 |
| C | 5.15673300  | -0.36911000 | 1.61393500  |
| H | 4.89343000  | 0.50672200  | 2.21411100  |
| H | 5.30077100  | -1.21809800 | 2.28967600  |
| H | 6.11453100  | -0.15131300 | 1.13213400  |
| C | 1.31387400  | 4.31801700  | 0.16783500  |
| C | 2.49057500  | 4.89075700  | 0.67048800  |
| C | 0.09306800  | 4.68590900  | 0.75465400  |
| C | 2.44918900  | 5.79822400  | 1.73252800  |
| H | 3.44702400  | 4.62127600  | 0.23219400  |
| C | 0.04781300  | 5.59344800  | 1.81459800  |
| H | -0.83283100 | 4.26512600  | 0.36934000  |
| C | 1.22847500  | 6.15206100  | 2.31032300  |
| H | 3.37383500  | 6.22819700  | 2.10782700  |
| H | -0.90927300 | 5.86338500  | 2.25245800  |
| H | 1.19686200  | 6.85566700  | 3.13716100  |
| C | 1.05398000  | 4.18425400  | -2.32287300 |
| H | 0.08266400  | 4.68166800  | -2.25028600 |
| H | 1.80668300  | 4.96390300  | -2.47540800 |
| H | 1.04208500  | 3.53730900  | -3.20595200 |
| C | -5.27033000 | -2.44113400 | 2.04227200  |
| C | 5.83648700  | 2.31890100  | -3.07805800 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 6.73883100  | 1.72889400  | -2.89720800 |
| H  | 5.51083000  | 2.12145700  | -4.10639400 |
| H  | 6.10661900  | 3.37904200  | -3.02578600 |
| H  | -5.50994400 | -2.84907000 | 1.05247900  |
| H  | -5.24349300 | -3.28144300 | 2.74320300  |
| H  | -6.08812600 | -1.77582100 | 2.33325800  |
| C  | -3.73544300 | -2.60945100 | -1.82959900 |
| F  | -4.78882200 | -0.81136800 | -2.93833200 |
| F  | -4.92769400 | -3.20007600 | -1.60147800 |
| F  | -2.62211700 | -4.43916700 | -0.82212300 |
| F  | -0.21191100 | -3.27861900 | -1.22829600 |
| C  | -1.23040100 | -1.31313300 | -2.15829300 |
| C  | -2.43020600 | -0.74046100 | -2.66607300 |
| C  | -2.25366800 | 0.43628100  | -3.59809700 |
| C  | -0.74256600 | 0.52357300  | -3.92827400 |
| C  | -0.01551100 | -0.76452800 | -3.49478000 |
| Ni | 0.15134500  | -0.31214200 | -1.37565000 |
| H  | -2.85476500 | 0.27538400  | -4.50038100 |
| H  | -2.60946200 | 1.37574200  | -3.15974700 |
| H  | -0.58609800 | 0.69811000  | -5.00184700 |
| H  | -0.29613100 | 1.37553500  | -3.40429500 |
| C  | -0.25367300 | -1.92877300 | -4.47141800 |
| H  | -1.31502200 | -2.09119700 | -4.67551600 |
| H  | 0.24770800  | -1.70773000 | -5.42357200 |
| H  | 0.16499000  | -2.86152700 | -4.08170500 |
| C  | 1.51334400  | -0.55166200 | -3.42444400 |
| H  | 1.85732500  | -0.26415700 | -4.43029000 |
| H  | 1.83130600  | 0.25645400  | -2.75256800 |
| H  | 2.04331500  | -1.46497300 | -3.14362400 |

$3^{C-H}_{exo}$

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.56325600 | -1.11510100 | -0.00429400 |
| C | -0.17526900 | -1.26117900 | -0.01066400 |
| C | -1.30446200 | 1.28278000  | -0.00847500 |
| C | -2.12965500 | 0.15816300  | -0.00492900 |
| F | -1.87361700 | 2.50401700  | 0.00252100  |
| F | -3.46428500 | 0.29174900  | -0.00166700 |
| F | -2.35956000 | -2.19487800 | 0.00375000  |
| F | 0.33133500  | -2.51253800 | 0.01129300  |
| C | 0.64765900  | -0.14424000 | -0.03682300 |
| C | 0.07305800  | 1.13448100  | -0.02536100 |
| C | 1.13643400  | 2.20624000  | 0.00473000  |
| C | 2.41337100  | 1.42693300  | -0.39185700 |

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 2.17350900 | -0.07005300 | -0.01299900 |
| H | 0.91909700 | 3.03800500  | -0.67201600 |
| H | 1.21381500 | 2.63211400  | 1.01349400  |
| H | 2.55366400 | 1.49992000  | -1.47588700 |
| H | 3.31524800 | 1.82532600  | 0.08182500  |
| C | 2.84528000 | -1.01910700 | -1.02049900 |
| H | 2.45867700 | -0.85766100 | -2.03201900 |
| H | 3.92614100 | -0.84141300 | -1.03907600 |
| H | 2.67823700 | -2.06617100 | -0.75510400 |
| C | 2.68177500 | -0.37565300 | 1.41422300  |
| H | 3.77341000 | -0.29305800 | 1.45518100  |
| H | 2.25993000 | 0.31969500  | 2.14729800  |
| H | 2.40624600 | -1.39149800 | 1.71492700  |

**TS1<sub>cw</sub>**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -6.19735500 | -1.97066000 | -0.56262500 |
| C  | -5.27100100 | -1.68309600 | 0.43796200  |
| C  | -3.93983600 | -2.04833200 | 0.31000300  |
| C  | -3.48879400 | -2.72066600 | -0.83670300 |
| C  | -4.42732300 | -3.00232300 | -1.82812700 |
| C  | -2.04457700 | -3.13048800 | -1.01116900 |
| H  | -2.01721900 | -4.04460800 | -1.61711800 |
| H  | -1.63459900 | -3.38918300 | -0.02963000 |
| C  | -1.11191000 | -2.05908200 | -1.64937200 |
| H  | -1.56883600 | -0.80490600 | -0.62126700 |
| H  | -0.10792800 | -2.54901800 | -1.68677400 |
| C  | -1.50394800 | -1.65905600 | -3.05244000 |
| C  | -2.25878700 | -0.58339800 | -3.32291300 |
| H  | -2.59623200 | 0.07966900  | -2.53332100 |
| H  | -2.56344800 | -0.34449700 | -4.33903200 |
| Ni | -0.13622700 | -0.72715400 | -0.64766200 |
| H  | -3.24993200 | -1.79844700 | 1.10859200  |
| C  | 1.01249500  | 0.47683000  | 0.29938900  |
| C  | 2.94900500  | 1.75607200  | 0.81653800  |
| C  | 1.92866400  | 1.90871500  | 1.95825900  |
| H  | 3.90917500  | 1.37005800  | 1.16797600  |
| H  | 3.12873700  | 2.69183700  | 0.27997600  |
| H  | 2.27954500  | 1.47583800  | 2.89929600  |
| H  | 1.66260700  | 2.95311200  | 2.13706100  |
| N  | 0.76164000  | 1.14524500  | 1.45163600  |
| N  | 2.28134400  | 0.77872400  | -0.07529900 |
| C  | -0.46578500 | 1.04936700  | 2.19355200  |
| C  | -0.72827900 | -0.09588000 | 2.98634400  |
| C  | -1.39453800 | 2.10620000  | 2.13170900  |
| C  | -1.94872300 | -0.16339100 | 3.66374700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.60004400 | 1.98814900  | 2.83544500  |
| C | -2.90395800 | 0.85986600  | 3.59366200  |
| H | -2.17470900 | -1.03784900 | 4.26522100  |
| H | -3.32729500 | 2.79304100  | 2.76434200  |
| C | 2.90345600  | 0.29183700  | -1.27569600 |
| C | 3.85194700  | -0.74584000 | -1.19075600 |
| C | 2.57484500  | 0.87045900  | -2.52948200 |
| C | 4.46169300  | -1.20076000 | -2.36816000 |
| C | 3.20799400  | 0.37293700  | -3.67027900 |
| C | 4.15729900  | -0.65752300 | -3.61350100 |
| H | 5.17926500  | -2.01479700 | -2.30488600 |
| H | 2.96060800  | 0.79345100  | -4.63948100 |
| C | -1.12288200 | 3.39330300  | 1.34933900  |
| C | 0.29627600  | -1.22286500 | 3.11110700  |
| C | 4.25525600  | -1.38467500 | 0.14126600  |
| C | 1.56276500  | 2.01136700  | -2.63076200 |
| H | 0.76877800  | 1.79052900  | -1.91063400 |
| H | -0.22440100 | 3.22391900  | 0.74884200  |
| H | 0.74897800  | -1.34673900 | 2.12249800  |
| H | 3.58458700  | -0.98714900 | 0.90795800  |
| C | -2.24595800 | 3.70687100  | 0.35590100  |
| C | -3.07389800 | 4.83127600  | 0.46570800  |
| C | -2.45078200 | 2.83688700  | -0.72955400 |
| C | -4.07814100 | 5.07993100  | -0.47661100 |
| H | -2.94210400 | 5.52887600  | 1.28591000  |
| C | -3.44653900 | 3.08609600  | -1.67288100 |
| H | -1.82753100 | 1.95057000  | -0.82607300 |
| C | -4.26808000 | 4.21082200  | -1.54954900 |
| H | -4.70812000 | 5.95860800  | -0.36825600 |
| H | -3.58152200 | 2.40275300  | -2.50665900 |
| H | -5.04487900 | 4.40568100  | -2.28331700 |
| C | -0.81289800 | 4.54988700  | 2.32010900  |
| H | -1.66126500 | 4.76736700  | 2.97643600  |
| H | 0.03307100  | 4.29197500  | 2.96341500  |
| H | -0.55859500 | 5.46425000  | 1.77453300  |
| C | 1.43042500  | -0.90121700 | 4.08936500  |
| C | 1.23599400  | -0.11267800 | 5.23201500  |
| C | 2.70122100  | -1.45869800 | 3.87630900  |
| C | 2.28177100  | 0.11869600  | 6.12966200  |
| H | 0.26195900  | 0.32952200  | 5.41848600  |
| C | 3.74811800  | -1.22940900 | 4.77084600  |
| H | 2.86826800  | -2.08690300 | 3.00439800  |
| C | 3.54245200  | -0.43622600 | 5.90238000  |
| H | 2.10906700  | 0.73563200  | 7.00734200  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 4. 72369600  | -1. 66948700 | 4. 58288400  |
| H | 4. 35575100  | -0. 25321900 | 6. 59871400  |
| C | -0. 32144000 | -2. 59035500 | 3. 47589800  |
| H | -1. 13110500 | -2. 85455500 | 2. 78816000  |
| H | 0. 44693400  | -3. 36626300 | 3. 41332800  |
| H | -0. 71519000 | -2. 60562400 | 4. 49673400  |
| C | 4. 03427700  | -2. 90029000 | 0. 12410000  |
| C | 5. 08383800  | -3. 82766700 | 0. 10158800  |
| C | 2. 71801300  | -3. 39281000 | 0. 13162400  |
| C | 4. 82756900  | -5. 20300300 | 0. 08034600  |
| H | 6. 11383000  | -3. 48665900 | 0. 10558800  |
| C | 2. 45872100  | -4. 76256100 | 0. 11339700  |
| H | 1. 88701400  | -2. 69073200 | 0. 14612000  |
| C | 3. 51632900  | -5. 67660700 | 0. 08565200  |
| H | 5. 65914500  | -5. 90212100 | 0. 06280500  |
| H | 1. 43146900  | -5. 11684800 | 0. 12334900  |
| H | 3. 31824900  | -6. 74442600 | 0. 07192800  |
| C | 5. 68830900  | -0. 97044800 | 0. 52874600  |
| H | 5. 76384500  | 0. 11823900  | 0. 60240200  |
| H | 5. 97067100  | -1. 39790700 | 1. 49605400  |
| H | 6. 42222200  | -1. 29390000 | -0. 21556300 |
| C | 2. 14935700  | 3. 37400600  | -2. 24927000 |
| C | 3. 48374200  | 3. 71797000  | -2. 50708400 |
| C | 1. 31276800  | 4. 34429100  | -1. 67518700 |
| C | 3. 96956700  | 4. 99005700  | -2. 19256200 |
| H | 4. 15013000  | 2. 98466300  | -2. 95153500 |
| C | 1. 79482100  | 5. 61576900  | -1. 35985300 |
| H | 0. 27001900  | 4. 10275500  | -1. 48322500 |
| C | 3. 12873300  | 5. 94346600  | -1. 61555500 |
| H | 5. 00813800  | 5. 23420300  | -2. 39900700 |
| H | 1. 12815600  | 6. 34898900  | -0. 91416400 |
| H | 3. 50779100  | 6. 93098200  | -1. 36858400 |
| C | 0. 87448000  | 2. 11273300  | -4. 00908400 |
| H | 0. 08581600  | 2. 86914400  | -3. 96494200 |
| H | 1. 57093000  | 2. 41622400  | -4. 79681300 |
| H | 0. 41668000  | 1. 15939600  | -4. 29033700 |
| C | -4. 23813400 | 0. 71630300  | 4. 28621800  |
| C | 4. 82577200  | -1. 15423300 | -4. 87387700 |
| H | 4. 08646200  | -1. 46352000 | -5. 62084300 |
| H | 5. 43600400  | -0. 36837300 | -5. 33437400 |
| H | 5. 47770800  | -2. 00772600 | -4. 67032200 |
| H | -4. 70504200 | 1. 68932500  | 4. 46298700  |
| H | -4. 92535400 | 0. 12608200  | 3. 66894300  |
| H | -4. 13887200 | 0. 20328300  | 5. 24797900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -5.76675300 | -2.63731200 | -1.70421100 |
| C | -1.02828700 | -2.57378800 | -4.16082100 |
| H | -1.39971400 | -3.59508800 | -4.01348300 |
| H | -1.36293400 | -2.23123300 | -5.14459100 |
| H | 0.06755700  | -2.63347800 | -4.17147000 |
| F | -5.71038100 | -1.04314400 | 1.54153800  |
| F | -7.48444600 | -1.61709300 | -0.43289700 |
| F | -6.64186500 | -2.92705600 | -2.67833500 |
| F | -4.06203100 | -3.65727600 | -2.94974800 |

**IM2<sub>ew</sub>**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 7.47689800  | 1.41608300  | -0.94687100 |
| C  | 6.86426100  | 0.20411400  | -1.25573000 |
| C  | 5.55344600  | -0.05317000 | -0.87788100 |
| C  | 4.81072800  | 0.90521200  | -0.17501200 |
| C  | 5.43786800  | 2.11445300  | 0.12612900  |
| C  | 3.36664700  | 0.67393600  | 0.23603500  |
| H  | 3.23656800  | 1.00248500  | 1.27166700  |
| H  | 3.16809800  | -0.40026400 | 0.22131400  |
| C  | 2.38725900  | 1.43685700  | -0.65201200 |
| H  | 0.37395600  | 1.52139000  | 0.79363900  |
| H  | 2.50616300  | 2.51586300  | -0.58811000 |
| C  | 1.85634400  | 0.94523500  | -1.87663800 |
| C  | 1.46607200  | -0.40273900 | -1.98538500 |
| H  | 1.98185600  | -1.18560100 | -1.43745600 |
| H  | 0.94989400  | -0.73029800 | -2.88216300 |
| Ni | 0.54129700  | 0.61153000  | -0.35683500 |
| H  | 5.11552600  | -1.01186000 | -1.13349200 |
| C  | -1.09301100 | -0.22905700 | 0.12558200  |
| C  | -3.42623800 | -0.51382900 | 0.43408800  |
| C  | -2.68398700 | -1.54729500 | 1.29077800  |
| H  | -3.93850400 | 0.22800900  | 1.05350300  |
| H  | -4.14985600 | -0.96557500 | -0.24663300 |
| H  | -2.94655700 | -1.48760800 | 2.34852100  |
| H  | -2.86167300 | -2.56848500 | 0.94067800  |
| N  | -1.26378300 | -1.17062600 | 1.08790200  |
| N  | -2.32312000 | 0.12496200  | -0.32406300 |
| C  | -0.20895000 | -1.75160600 | 1.87601900  |
| C  | 0.28799400  | -1.04333500 | 2.99981600  |
| C  | 0.28091100  | -3.03900900 | 1.56595200  |
| C  | 1.33107500  | -1.61401900 | 3.73397100  |
| C  | 1.32456700  | -3.56212700 | 2.34051900  |
| C  | 1.87528400  | -2.86330100 | 3.41320500  |
| H  | 1.73377900  | -1.07741200 | 4.58661700  |
| H  | 1.72160300  | -4.54170500 | 2.09194900  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.58169900 | 1.03665300  | -1.40735900 |
| C | -2.93332200 | 2.37670300  | -1.14574400 |
| C | -2.53749000 | 0.55302700  | -2.74096400 |
| C | -3.19458000 | 3.22746500  | -2.22921300 |
| C | -2.80237900 | 1.44680800  | -3.78107900 |
| C | -3.12685000 | 2.78998600  | -3.54911800 |
| H | -3.44773400 | 4.26438800  | -2.02542600 |
| H | -2.76235700 | 1.09516100  | -4.80674100 |
| C | -0.35991800 | -3.92205000 | 0.48656700  |
| C | -0.32696100 | 0.28791100  | 3.43044900  |
| C | -3.11684800 | 2.92862100  | 0.27206300  |
| C | -2.24134000 | -0.91712600 | -3.03803700 |
| H | -1.46796800 | -1.23295200 | -2.33247600 |
| H | -0.98705300 | -3.27292500 | -0.12970900 |
| H | -0.56233700 | 0.83590900  | 2.51532900  |
| H | -2.63322400 | 2.22745700  | 0.95911700  |
| C | 0.64697100  | -4.57115900 | -0.46466500 |
| C | 1.24798100  | -5.81316800 | -0.20877000 |
| C | 0.97886300  | -3.91744400 | -1.66066200 |
| C | 2.16501900  | -6.36790900 | -1.10538900 |
| H | 0.99721300  | -6.36685100 | 0.69053400  |
| C | 1.89201200  | -4.46823000 | -2.56141500 |
| H | 0.51383100  | -2.96340600 | -1.88715200 |
| C | 2.49398900  | -5.69723000 | -2.28432700 |
| H | 2.61698500  | -7.33041800 | -0.88228000 |
| H | 2.12714200  | -3.93915100 | -3.48075900 |
| H | 3.20392100  | -6.13099200 | -2.98251900 |
| C | -1.28527200 | -4.96494000 | 1.15538900  |
| H | -0.72663000 | -5.63010600 | 1.82013900  |
| H | -2.04877700 | -4.47318300 | 1.76419800  |
| H | -1.78728800 | -5.57852200 | 0.40045300  |
| C | -1.63376700 | 0.11890700  | 4.21142300  |
| C | -1.85833000 | -0.95296800 | 5.08705300  |
| C | -2.63119100 | 1.10044800  | 4.09726800  |
| C | -3.04506600 | -1.04476900 | 5.81932300  |
| H | -1.10252300 | -1.72561500 | 5.19218400  |
| C | -3.81759400 | 1.01287200  | 4.82762800  |
| H | -2.46963800 | 1.94713200  | 3.43408200  |
| C | -4.03042300 | -0.06380100 | 5.69192000  |
| H | -3.19852200 | -1.88610400 | 6.48974300  |
| H | -4.57541700 | 1.78413200  | 4.72002700  |
| H | -4.95376700 | -0.13715500 | 6.25928000  |
| C | 0.63888100  | 1.19073600  | 4.22751100  |
| H | 1.57637900  | 1.33781500  | 3.68194500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.17758400  | 2.17037200  | 4.38234100  |
| H | 0.87016800  | 0.78185900  | 5.21607700  |
| C | -2.42029200 | 4.28067900  | 0.46432100  |
| C | -3.12072100 | 5.48565100  | 0.60989200  |
| C | -1.01645100 | 4.32260700  | 0.50049800  |
| C | -2.44122300 | 6.69687300  | 0.78071000  |
| H | -4.20540500 | 5.49440700  | 0.59741600  |
| C | -0.33757300 | 5.52811200  | 0.67273300  |
| H | -0.45597500 | 3.39648700  | 0.39599000  |
| C | -1.04789900 | 6.72430000  | 0.81263300  |
| H | -3.00790100 | 7.61739100  | 0.89202800  |
| H | 0.74889600  | 5.53261800  | 0.70245300  |
| H | -0.52017600 | 7.66409000  | 0.94841000  |
| C | -4.62019800 | 2.96919700  | 0.61946700  |
| H | -5.06773100 | 1.97657300  | 0.52710000  |
| H | -4.77809100 | 3.32117500  | 1.64403600  |
| H | -5.16906900 | 3.62992100  | -0.05844200 |
| C | -3.45178500 | -1.83107000 | -2.81728700 |
| C | -4.76598700 | -1.40735900 | -3.06013800 |
| C | -3.24741200 | -3.16162700 | -2.41955200 |
| C | -5.84294100 | -2.28373100 | -2.90162500 |
| H | -4.94996600 | -0.38271600 | -3.36888100 |
| C | -4.32063900 | -4.04004800 | -2.26014300 |
| H | -2.23467100 | -3.51641100 | -2.24319600 |
| C | -5.62570400 | -3.60269200 | -2.49879600 |
| H | -6.85327400 | -1.93255400 | -3.09289200 |
| H | -4.13683300 | -5.06471400 | -1.94889300 |
| H | -6.46328400 | -4.28255900 | -2.37253400 |
| C | -1.67295900 | -1.16361500 | -4.45322000 |
| H | -1.35299100 | -2.20563500 | -4.54344500 |
| H | -2.42115300 | -0.98699400 | -5.23194300 |
| H | -0.80972300 | -0.52103000 | -4.65291100 |
| C | 3.02858300  | -3.43029300 | 4.20700900  |
| C | -3.38361600 | 3.73035200  | -4.70291700 |
| H | -2.45154600 | 3.97558600  | -5.22614800 |
| H | -4.05735400 | 3.28254100  | -5.44114000 |
| H | -3.82774400 | 4.66917100  | -4.36146100 |
| H | 2.93459700  | -3.19534600 | 5.27188700  |
| H | 3.09216600  | -4.51688300 | 4.10056400  |
| H | 3.98377400  | -3.01101000 | 3.86751500  |
| C | 6.75291900  | 2.37804200  | -0.24848100 |
| C | 1.41767500  | 1.93975300  | -2.93258400 |
| H | 2.21398500  | 2.05974900  | -3.67811700 |
| H | 0.51633100  | 1.60755100  | -3.45557300 |

|                         |              |              |              |
|-------------------------|--------------|--------------|--------------|
| H                       | 1. 22154700  | 2. 92467000  | -2. 49852000 |
| F                       | 7. 57758100  | -0. 71812000 | -1. 92834600 |
| F                       | 8. 74369000  | 1. 66128100  | -1. 31171700 |
| F                       | 7. 32596200  | 3. 54989800  | 0. 06027000  |
| F                       | 4. 77087000  | 3. 07357000  | 0. 80236700  |
| <b>TS2<sub>cw</sub></b> |              |              |              |
| C                       | -7. 20561700 | -0. 88721100 | -1. 38503400 |
| C                       | -6. 57470700 | 0. 15484000  | -2. 05972300 |
| C                       | -5. 24934200 | 0. 47737800  | -1. 80144900 |
| C                       | -4. 50786100 | -0. 24111300 | -0. 85343600 |
| C                       | -5. 15469900 | -1. 28230800 | -0. 18803600 |
| C                       | -3. 04789500 | 0. 06773100  | -0. 56101200 |
| H                       | -2. 90950000 | 0. 12102600  | 0. 52263600  |
| H                       | -2. 82332900 | 1. 06481900  | -0. 94701100 |
| C                       | -2. 11076600 | -0. 97902200 | -1. 15286900 |
| H                       | 0. 25823500  | 0. 88739000  | -2. 38029500 |
| H                       | -2. 27577400 | -1. 98112900 | -0. 76223500 |
| C                       | -1. 52979500 | -0. 90193000 | -2. 43133900 |
| C                       | -1. 13105400 | 0. 36274500  | -3. 01266100 |
| H                       | -1. 74535900 | 1. 24560400  | -2. 84928800 |
| H                       | -0. 73113300 | 0. 31987500  | -4. 02273600 |
| Ni                      | -0. 15433100 | -0. 02595600 | -1. 25565800 |
| H                       | -4. 79889600 | 1. 30076100  | -2. 34497600 |
| C                       | 1. 10508900  | 0. 20740800  | 0. 12428100  |
| C                       | 2. 32188400  | 1. 09049500  | 1. 96516600  |
| C                       | 3. 19141200  | 0. 04555800  | 1. 25889000  |
| H                       | 2. 71308800  | 2. 10333900  | 1. 81923400  |
| H                       | 2. 21633500  | 0. 90617100  | 3. 03553200  |
| H                       | 4. 16928600  | 0. 43348200  | 0. 96690700  |
| H                       | 3. 33695300  | -0. 84568200 | 1. 87885700  |
| N                       | 2. 37890700  | -0. 27784800 | 0. 06458600  |
| N                       | 1. 02030500  | 0. 93840500  | 1. 27181000  |
| C                       | 2. 89129000  | -1. 09545800 | -0. 99960600 |
| C                       | 3. 40060800  | -0. 47247500 | -2. 16722000 |
| C                       | 2. 93141800  | -2. 49798200 | -0. 86165100 |
| C                       | 3. 88712800  | -1. 28475400 | -3. 19393100 |
| C                       | 3. 43444800  | -3. 26459600 | -1. 92166300 |
| C                       | 3. 90491100  | -2. 68271900 | -3. 09677700 |
| H                       | 4. 26772900  | -0. 82506400 | -4. 10036000 |
| H                       | 3. 44852000  | -4. 34690800 | -1. 82457700 |
| C                       | -0. 17091500 | 1. 55840700  | 1. 78091200  |
| C                       | -0. 42359900 | 2. 92380000  | 1. 53981900  |
| C                       | -1. 05751900 | 0. 79501700  | 2. 58424300  |
| C                       | -1. 58531600 | 3. 49923400  | 2. 07395400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.20004200 | 1.41962300  | 3.09075500  |
| C | -2.48733800 | 2.76858100  | 2.84307600  |
| H | -1.78848600 | 4.54763400  | 1.87233000  |
| H | -2.89278100 | 0.84718700  | 3.69885400  |
| C | 2.52107600  | -3.20510200 | 0.43476300  |
| C | 3.43520100  | 1.05021800  | -2.28644400 |
| C | 0.55589400  | 3.82251600  | 0.77655900  |
| C | -0.76081100 | -0.66795400 | 2.91472900  |
| H | -0.32894500 | -1.11351500 | 2.01382400  |
| H | 2.00062000  | -2.46865000 | 1.05172300  |
| H | 2.51382600  | 1.41680000  | -1.82705200 |
| H | 1.27251900  | 3.16686800  | 0.27372600  |
| C | 1.52863600  | -4.34786800 | 0.21020100  |
| C | 1.91942300  | -5.69169100 | 0.12663300  |
| C | 0.16048400  | -4.05135200 | 0.09965100  |
| C | 0.97623700  | -6.70503900 | -0.06987100 |
| H | 2.96566500  | -5.96303900 | 0.22516900  |
| C | -0.78445500 | -5.06050300 | -0.09034900 |
| H | -0.16529100 | -3.01584900 | 0.15688900  |
| C | -0.37936200 | -6.39496800 | -0.17812000 |
| H | 1.30536800  | -7.73880400 | -0.13025200 |
| H | -1.83810800 | -4.80493600 | -0.16327800 |
| H | -1.11281100 | -7.18285100 | -0.32311600 |
| C | 3.78254900  | -3.64793800 | 1.20783200  |
| H | 4.39038900  | -4.34553800 | 0.62412100  |
| H | 4.41589800  | -2.78609600 | 1.43561000  |
| H | 3.51272800  | -4.13543300 | 2.15023900  |
| C | 4.60224500  | 1.68649700  | -1.52639700 |
| C | 5.86500900  | 1.08275800  | -1.44313600 |
| C | 4.43103600  | 2.94790200  | -0.93481200 |
| C | 6.92151400  | 1.71756000  | -0.78471300 |
| H | 6.02136800  | 0.10533800  | -1.89022500 |
| C | 5.48414100  | 3.58599600  | -0.27698600 |
| H | 3.46196400  | 3.43771200  | -0.99886400 |
| C | 6.73579800  | 2.97080400  | -0.19768300 |
| H | 7.89095400  | 1.22965200  | -0.73027200 |
| H | 5.32608900  | 4.56153900  | 0.17473600  |
| H | 7.55662500  | 3.46249300  | 0.31644200  |
| C | 3.42672700  | 1.56094500  | -3.74293900 |
| H | 2.58783100  | 1.13479400  | -4.30249900 |
| H | 3.32354200  | 2.65002000  | -3.74767000 |
| H | 4.35499900  | 1.32177600  | -4.27112000 |
| C | -0.13657800 | 4.63027300  | -0.32415400 |
| C | -0.46278500 | 5.98639700  | -0.18806000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.46425800 | 3.98894800  | -1.52953700 |
| C | -1.10598000 | 6.67813000  | -1.21984200 |
| H | -0.21244700 | 6.52089300  | 0.72254700  |
| C | -1.10307600 | 4.67654900  | -2.56116500 |
| H | -0.21227100 | 2.93861900  | -1.65355500 |
| C | -1.42979200 | 6.02732700  | -2.40982700 |
| H | -1.34820900 | 7.72942400  | -1.09017900 |
| H | -1.34044600 | 4.15931400  | -3.48717700 |
| H | -1.92566700 | 6.56567400  | -3.21246900 |
| C | 1.34244200  | 4.70193600  | 1.77147000  |
| H | 1.89426200  | 4.08023700  | 2.48138800  |
| H | 2.05819900  | 5.34294600  | 1.24674800  |
| H | 0.67559000  | 5.34126800  | 2.35753900  |
| C | 0.27173700  | -0.83332700 | 4.03538700  |
| C | 0.37913600  | 0.07361400  | 5.09921700  |
| C | 1.10072300  | -1.96599600 | 4.04480700  |
| C | 1.29418900  | -0.13963000 | 6.13393600  |
| H | -0.25175700 | 0.95734500  | 5.11599000  |
| C | 2.01551100  | -2.18281200 | 5.07671700  |
| H | 1.01906600  | -2.69244200 | 3.23974800  |
| C | 2.11820000  | -1.26646000 | 6.12616400  |
| H | 1.36208000  | 0.57849900  | 6.94662400  |
| H | 2.64779000  | -3.06628000 | 5.05978400  |
| H | 2.83116100  | -1.43000500 | 6.92909300  |
| C | -2.01506600 | -1.50075300 | 3.26166600  |
| H | -1.73402100 | -2.55299500 | 3.36294700  |
| H | -2.45803000 | -1.19315400 | 4.21389900  |
| H | -2.77817400 | -1.42797300 | 2.48212700  |
| C | 4.41156600  | -3.52773700 | -4.24197000 |
| C | -3.74750800 | 3.39938700  | 3.38708900  |
| H | -3.91953700 | 3.11257400  | 4.42972400  |
| H | -3.70223300 | 4.49065500  | 3.33657600  |
| H | -4.62735000 | 3.07815700  | 2.81638400  |
| H | 3.66924500  | -3.58654000 | -5.04735200 |
| H | 5.32384800  | -3.10642300 | -4.67693900 |
| H | 4.62805400  | -4.54985000 | -3.91935300 |
| C | -6.48420100 | -1.61030300 | -0.43944700 |
| C | -1.05794900 | -2.16768200 | -3.12069500 |
| H | -1.74215600 | -2.42669700 | -3.93967800 |
| H | -0.06145700 | -2.04201200 | -3.55805700 |
| H | -1.02396300 | -3.01554500 | -2.43197900 |
| F | -7.28444000 | 0.84860000  | -2.96862000 |
| F | -8.48625200 | -1.19626400 | -1.63440000 |
| F | -7.07304200 | -2.61646300 | 0.22220200  |

|                         |             |             |             |
|-------------------------|-------------|-------------|-------------|
| F                       | -4.49194700 | -2.01642500 | 0.73482900  |
| <b>1<sub>cw</sub></b>   |             |             |             |
| C                       | 2.55570000  | 0.31954600  | 0.28062400  |
| C                       | 1.77418900  | 1.43078000  | -0.02745000 |
| C                       | 0.48219200  | 1.28540300  | -0.51338500 |
| C                       | -0.06840800 | 0.01186500  | -0.70731800 |
| C                       | 0.72423400  | -1.09093900 | -0.39221000 |
| C                       | -1.48405100 | -0.18656900 | -1.22092000 |
| H                       | -1.46981700 | -0.97853000 | -1.98075100 |
| H                       | -1.80477400 | 0.72791000  | -1.72393700 |
| C                       | -2.44304500 | -0.58115600 | -0.11928200 |
| H                       | -5.03279100 | 1.30273000  | -0.62757600 |
| H                       | -2.19978700 | -1.52592300 | 0.36556300  |
| C                       | -3.52531500 | 0.08422400  | 0.31262700  |
| C                       | -4.01278100 | 1.40321500  | -0.23468100 |
| H                       | -3.38583600 | 1.80536100  | -1.03240500 |
| H                       | -4.06269700 | 2.15397600  | 0.56447500  |
| H                       | -0.09164000 | 2.17673600  | -0.74239700 |
| C                       | 2.02163100  | -0.95212500 | 0.09528000  |
| C                       | -4.37216100 | -0.47650400 | 1.43114500  |
| H                       | -4.41319900 | 0.22019700  | 2.27885500  |
| H                       | -5.40916100 | -0.62502800 | 1.10239400  |
| H                       | -3.98963700 | -1.43394300 | 1.79495600  |
| F                       | 2.30371400  | 2.65367100  | 0.15515500  |
| F                       | 3.80310000  | 0.46358100  | 0.74826700  |
| F                       | 2.75723600  | -2.03386300 | 0.38414100  |
| F                       | 0.24108700  | -2.34004900 | -0.55709100 |
| <b>IM3<sub>cw</sub></b> |             |             |             |
| C                       | -7.22327000 | -1.08941200 | -1.68437000 |
| C                       | -6.65728200 | 0.02439400  | -2.29928000 |
| C                       | -5.37788600 | 0.45138700  | -1.97067200 |
| C                       | -4.61872600 | -0.23000400 | -1.00932500 |
| C                       | -5.20037900 | -1.34380200 | -0.40362100 |
| C                       | -3.20604800 | 0.19152400  | -0.64134200 |
| H                       | -3.11517400 | 0.19982000  | 0.45040900  |
| H                       | -3.05125500 | 1.21953600  | -0.97603400 |
| C                       | -2.15330100 | -0.74724800 | -1.22097600 |
| H                       | -0.70253400 | 0.85825800  | -3.84812800 |
| H                       | -2.23374800 | -1.76468100 | -0.83150700 |
| C                       | -1.47794700 | -0.59619900 | -2.44601500 |
| C                       | -1.64442100 | 0.61714900  | -3.34066200 |
| H                       | -1.96667400 | 1.51049000  | -2.80047900 |
| H                       | -2.38649800 | 0.42043100  | -4.13075600 |
| Ni                      | -0.28872400 | -0.20535500 | -0.86765000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.97674500 | 1.32612700  | -2.47061000 |
| C | 1.17772300  | 0.19435400  | 0.28558700  |
| C | 2.40809600  | 0.75549000  | 2.24237800  |
| C | 3.39569800  | 0.47101100  | 1.10013800  |
| H | 2.55203900  | 1.74703400  | 2.67830300  |
| H | 2.46342100  | 0.01465200  | 3.04557100  |
| H | 3.95243400  | 1.35984500  | 0.78929000  |
| H | 4.11317900  | -0.31163400 | 1.35722700  |
| N | 2.49669600  | 0.02478300  | 0.00797900  |
| N | 1.09596300  | 0.66627300  | 1.55701600  |
| C | 3.01429600  | -0.48443700 | -1.23128300 |
| C | 3.11728800  | 0.36576700  | -2.36208200 |
| C | 3.45001300  | -1.82232500 | -1.29946100 |
| C | 3.64407100  | -0.16480900 | -3.54168300 |
| C | 3.97252600  | -2.30136800 | -2.50857700 |
| C | 4.07788100  | -1.49441000 | -3.63832400 |
| H | 3.72301900  | 0.46825600  | -4.41951700 |
| H | 4.29006800  | -3.33939700 | -2.56654400 |
| C | -0.12567200 | 0.99760900  | 2.23641600  |
| C | -0.50964300 | 2.34864000  | 2.34239600  |
| C | -0.91645400 | -0.02390300 | 2.82097900  |
| C | -1.69311900 | 2.66438400  | 3.02342300  |
| C | -2.08731500 | 0.34727300  | 3.48693500  |
| C | -2.49379200 | 1.68380700  | 3.60361400  |
| H | -1.99976500 | 3.70562400  | 3.08432800  |
| H | -2.71181900 | -0.42208200 | 3.92916300  |
| C | 3.39822800  | -2.76811000 | -0.09617000 |
| C | 2.66957200  | 1.82532000  | -2.29311800 |
| C | 0.32850500  | 3.48859600  | 1.75910100  |
| C | -0.50580400 | -1.49242100 | 2.72582500  |
| H | -0.06169500 | -1.62864000 | 1.73475500  |
| H | 2.85883000  | -2.25049800 | 0.70141100  |
| H | 1.75934400  | 1.84482000  | -1.68462200 |
| H | 1.13373600  | 3.03412800  | 1.17523900  |
| C | 2.58969900  | -4.03162800 | -0.40508700 |
| C | 3.17390800  | -5.29535100 | -0.55971100 |
| C | 1.19375500  | -3.92728300 | -0.53363400 |
| C | 2.39060100  | -6.42068200 | -0.83843600 |
| H | 4.24730100  | -5.41725900 | -0.45819600 |
| C | 0.41013800  | -5.04838100 | -0.80553900 |
| H | 0.72111600  | -2.95182600 | -0.42961800 |
| C | 1.00694900  | -6.30324000 | -0.96134100 |
| H | 2.86789100  | -7.38993100 | -0.95433300 |
| H | -0.66787700 | -4.94328800 | -0.89414000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.39827300  | -7.17764800 | -1.17279500 |
| C | 4.82003800  | -3.05639900 | 0.42513800  |
| H | 5.44352800  | -3.53810200 | -0.33409500 |
| H | 5.32019000  | -2.12527800 | 0.70660400  |
| H | 4.78917500  | -3.70640900 | 1.30529700  |
| C | 3.68866600  | 2.74117200  | -1.60882800 |
| C | 5.07113500  | 2.52898000  | -1.70371100 |
| C | 3.23688000  | 3.87226700  | -0.91099300 |
| C | 5.97466500  | 3.41531700  | -1.11121800 |
| H | 5.44413400  | 1.66046800  | -2.23842600 |
| C | 4.13679900  | 4.75996300  | -0.31835500 |
| H | 2.16866400  | 4.06240600  | -0.83864300 |
| C | 5.51200000  | 4.53298900  | -0.41418100 |
| H | 7.04204800  | 3.22942800  | -1.19453500 |
| H | 3.76296800  | 5.62780200  | 0.21815800  |
| H | 6.21462400  | 5.21990100  | 0.04877900  |
| C | 2.29011700  | 2.42375300  | -3.66514400 |
| H | 1.56319600  | 1.79215700  | -4.18546400 |
| H | 1.84461300  | 3.41220600  | -3.52149400 |
| H | 3.16319300  | 2.55234000  | -4.31237900 |
| C | -0.48268100 | 4.33901900  | 0.77687300  |
| C | -0.82484700 | 5.67455000  | 1.02403900  |
| C | -0.89720300 | 3.76277300  | -0.43734900 |
| C | -1.56090000 | 6.41359600  | 0.09129600  |
| H | -0.51599100 | 6.15505600  | 1.94631300  |
| C | -1.62608500 | 4.49922000  | -1.37036800 |
| H | -0.64799600 | 2.72301200  | -0.64558400 |
| C | -1.96373500 | 5.83092500  | -1.10902500 |
| H | -1.81397900 | 7.44798800  | 0.30726500  |
| H | -1.92859600 | 4.03569800  | -2.30561800 |
| H | -2.53139300 | 6.40555600  | -1.83523500 |
| C | 0.98852900  | 4.30383900  | 2.88846400  |
| H | 1.60190200  | 3.65380800  | 3.51883500  |
| H | 1.63343700  | 5.08862200  | 2.48052300  |
| H | 0.24560800  | 4.77535600  | 3.53910100  |
| C | 0.55693800  | -1.89453500 | 3.75314300  |
| C | 0.62601400  | -1.31991400 | 5.02996100  |
| C | 1.46280600  | -2.91950600 | 3.43692300  |
| C | 1.57520000  | -1.75217700 | 5.96028300  |
| H | -0.06317700 | -0.52456200 | 5.29750400  |
| C | 2.41219500  | -3.35350100 | 4.36370200  |
| H | 1.41622600  | -3.38770600 | 2.45658600  |
| C | 2.47340100  | -2.76892900 | 5.63118000  |
| H | 1.61194800  | -1.29093200 | 6.94353200  |



|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 3. 10346600  | -4. 14769300 | 4. 09501000  |
| H | 3. 21272900  | -3. 10243600 | 6. 35372600  |
| C | -1. 69627200 | -2. 47372000 | 2. 80693500  |
| H | -1. 34901500 | -3. 48659700 | 2. 58299300  |
| H | -2. 13923100 | -2. 49846100 | 3. 80742900  |
| H | -2. 47701400 | -2. 21117000 | 2. 08736800  |
| C | 4. 63047800  | -2. 02892500 | -4. 93879400 |
| C | -3. 75835800 | 2. 03995300  | 4. 34946900  |
| H | -4. 59317200 | 1. 39885900  | 4. 04752700  |
| H | -3. 62960400 | 1. 91042100  | 5. 43101600  |
| H | -4. 04702700 | 3. 07953400  | 4. 17265100  |
| H | 5. 42870700  | -1. 38640900 | -5. 32647100 |
| H | 5. 03645700  | -3. 03645400 | -4. 81579600 |
| H | 3. 85289100  | -2. 07422100 | -5. 71037400 |
| C | -6. 48343400 | -1. 77728700 | -0. 72692800 |
| C | -0. 95618000 | -1. 81610400 | -3. 18389700 |
| H | -1. 63855700 | -2. 09486100 | -4. 00309500 |
| H | 0. 02265200  | -1. 62238500 | -3. 63984300 |
| H | -0. 85317900 | -2. 68332900 | -2. 52653300 |
| F | -7. 38434300 | 0. 68284100  | -3. 22092800 |
| F | -8. 45953100 | -1. 50019000 | -2. 00220600 |
| F | -7. 01079200 | -2. 85088000 | -0. 12166500 |
| F | -4. 51977300 | -2. 04591000 | 0. 53035500  |

#### IM4<sub>ew</sub>

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | 5. 63637300  | 1. 78624100  | -1. 19986300 |
| C  | 4. 36450600  | 2. 34119700  | -1. 11815400 |
| C  | 3. 27867900  | 1. 75406200  | -1. 75209900 |
| C  | 3. 44179500  | 0. 58510600  | -2. 50434300 |
| C  | 4. 72561500  | 0. 04097000  | -2. 57971700 |
| C  | 2. 31271500  | -0. 09883600 | -3. 24961700 |
| H  | 2. 58836600  | -0. 10347100 | -4. 31790300 |
| H  | 2. 30822900  | -1. 15371000 | -2. 96075800 |
| C  | 0. 93508100  | 0. 51001000  | -3. 08102100 |
| C  | -0. 26336600 | -0. 18013400 | -3. 36628500 |
| Ni | -0. 06298700 | 0. 09663600  | -1. 40114500 |
| H  | 2. 29915600  | 2. 20103100  | -1. 64111300 |
| C  | -0. 83354900 | -0. 20466700 | 0. 33583100  |
| C  | -2. 44318800 | -0. 64485000 | 2. 03603800  |
| C  | -1. 07750700 | -0. 42535300 | 2. 69387400  |
| H  | -3. 14439100 | 0. 15978300  | 2. 27925700  |
| H  | -2. 89967100 | -1. 59800700 | 2. 30743800  |
| H  | -1. 08736400 | 0. 36408500  | 3. 44770700  |
| H  | -0. 69629800 | -1. 34296200 | 3. 15244100  |
| N  | -0. 22648500 | -0. 03706100 | 1. 54225800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -2.10618200 | -0.61629300 | 0.59175300  |
| C | 1.13509300  | 0.37034700  | 1.76085100  |
| C | 1.45055600  | 1.75296800  | 1.80749700  |
| C | 2.12872700  | -0.59611500 | 2.01486100  |
| C | 2.76369300  | 2.12462200  | 2.10113800  |
| C | 3.43304400  | -0.16591400 | 2.29709800  |
| C | 3.77209200  | 1.18338700  | 2.34864600  |
| H | 3.02397700  | 3.17661700  | 2.12819800  |
| H | 4.20251100  | -0.91377500 | 2.47091200  |
| C | -3.11034900 | -0.86610400 | -0.40582600 |
| C | -4.03191500 | 0.14386700  | -0.74756200 |
| C | -3.19871600 | -2.15271900 | -0.99628600 |
| C | -5.00360600 | -0.13216500 | -1.71934100 |
| C | -4.18870100 | -2.37342800 | -1.95665400 |
| C | -5.09519700 | -1.37544200 | -2.34060500 |
| H | -5.70145900 | 0.65268600  | -1.99916700 |
| H | -4.26609100 | -3.34819600 | -2.42691100 |
| C | 1.83693100  | -2.09959300 | 2.04085600  |
| C | 0.38171900  | 2.81534300  | 1.55221300  |
| C | -4.05785200 | 1.50502800  | -0.04389400 |
| C | -2.24657400 | -3.27507200 | -0.57790700 |
| H | -1.24795100 | -2.83144900 | -0.50587500 |
| H | 0.82049600  | -2.24172100 | 1.66320600  |
| H | -0.25330600 | 2.43354400  | 0.74632100  |
| H | -3.15514400 | 1.57058900  | 0.56754300  |
| C | 2.76103100  | -2.87097800 | 1.09353000  |
| C | 3.77979300  | -3.72014300 | 1.54474800  |
| C | 2.58776900  | -2.72257300 | -0.29303500 |
| C | 4.60682300  | -4.39522200 | 0.64057300  |
| H | 3.93774200  | -3.86784800 | 2.60785100  |
| C | 3.41103600  | -3.39388900 | -1.19630000 |
| H | 1.79988200  | -2.06556900 | -0.65950400 |
| C | 4.42779800  | -4.23410500 | -0.73205900 |
| H | 5.39063700  | -5.04758000 | 1.01568000  |
| H | 3.26699200  | -3.26027500 | -2.26449300 |
| H | 5.07013600  | -4.75660400 | -1.43498100 |
| C | 1.87018200  | -2.62463300 | 3.49054600  |
| H | 2.85214500  | -2.48045600 | 3.95130300  |
| H | 1.14480000  | -2.09053300 | 4.11007800  |
| H | 1.62983000  | -3.69206300 | 3.52702500  |
| C | -0.52857200 | 3.06664700  | 2.75859900  |
| C | -0.07007200 | 2.95814700  | 4.07910300  |
| C | -1.85047000 | 3.48929000  | 2.54854100  |
| C | -0.91027600 | 3.25213900  | 5.15655400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.94992800  | 2.63613200  | 4.26684800  |
| C | -2.69219700 | 3.78493000  | 3.62241100  |
| H | -2.21978500 | 3.59879400  | 1.53162000  |
| C | -2.22531000 | 3.66436900  | 4.93356500  |
| H | -0.53409700 | 3.15815900  | 6.17166500  |
| H | -3.71194500 | 4.10958700  | 3.43415400  |
| H | -2.87859800 | 3.89072800  | 5.77128300  |
| C | 0.95563600  | 4.16479700  | 1.06433200  |
| H | 1.65002900  | 4.02821700  | 0.23047400  |
| H | 0.13839400  | 4.81234200  | 0.73397800  |
| H | 1.48442000  | 4.69274700  | 1.86406000  |
| C | -3.99262100 | 2.68604900  | -1.01567600 |
| C | -5.12470000 | 3.41081500  | -1.41404200 |
| C | -2.74373300 | 3.08351400  | -1.52046200 |
| C | -5.01411800 | 4.49206300  | -2.29365000 |
| H | -6.10552400 | 3.14454600  | -1.03348500 |
| C | -2.62874500 | 4.16619600  | -2.39295000 |
| H | -1.85494500 | 2.52330600  | -1.23693600 |
| C | -3.76653400 | 4.87651900  | -2.78485700 |
| H | -5.90688200 | 5.03753200  | -2.58700200 |
| H | -1.64983900 | 4.45649700  | -2.76500700 |
| H | -3.67993400 | 5.72131400  | -3.46205600 |
| C | -5.26794800 | 1.57682700  | 0.91180600  |
| H | -5.22322000 | 0.76992400  | 1.64860200  |
| H | -5.28553600 | 2.53122000  | 1.44753800  |
| H | -6.21565800 | 1.46776500  | 0.37637300  |
| C | -2.58003100 | -3.86023500 | 0.79765000  |
| C | -3.90248200 | -4.03301100 | 1.23074600  |
| C | -1.54432900 | -4.30834100 | 1.63102000  |
| C | -4.18058000 | -4.62328100 | 2.46615100  |
| H | -4.72040000 | -3.69546000 | 0.60076900  |
| C | -1.81826500 | -4.89855000 | 2.86658900  |
| H | -0.51333600 | -4.20108600 | 1.30246900  |
| C | -3.13976400 | -5.05532100 | 3.29097900  |
| H | -5.21263500 | -4.74398800 | 2.78396500  |
| H | -0.99962900 | -5.23506500 | 3.49679700  |
| H | -3.35590900 | -5.51087500 | 4.25301400  |
| C | -2.14942000 | -4.43269000 | -1.59488200 |
| H | -1.36649800 | -5.12801200 | -1.27891000 |
| H | -3.08266200 | -5.00130600 | -1.65524200 |
| H | -1.89874500 | -4.07027800 | -2.59584100 |
| C | 5.18333500  | 1.63358800  | 2.64569800  |
| C | -6.13200600 | -1.64635300 | -3.40540200 |
| H | -6.91145100 | -0.87961400 | -3.40792600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.67798900 | -1.65961800 | -4.40370700 |
| H | -6.61122300 | -2.61984600 | -3.25799300 |
| H | 5.82047200  | 0.79066900  | 2.92633900  |
| H | 5.63500900  | 2.12027100  | 1.77452500  |
| H | 5.20317700  | 2.36112000  | 3.46473500  |
| C | 5.81597100  | 0.61921200  | -1.93736000 |
| F | 4.20725700  | 3.46442500  | -0.38651900 |
| F | 6.67475200  | 2.34656600  | -0.55621400 |
| F | 7.03257500  | 0.06252000  | -2.02210200 |
| F | 4.93618400  | -1.08895000 | -3.28808700 |
| H | 0.90411600  | 1.59163200  | -3.23906800 |
| C | -1.45887000 | 0.58017300  | -3.91049000 |
| C | -0.28748400 | -1.65215500 | -3.73418300 |
| H | -1.42040700 | 1.64302600  | -3.66135000 |
| H | -1.49247800 | 0.49399300  | -5.00898300 |
| H | -2.40372200 | 0.17703100  | -3.52948100 |
| H | 0.48370400  | -2.23890100 | -3.22985700 |
| H | -1.25966200 | -2.08880000 | -3.48585400 |
| H | -0.14603600 | -1.78046600 | -4.81959200 |

#### IM4'<sub>cw</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -5.80380500 | -0.77457400 | -0.84274000 |
| C  | -4.81606600 | -1.75498100 | -0.84327300 |
| C  | -3.68764400 | -1.63537000 | -1.64194000 |
| C  | -3.50998400 | -0.51992300 | -2.46976700 |
| C  | -4.51603900 | 0.44617800  | -2.46896200 |
| C  | -2.27473200 | -0.33684500 | -3.32251100 |
| H  | -1.74758100 | -1.29277900 | -3.37949800 |
| H  | -2.59810100 | -0.09962700 | -4.34810500 |
| C  | -1.35903300 | 0.77349300  | -2.81324600 |
| C  | -0.02000500 | 0.94291000  | -3.21435800 |
| Ni | -0.12309600 | 0.36819000  | -1.30059100 |
| H  | -2.93672100 | -2.41662300 | -1.61206200 |
| C  | 0.79097500  | 0.09546000  | 0.35426800  |
| C  | 2.53446100  | -0.10437800 | 1.96060400  |
| C  | 1.19832300  | 0.00089100  | 2.69342500  |
| H  | 2.95303000  | -1.11502200 | 2.03189700  |
| H  | 3.27748700  | 0.61096000  | 2.31489400  |
| H  | 1.04802500  | -0.79020900 | 3.42873400  |
| H  | 1.07929200  | 0.97224600  | 3.19055800  |
| N  | 0.22851400  | -0.11954300 | 1.57718400  |
| N  | 2.13652300  | 0.18948000  | 0.56249700  |
| C  | -1.17142700 | -0.25650000 | 1.86830900  |
| C  | -1.72546300 | -1.55788800 | 1.96869100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.95115000 | 0.88138100  | 2.16324600  |
| C | -3.05707900 | -1.68448000 | 2.37122400  |
| C | -3.27546000 | 0.69102400  | 2.58694400  |
| C | -3.84772900 | -0.57531300 | 2.69426800  |
| H | -3.50245600 | -2.67123300 | 2.43549600  |
| H | -3.87976800 | 1.55886300  | 2.83532600  |
| C | 3.11647100  | 0.33901500  | -0.47689500 |
| C | 3.67490700  | -0.79779500 | -1.09512700 |
| C | 3.55096700  | 1.64007400  | -0.83419700 |
| C | 4.62311500  | -0.61424800 | -2.11053600 |
| C | 4.50199400  | 1.76572100  | -1.85020800 |
| C | 5.04235900  | 0.65344600  | -2.50961400 |
| H | 5.03983700  | -1.48968000 | -2.60183200 |
| H | 4.83695400  | 2.75432300  | -2.14710200 |
| C | -1.39385200 | 2.29724400  | 2.06250100  |
| C | -0.89348800 | -2.79814400 | 1.64059000  |
| C | 3.34708700  | -2.22255900 | -0.63599900 |
| C | 3.00654000  | 2.87171900  | -0.10894600 |
| H | 1.93790900  | 2.69539300  | 0.05063400  |
| H | -0.32358800 | 2.21258400  | 1.85723600  |
| H | -0.25152200 | -2.53072300 | 0.79504100  |
| H | 2.48824700  | -2.15552000 | 0.03566000  |
| C | -1.97296000 | 3.14423100  | 0.91747900  |
| C | -1.29634000 | 4.32359900  | 0.56031800  |
| C | -3.14603800 | 2.83035000  | 0.21989600  |
| C | -1.77742300 | 5.16190300  | -0.44497300 |
| H | -0.37805800 | 4.59183200  | 1.07751500  |
| C | -3.63544700 | 3.66799100  | -0.78795200 |
| H | -3.68457800 | 1.91934200  | 0.45210300  |
| C | -2.95542500 | 4.83797600  | -1.12425900 |
| H | -1.23237100 | 6.06716700  | -0.69808100 |
| H | -4.54320600 | 3.39058900  | -1.31509200 |
| H | -3.33406200 | 5.48843800  | -1.90734300 |
| C | -1.53643400 | 3.04766300  | 3.41040400  |
| H | -2.58632500 | 3.21568100  | 3.66734700  |
| H | -1.07482800 | 2.47681300  | 4.22255700  |
| H | -1.05012500 | 4.02615700  | 3.35965300  |
| C | 0.02940700  | -3.23878200 | 2.78113300  |
| C | -0.34324300 | -3.12681900 | 4.12837300  |
| C | 1.25890400  | -3.84463300 | 2.48118600  |
| C | 0.49280800  | -3.59636400 | 5.14474400  |
| H | -1.29067900 | -2.66197300 | 4.38507000  |
| C | 2.09671400  | -4.31572400 | 3.49398000  |
| H | 1.55685400  | -3.95750800 | 1.44152000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 1. 71723300  | -4. 19051800 | 4. 83236700  |
| H | 0. 18558700  | -3. 49586500 | 6. 18213900  |
| H | 3. 04533300  | -4. 77898700 | 3. 23696700  |
| H | 2. 36817300  | -4. 55286300 | 5. 62274800  |
| C | -1. 74290300 | -4. 01018500 | 1. 19511400  |
| H | -2. 46553200 | -3. 73466600 | 0. 42232700  |
| H | -1. 08744300 | -4. 79012600 | 0. 79717200  |
| H | -2. 29397800 | -4. 44718400 | 2. 03354900  |
| C | 2. 91547600  | -3. 14247000 | -1. 77998700 |
| C | 1. 58407100  | -3. 09653500 | -2. 22414800 |
| C | 3. 78643700  | -4. 05016900 | -2. 39858400 |
| C | 1. 13859700  | -3. 92820500 | -3. 25179000 |
| H | 0. 89679900  | -2. 38818600 | -1. 76476300 |
| C | 3. 34451400  | -4. 88065100 | -3. 43317900 |
| H | 4. 81848100  | -4. 12644100 | -2. 07159400 |
| C | 2. 01892300  | -4. 82494800 | -3. 86331300 |
| H | 0. 10182800  | -3. 87859400 | -3. 57411000 |
| H | 4. 03913800  | -5. 57628600 | -3. 89604800 |
| H | 1. 67342300  | -5. 47474700 | -4. 66223900 |
| C | 4. 52980300  | -2. 78704400 | 0. 18055600  |
| H | 4. 73200500  | -2. 15422400 | 1. 04915000  |
| H | 4. 31275700  | -3. 79970100 | 0. 53551700  |
| H | 5. 44981800  | -2. 82231800 | -0. 41036500 |
| C | 3. 64190100  | 3. 07894300  | 1. 26960500  |
| C | 5. 01038000  | 2. 86971900  | 1. 49403100  |
| C | 2. 86263200  | 3. 55851700  | 2. 33262500  |
| C | 5. 57945200  | 3. 12591700  | 2. 74363700  |
| H | 5. 63392100  | 2. 49616300  | 0. 68696800  |
| C | 3. 42700000  | 3. 81640500  | 3. 58364800  |
| H | 1. 80111500  | 3. 73357400  | 2. 17660900  |
| C | 4. 79038600  | 3. 59911400  | 3. 79445200  |
| H | 6. 64147600  | 2. 95376800  | 2. 89579900  |
| H | 2. 80136600  | 4. 18423200  | 4. 39223900  |
| H | 5. 23269200  | 3. 79537000  | 4. 76685700  |
| C | 3. 12996000  | 4. 18361000  | -0. 91385800 |
| H | 2. 61143600  | 4. 98622200  | -0. 38133500 |
| H | 4. 17280900  | 4. 49439400  | -1. 03006700 |
| H | 2. 68246700  | 4. 08817500  | -1. 90706900 |
| C | -5. 28795500 | -0. 75456900 | 3. 11326500  |
| C | 6. 04260400  | 0. 83254400  | -3. 62751400 |
| H | 6. 59908200  | -0. 08937900 | -3. 81759700 |
| H | 5. 54256200  | 1. 11400600  | -4. 56236500 |
| H | 6. 76197500  | 1. 62480900  | -3. 39661700 |
| H | -5. 39757500 | -1. 58606200 | 3. 81703800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.68170000 | 0.14841400  | 3.58805200  |
| H | -5.92097900 | -0.97807400 | 2.24732300  |
| C | -5.64650600 | 0.33788300  | -1.66393300 |
| F | -4.41070100 | 1.54250700  | -3.24945900 |
| F | -6.57390300 | 1.30725400  | -1.66933700 |
| F | -6.88376900 | -0.88394100 | -0.05076800 |
| F | -4.97388500 | -2.82085500 | -0.03275200 |
| C | 0.56719100  | 2.34258700  | -3.26468100 |
| C | 0.69950900  | -0.03629600 | -4.12089200 |
| H | 0.48660200  | 2.75248800  | -4.28500400 |
| H | 0.05104100  | 3.02951700  | -2.58823100 |
| H | 1.63175600  | 2.33652800  | -3.00765600 |
| H | 0.31931500  | -1.05638600 | -4.04354200 |
| H | 0.60446500  | 0.27612100  | -5.17351700 |
| H | 1.77059300  | -0.06639600 | -3.89221700 |
| H | -1.89757600 | 1.67607300  | -2.51962700 |

### IMS<sub>ew</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.83307900  | -1.55225300 | -0.15561700 |
| C  | 3.51424900  | -1.11730400 | -0.17501300 |
| C  | 2.68763400  | -1.13660400 | -1.29239600 |
| C  | 3.26844400  | -1.61727500 | -2.48269200 |
| C  | 4.59381500  | -2.05482400 | -2.48447700 |
| C  | 2.47946500  | -1.67471800 | -3.77215700 |
| H  | 3.11981400  | -1.37009300 | -4.60820600 |
| H  | 2.20458600  | -2.71692600 | -3.98600200 |
| C  | 1.22498000  | -0.80266900 | -3.74821500 |
| C  | 0.20888600  | -1.07711100 | -2.63082200 |
| Ni | 0.90956900  | -0.52615100 | -0.89792900 |
| H  | 1.51466200  | 0.25586100  | -3.71884000 |
| C  | -0.62279400 | 0.13666700  | 0.25905100  |
| C  | -1.52071700 | 1.57410700  | 1.92456900  |
| C  | -2.09503000 | 0.17112500  | 2.12838800  |
| H  | -0.84227700 | 1.85654600  | 2.73432000  |
| H  | -2.28872800 | 2.34181500  | 1.82454100  |
| H  | -1.88608300 | -0.23375100 | 3.11967500  |
| H  | -3.17551900 | 0.13161900  | 1.95638700  |
| N  | -1.37694100 | -0.61999000 | 1.09264700  |
| N  | -0.75073100 | 1.42734900  | 0.65930700  |
| C  | -1.54202300 | -2.05269400 | 1.08116700  |
| C  | -0.57212100 | -2.87175200 | 1.71177500  |
| C  | -2.73204800 | -2.61427200 | 0.56598000  |
| C  | -0.80242900 | -4.24848700 | 1.77150200  |
| C  | -2.92532700 | -3.99798000 | 0.69634000  |
| C  | -1.97246600 | -4.83356800 | 1.27564500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.05985200 | -4.88883700 | 2.23557700  |
| H | -3.85121300 | -4.43452900 | 0.33340500  |
| C | -0.33354900 | 2.60570900  | -0.06377300 |
| C | 0.92667300  | 3.19594000  | 0.17407200  |
| C | -1.25743600 | 3.22161200  | -0.94859600 |
| C | 1.25303000  | 4.37621300  | -0.50759200 |
| C | -0.86432600 | 4.38417900  | -1.61846800 |
| C | 0.38474300  | 4.97924100  | -1.41453300 |
| H | 2.22545700  | 4.82497100  | -0.32773200 |
| H | -1.55330600 | 4.85150600  | -2.31467300 |
| C | -3.84971700 | -1.77060000 | -0.04280300 |
| C | 0.68045500  | -2.27151400 | 2.34465300  |
| C | 1.92765000  | 2.65159400  | 1.19691900  |
| C | -2.67392200 | 2.68203900  | -1.14767900 |
| H | -2.64306600 | 1.60628000  | -0.95671000 |
| H | -3.52502500 | -0.72708800 | -0.01048100 |
| H | 1.00677600  | -1.45393300 | 1.70069700  |
| H | 1.71114700  | 1.58788700  | 1.34140400  |
| C | -4.19609300 | -2.04644600 | -1.51661500 |
| C | -5.01284500 | -1.11168900 | -2.17802100 |
| C | -3.76667300 | -3.16240300 | -2.24513500 |
| C | -5.39135800 | -1.28510100 | -3.50815400 |
| H | -5.35886100 | -0.23012500 | -1.64431500 |
| C | -4.14405700 | -3.34175700 | -3.58035700 |
| H | -3.11966500 | -3.89737000 | -1.78245900 |
| C | -4.95851900 | -2.40796200 | -4.21843300 |
| H | -6.02111200 | -0.54239000 | -3.98997800 |
| H | -3.79238500 | -4.21692800 | -4.11962300 |
| H | -5.24925700 | -2.54806900 | -5.25543500 |
| C | -5.12719800 | -1.87866700 | 0.83104200  |
| H | -5.53449900 | -2.89359300 | 0.80816600  |
| H | -4.90919500 | -1.62653000 | 1.87357300  |
| H | -5.90588600 | -1.20108400 | 0.46976400  |
| C | 0.42515000  | -1.66427100 | 3.72753600  |
| C | -0.46849200 | -2.23362200 | 4.64570100  |
| C | 1.15220600  | -0.53036500 | 4.12266100  |
| C | -0.63647400 | -1.68163500 | 5.91846000  |
| H | -1.04216800 | -3.11120300 | 4.36217800  |
| C | 0.98732900  | 0.02272400  | 5.39391900  |
| H | 1.86305100  | -0.08861900 | 3.42891900  |
| C | 0.08862400  | -0.55011200 | 6.29719900  |
| H | -1.33604700 | -2.13765400 | 6.61373200  |
| H | 1.56056300  | 0.90099500  | 5.67792400  |
| H | -0.04389700 | -0.11994600 | 7.28573000  |



|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 1. 87263100  | -3. 24958100 | 2. 41807600  |
| H | 2. 06966100  | -3. 70144500 | 1. 44086800  |
| H | 2. 76794300  | -2. 70331600 | 2. 72415400  |
| H | 1. 70739300  | -4. 04946000 | 3. 14642300  |
| C | 3. 37383100  | 2. 74463300  | 0. 69237600  |
| C | 4. 40209500  | 3. 33732600  | 1. 43693800  |
| C | 3. 70079000  | 2. 20456800  | -0. 56261100 |
| C | 5. 71199500  | 3. 38792100  | 0. 94652200  |
| H | 4. 19708200  | 3. 76759100  | 2. 41087900  |
| C | 5. 00352300  | 2. 25126600  | -1. 05431300 |
| H | 2. 92395500  | 1. 73390300  | -1. 15731200 |
| C | 6. 01916600  | 2. 84677200  | -0. 30037400 |
| H | 6. 48926300  | 3. 85394400  | 1. 54599400  |
| H | 5. 22641800  | 1. 81827700  | -2. 02559800 |
| H | 7. 03568600  | 2. 88506700  | -0. 68131300 |
| C | 1. 71736400  | 3. 35838200  | 2. 55290200  |
| H | 0. 67353300  | 3. 29506200  | 2. 86666400  |
| H | 2. 33085400  | 2. 90363700  | 3. 33672200  |
| H | 1. 97428300  | 4. 42058800  | 2. 48776800  |
| C | -3. 69342200 | 3. 28048500  | -0. 16641100 |
| C | -3. 62392900 | 4. 60670800  | 0. 28397500  |
| C | -4. 77956900 | 2. 49768500  | 0. 25621400  |
| C | -4. 60621000 | 5. 13020300  | 1. 12856000  |
| H | -2. 79212400 | 5. 23456700  | -0. 01858200 |
| C | -5. 76317600 | 3. 01631000  | 1. 09977400  |
| H | -4. 85561300 | 1. 46759600  | -0. 08224800 |
| C | -5. 67956600 | 4. 33869700  | 1. 54075300  |
| H | -4. 52839700 | 6. 15988200  | 1. 46649000  |
| H | -6. 59140500 | 2. 38695500  | 1. 41334200  |
| H | -6. 44077100 | 4. 74618400  | 2. 19960000  |
| C | -3. 20097600 | 2. 85480600  | -2. 59154000 |
| H | -4. 14393500 | 2. 31231100  | -2. 70460000 |
| H | -3. 39937000 | 3. 90340700  | -2. 83126600 |
| H | -2. 48953600 | 2. 45973400  | -3. 32200200 |
| C | -2. 18575800 | -6. 32626800 | 1. 35749700  |
| C | 0. 78193000  | 6. 22584800  | -2. 16871500 |
| H | 1. 57411100  | 6. 77167600  | -1. 64877600 |
| H | 1. 15804000  | 5. 97610600  | -3. 16846800 |
| H | -0. 06914600 | 6. 90062600  | -2. 30301900 |
| H | -3. 24519400 | -6. 58454400 | 1. 27481800  |
| H | -1. 65712400 | -6. 84283500 | 0. 54698900  |
| H | -1. 80639500 | -6. 73319700 | 2. 29995300  |
| C | 5. 38390200  | -2. 03290300 | -1. 33917500 |
| F | 3. 02854100  | -0. 61275800 | 1. 01367100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | 5.57821400  | -1.50517300 | 0.96571500  |
| F | 6.66034800  | -2.45905800 | -1.37177400 |
| F | 5.15841100  | -2.52291400 | -3.62553400 |
| H | 0.70838800  | -0.94845700 | -4.71247800 |
| C | -1.04136300 | -0.23743200 | -2.88753600 |
| C | -0.14091200 | -2.55942400 | -2.50472800 |
| H | -0.80619100 | 0.83098200  | -2.92301200 |
| H | -1.48620200 | -0.50963200 | -3.85932100 |
| H | -1.80774300 | -0.39911600 | -2.12722300 |
| H | 0.73466600  | -3.17782400 | -2.29042900 |
| H | -0.87374100 | -2.72698500 | -1.71254400 |
| H | -0.58911500 | -2.92724600 | -3.44365900 |

**IM5'**<sub>cw</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -4.62514100 | -2.36028000 | -1.43542300 |
| C  | -3.29850900 | -2.18515000 | -1.04082400 |
| C  | -2.56693000 | -1.05412400 | -1.35823400 |
| C  | -3.20551700 | -0.06351600 | -2.13812200 |
| C  | -4.52401700 | -0.22229800 | -2.54029000 |
| C  | -2.30071300 | 1.08527300  | -2.50578400 |
| H  | -2.55119300 | 1.50673600  | -3.49059100 |
| H  | -2.41724200 | 1.90350600  | -1.78733100 |
| C  | -0.86586000 | 0.51667200  | -2.45530200 |
| C  | -0.55290600 | -0.32143400 | -3.71220900 |
| Ni | -0.84460900 | -0.48130900 | -0.76600000 |
| H  | -1.44968800 | -0.91587600 | -3.93187800 |
| C  | 0.65691400  | 0.21922500  | 0.37103000  |
| C  | 2.66439000  | 0.67909700  | 1.54945900  |
| C  | 1.47851200  | 1.06483200  | 2.43694800  |
| H  | 3.20667800  | -0.18792200 | 1.94083500  |
| H  | 3.37111700  | 1.49514600  | 1.39747600  |
| H  | 1.48478100  | 0.56295700  | 3.40570100  |
| H  | 1.41990900  | 2.14596900  | 2.60207700  |
| N  | 0.32055000  | 0.61160700  | 1.62400800  |
| N  | 2.00120200  | 0.31432700  | 0.26852900  |
| C  | -1.00461400 | 0.62984200  | 2.18942400  |
| C  | -1.51985100 | -0.55137900 | 2.78067600  |
| C  | -1.72015100 | 1.84531100  | 2.25999300  |
| C  | -2.77411400 | -0.49014800 | 3.39477800  |
| C  | -2.95088600 | 1.85285900  | 2.93093300  |
| C  | -3.50452400 | 0.69940300  | 3.48594300  |
| H  | -3.19134100 | -1.38805400 | 3.83781500  |
| H  | -3.49464600 | 2.78880500  | 3.02060500  |
| C  | 2.81169600  | -0.05460900 | -0.86127200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.29284800  | -1.37358600 | -0.98304200 |
| C | 3.18947200  | 0.94580300  | -1.79016100 |
| C | 4.11013500  | -1.68650900 | -2.07705700 |
| C | 4.01207400  | 0.57765200  | -2.85795000 |
| C | 4.47604100  | -0.73354400 | -3.02547500 |
| H | 4.46463600  | -2.70717400 | -2.19151800 |
| H | 4.30061200  | 1.32530800  | -3.58951400 |
| C | -1.16264500 | 3.15446100  | 1.71087700  |
| C | -0.71577700 | -1.85179400 | 2.80857800  |
| C | 3.01837500  | -2.45431700 | 0.06906700  |
| C | 2.72819300  | 2.39384600  | -1.62224100 |
| H | 1.71667300  | 2.35955500  | -1.20647400 |
| H | -0.18847800 | 2.93506400  | 1.26492400  |
| H | -0.14458200 | -1.90349100 | 1.87727100  |
| H | 2.31531200  | -2.03352200 | 0.79126400  |
| C | -1.98465700 | 3.83215900  | 0.60162600  |
| C | -1.38957100 | 4.90535400  | -0.08583700 |
| C | -3.28604500 | 3.46704500  | 0.23418900  |
| C | -2.06932300 | 5.59606000  | -1.08751600 |
| H | -0.37684600 | 5.20842800  | 0.16888600  |
| C | -3.97436900 | 4.16020000  | -0.76810200 |
| H | -3.77245900 | 2.62751900  | 0.71606100  |
| C | -3.37323500 | 5.22840200  | -1.43099800 |
| H | -1.58038000 | 6.41936400  | -1.60088100 |
| H | -4.98154500 | 3.85100400  | -1.03285000 |
| H | -3.90790500 | 5.76367300  | -2.21012400 |
| C | -0.91701000 | 4.14928500  | 2.87588900  |
| H | -1.85925700 | 4.44553500  | 3.34611500  |
| H | -0.28296900 | 3.69792900  | 3.64569500  |
| H | -0.42466300 | 5.05696400  | 2.51643300  |
| C | 0.30902400  | -1.89839100 | 3.94927000  |
| C | 0.10409200  | -1.25440100 | 5.17754800  |
| C | 1.47614300  | -2.66175600 | 3.78798000  |
| C | 1.04139000  | -1.36335400 | 6.20878400  |
| H | -0.79076600 | -0.65873900 | 5.32958300  |
| C | 2.41419500  | -2.77258700 | 4.81540100  |
| H | 1.64427500  | -3.18500000 | 2.84974300  |
| C | 2.20120500  | -2.11956400 | 6.03192700  |
| H | 0.86253800  | -0.85388700 | 7.15169700  |
| H | 3.31063400  | -3.36768600 | 4.66478200  |
| H | 2.93041500  | -2.20072600 | 6.83273500  |
| C | -1.59173400 | -3.12355200 | 2.84574600  |
| H | -2.31590400 | -3.12282600 | 2.02788400  |
| H | -0.95391900 | -4.00521200 | 2.73526800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.12250700 | -3.22692500 | 3.79663000  |
| C | 2.33481500  | -3.69822000 | -0.50571200 |
| C | 0.93472000  | -3.72567800 | -0.59589900 |
| C | 3.04154200  | -4.83101000 | -0.93383600 |
| C | 0.25637600  | -4.83557100 | -1.09975700 |
| H | 0.36329200  | -2.85848300 | -0.27459600 |
| C | 2.36889800  | -5.94486700 | -1.44551100 |
| H | 4.12430400  | -4.86110200 | -0.86107000 |
| C | 0.97576200  | -5.95289600 | -1.53051800 |
| H | -0.82838000 | -4.81745800 | -1.14626400 |
| H | 2.93871900  | -6.81099100 | -1.77069600 |
| H | 0.45590300  | -6.82229300 | -1.92243900 |
| C | 4.31620800  | -2.78060600 | 0.83935600  |
| H | 4.71173700  | -1.88225800 | 1.32263700  |
| H | 4.13011600  | -3.53368500 | 1.61153400  |
| H | 5.09994300  | -3.15961400 | 0.17750700  |
| C | 3.58477000  | 3.18759700  | -0.62960800 |
| C | 4.97570700  | 3.03049700  | -0.54805500 |
| C | 2.97675900  | 4.15093600  | 0.18927000  |
| C | 5.73365900  | 3.80963900  | 0.32962600  |
| H | 5.46875500  | 2.28723200  | -1.16762100 |
| C | 3.73041400  | 4.93127600  | 1.06804400  |
| H | 1.89997100  | 4.29122200  | 0.13233400  |
| C | 5.11483600  | 4.76184200  | 1.14222600  |
| H | 6.80994800  | 3.66935000  | 0.37910500  |
| H | 3.23632100  | 5.66853200  | 1.69476900  |
| H | 5.70458500  | 5.36453100  | 1.82674400  |
| C | 2.63738700  | 3.17719100  | -2.94998600 |
| H | 2.17576400  | 4.15175900  | -2.76735400 |
| H | 3.62466800  | 3.36273000  | -3.38345600 |
| H | 2.02958400  | 2.64277600  | -3.68572800 |
| C | -4.85762900 | 0.72786500  | 4.15559700  |
| C | 5.33095300  | -1.10122200 | -4.21494300 |
| H | 5.88270800  | -2.02880900 | -4.03972600 |
| H | 4.71395900  | -1.24920700 | -5.10963600 |
| H | 6.05263600  | -0.31191500 | -4.44786400 |
| H | -4.90731200 | 0.01866300  | 4.98721700  |
| H | -5.09274900 | 1.72464300  | 4.53952600  |
| H | -5.64991500 | 0.45403400  | 3.44817000  |
| C | -5.24291700 | -1.36660900 | -2.18893300 |
| F | -5.15168800 | 0.71687700  | -3.29041800 |
| F | -6.52433000 | -1.51690600 | -2.57745300 |
| F | -5.31647400 | -3.46997300 | -1.10394000 |
| F | -2.73594600 | -3.20134100 | -0.31151300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.61662400  | -1.30001100 | -3.56407300 |
| C | -0.29778000 | 0.59720300  | -4.92781300 |
| H | 1.55099500  | -0.77395500 | -3.35103700 |
| H | 0.43836800  | -2.01051900 | -2.75332900 |
| H | 0.75985400  | -1.86998900 | -4.49066600 |
| H | -1.11149000 | 1.31071300  | -5.09114400 |
| H | 0.62806000  | 1.16993900  | -4.79474000 |
| H | -0.18892300 | 0.00442000  | -5.84368600 |
| H | -0.11621900 | 1.30744300  | -2.32485600 |

**IM8**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -6.15845600 | -0.79299600 | -0.88734100 |
| C  | -5.38972300 | -1.81500600 | -0.33990600 |
| C  | -4.42243300 | -2.44223300 | -1.11814000 |
| C  | -4.15421600 | -2.05021600 | -2.43031600 |
| C  | -4.95096600 | -1.03195600 | -2.97083800 |
| C  | -2.99112100 | -2.65665500 | -3.17975300 |
| H  | -3.05035100 | -2.35954200 | -4.23139400 |
| H  | -3.06716800 | -3.75011700 | -3.15068400 |
| C  | -1.60742100 | -2.24611600 | -2.58389100 |
| H  | -1.59710200 | -2.54785500 | -1.53164000 |
| H  | -0.84097000 | -2.84912700 | -3.08801200 |
| C  | -1.26247400 | -0.76823500 | -2.71432000 |
| C  | -1.85311200 | 0.17639200  | -1.85516600 |
| H  | -2.56540200 | -0.12189100 | -1.08812000 |
| H  | -1.92598900 | 1.22186600  | -2.15331500 |
| Ni | -0.06786900 | -0.20769900 | -1.17121500 |
| C  | 1.04474000  | 0.27834500  | 0.30127700  |
| C  | 2.95237200  | 0.66850500  | 1.67097800  |
| C  | 1.68983400  | 1.09276500  | 2.44331700  |
| H  | 3.47635300  | -0.15529600 | 2.16542100  |
| H  | 3.65808300  | 1.49027300  | 1.52795700  |
| H  | 1.56440400  | 0.54682000  | 3.38073300  |
| H  | 1.68833300  | 2.16429500  | 2.66430100  |
| N  | 0.60111400  | 0.75286000  | 1.49515200  |
| N  | 2.40010000  | 0.22882500  | 0.36743300  |
| C  | -0.79097000 | 0.90769400  | 1.82274500  |
| C  | -1.55171000 | -0.22758600 | 2.20681100  |
| C  | -1.39018300 | 2.18002700  | 1.75955500  |
| C  | -2.91560000 | -0.05789800 | 2.45276600  |
| C  | -2.76173000 | 2.29538400  | 2.02998800  |
| C  | -3.54447400 | 1.19243300  | 2.36044200  |
| H  | -3.52191900 | -0.91973500 | 2.71080000  |
| H  | -3.22826300 | 3.27423500  | 1.95461400  |
| C  | 3.24544300  | -0.19239200 | -0.71498100 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 3. 78996100  | -1. 49071600 | -0. 71100300 |
| C | 3. 54679600  | 0. 71157600  | -1. 76648300 |
| C | 4. 62509900  | -1. 87765600 | -1. 76841500 |
| C | 4. 38044400  | 0. 27238300  | -2. 79691100 |
| C | 4. 93151200  | -1. 01677700 | -2. 81877400 |
| H | 5. 02936800  | -2. 88682800 | -1. 77263900 |
| H | 4. 61393900  | 0. 94738000  | -3. 61380000 |
| C | -0. 59021900 | 3. 44954700  | 1. 45093500  |
| C | -0. 89571800 | -1. 60026600 | 2. 35898800  |
| C | 3. 52498200  | -2. 48739300 | 0. 41956200  |
| C | 2. 98069800  | 2. 13054300  | -1. 76811600 |
| H | 1. 95280400  | 2. 05551200  | -1. 39948800 |
| H | 0. 39612200  | 3. 13445600  | 1. 10032700  |
| H | -0. 24100400 | -1. 73505000 | 1. 49131700  |
| H | 2. 75968200  | -2. 04824900 | 1. 06499400  |
| C | -1. 20284500 | 4. 26235800  | 0. 30799000  |
| C | -1. 90431500 | 5. 45867700  | 0. 50689500  |
| C | -1. 04941900 | 3. 79662100  | -1. 00876400 |
| C | -2. 44308100 | 6. 16406200  | -0. 57443000 |
| H | -2. 03214400 | 5. 85696600  | 1. 50812000  |
| C | -1. 58178100 | 4. 49945500  | -2. 08934500 |
| H | -0. 51742800 | 2. 86386400  | -1. 18027800 |
| C | -2. 28446200 | 5. 68903500  | -1. 87577200 |
| H | -2. 98376900 | 7. 08924000  | -0. 39441000 |
| H | -1. 44625800 | 4. 11974700  | -3. 09851100 |
| H | -2. 69963400 | 6. 23937800  | -2. 71517700 |
| C | -0. 38201800 | 4. 26659800  | 2. 74244100  |
| H | -1. 33443300 | 4. 57419100  | 3. 18470500  |
| H | 0. 14065600  | 3. 66696800  | 3. 49305900  |
| H | 0. 21178400  | 5. 16545100  | 2. 54722700  |
| C | -0. 01941000 | -1. 70611600 | 3. 61025600  |
| C | -0. 34063100 | -1. 04549600 | 4. 80461200  |
| C | 1. 10655000  | -2. 54375800 | 3. 59831300  |
| C | 0. 44690300  | -1. 20649500 | 5. 94758500  |
| H | -1. 20937700 | -0. 39471400 | 4. 83849300  |
| C | 1. 89631800  | -2. 70678300 | 4. 73808700  |
| H | 1. 35936400  | -3. 08232900 | 2. 68806800  |
| C | 1. 57080600  | -2. 03459200 | 5. 91869600  |
| H | 0. 18051900  | -0. 68243500 | 6. 86150800  |
| H | 2. 76517300  | -3. 35842000 | 4. 70313900  |
| H | 2. 18476300  | -2. 15688300 | 6. 80636700  |
| C | -1. 89137600 | -2. 77982600 | 2. 34940600  |
| H | -2. 53532600 | -2. 76133100 | 1. 46705700  |
| H | -1. 33558000 | -3. 72204300 | 2. 34487900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.52507500 | -2.78289900 | 3.24205100  |
| C | 2.93382800  | -3.79692000 | -0.11028400 |
| C | 3.62968700  | -5.01241600 | -0.09488000 |
| C | 1.62866400  | -3.78725800 | -0.63222000 |
| C | 3.04332000  | -6.18278200 | -0.58892600 |
| H | 4.63574500  | -5.06023000 | 0.30833400  |
| C | 1.04060200  | -4.95236500 | -1.12185500 |
| H | 1.07167200  | -2.85191500 | -0.65675700 |
| C | 1.74789800  | -6.15853900 | -1.10322500 |
| H | 3.60354600  | -7.11353400 | -0.56588600 |
| H | 0.02839300  | -4.91963400 | -1.51520000 |
| H | 1.29113800  | -7.06786700 | -1.48322300 |
| C | 4.79292100  | -2.67772800 | 1.27470900  |
| H | 5.12422800  | -1.71807400 | 1.68138900  |
| H | 4.60423000  | -3.35612800 | 2.11295300  |
| H | 5.62274400  | -3.08261000 | 0.68728800  |
| C | 3.72863100  | 3.07998700  | -0.82761800 |
| C | 5.10469100  | 2.96662600  | -0.58410100 |
| C | 3.03433900  | 4.14260600  | -0.22812900 |
| C | 5.76470700  | 3.88200000  | 0.24042800  |
| H | 5.66362800  | 2.15317900  | -1.03719400 |
| C | 3.69036900  | 5.05878100  | 0.59590300  |
| H | 1.96987500  | 4.25825800  | -0.41797200 |
| C | 5.06066000  | 4.93021000  | 0.83593700  |
| H | 6.83134500  | 3.77320200  | 0.41735500  |
| H | 3.13049000  | 5.87145000  | 1.05063700  |
| H | 5.57351300  | 5.63936100  | 1.47932400  |
| C | 2.89129700  | 2.76209200  | -3.17425200 |
| H | 2.35382600  | 3.71278000  | -3.11397700 |
| H | 3.87956800  | 2.97416700  | -3.59382600 |
| H | 2.35274400  | 2.10709900  | -3.86664500 |
| C | -5.02814100 | 1.32312700  | 2.61654800  |
| C | 5.81793500  | -1.45345000 | -3.96141500 |
| H | 6.28783400  | -2.41889200 | -3.75574600 |
| H | 5.24455200  | -1.55330300 | -4.89068500 |
| H | 6.61153700  | -0.72277100 | -4.15182800 |
| H | -5.35958300 | 2.36048900  | 2.51970200  |
| H | -5.61048800 | 0.71744900  | 1.91333200  |
| H | -5.28833700 | 0.97929500  | 3.62435300  |
| C | -5.93674100 | -0.41777800 | -2.20963100 |
| C | -0.71498900 | -0.34909800 | -4.06668800 |
| H | -1.42040500 | -0.57064200 | -4.88354300 |
| H | -0.50635000 | 0.72480800  | -4.09810800 |
| H | 0.21656100  | -0.87886900 | -4.30578400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | -5.57258200 | -2.17416700 | 0.94006700  |
| F | -7.07886300 | -0.17169100 | -0.13283400 |
| F | -6.68909400 | 0.56868100  | -2.72922300 |
| H | -4.78998300 | -0.68855400 | -3.98666400 |
| F | -3.69812500 | -3.42889200 | -0.54234900 |

## TS5

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.07404000 | -2.83993300 | 0.34987900  |
| C  | -1.76881800 | -2.52975100 | 0.01816600  |
| C  | -1.39022800 | -2.16528000 | -1.29239800 |
| C  | -2.36638700 | -2.28345000 | -2.31723400 |
| C  | -3.69333300 | -2.57582900 | -1.95680900 |
| C  | -2.08759100 | -2.04889800 | -3.79116800 |
| H  | -2.53114300 | -1.08905800 | -4.09086300 |
| H  | -2.63199900 | -2.80958700 | -4.36282400 |
| C  | -0.62338900 | -2.08157300 | -4.22147400 |
| H  | -0.18358100 | -3.04647500 | -3.95021200 |
| H  | -0.58603700 | -2.02760700 | -5.32054100 |
| C  | 0.25604700  | -0.97632500 | -3.67265200 |
| C  | -0.23577600 | 0.25484300  | -3.27576300 |
| H  | -1.29290100 | 0.49556900  | -3.32435100 |
| H  | 0.43047200  | 1.10666700  | -3.18253300 |
| Ni | 0.03972400  | -0.84373900 | -1.51431300 |
| C  | 0.35214800  | 0.29123200  | 0.11242600  |
| C  | 1.72104500  | 1.62948300  | 1.52395700  |
| C  | 0.27312100  | 2.04417800  | 1.70508800  |
| H  | 2.09107600  | 1.06485300  | 2.38680300  |
| H  | 2.39172300  | 2.46648400  | 1.33277000  |
| H  | -0.03327900 | 2.10869200  | 2.74772400  |
| H  | 0.06307700  | 2.99957200  | 1.21087700  |
| N  | -0.44504600 | 0.95016900  | 0.99824400  |
| N  | 1.62200300  | 0.73980200  | 0.33938500  |
| C  | -1.84269600 | 0.73367300  | 1.26595600  |
| C  | -2.20228900 | -0.04542300 | 2.39625400  |
| C  | -2.83386300 | 1.37035600  | 0.48678100  |
| C  | -3.56127200 | -0.26409700 | 2.63988000  |
| C  | -4.17944800 | 1.12528900  | 0.78905200  |
| C  | -4.56313000 | 0.28200100  | 1.83121200  |
| H  | -3.85535300 | -0.89409400 | 3.47220700  |
| H  | -4.94578100 | 1.59522600  | 0.17949700  |
| C  | 2.81028900  | 0.37100000  | -0.38356900 |
| C  | 3.55498100  | -0.77269500 | -0.01406700 |
| C  | 3.27951200  | 1.23553000  | -1.40704200 |
| C  | 4.72521000  | -1.06421000 | -0.72711300 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 4.46004700  | 0.89710800  | -2.07541600 |
| C | 5.19139500  | -0.25330600 | -1.76060400 |
| H | 5.28896400  | -1.95302800 | -0.45970600 |
| H | 4.82495900  | 1.54079200  | -2.86931900 |
| C | -2.48462300 | 2.41537400  | -0.57670900 |
| C | -1.15137600 | -0.60698200 | 3.35800000  |
| C | 3.19892300  | -1.63927400 | 1.20300200  |
| C | 2.53586700  | 2.52207200  | -1.77065100 |
| H | 1.47192800  | 2.33287900  | -1.60010500 |
| H | -1.46032100 | 2.21017800  | -0.90927700 |
| H | -0.25643900 | -0.81842100 | 2.76749500  |
| H | 2.13525400  | -1.49367300 | 1.41281600  |
| C | -3.37515600 | 2.36311300  | -1.82589800 |
| C | -3.78695700 | 3.52685400  | -2.49271200 |
| C | -3.77292400 | 1.12928700  | -2.36722600 |
| C | -4.56196300 | 3.46267400  | -3.65490300 |
| H | -3.50985400 | 4.50321900  | -2.11198200 |
| C | -4.55249000 | 1.06134500  | -3.52253400 |
| H | -3.48327900 | 0.21025900  | -1.87000000 |
| C | -4.95123800 | 2.22983100  | -4.17597700 |
| H | -4.86469900 | 4.38332200  | -4.14624500 |
| H | -4.85507000 | 0.09138300  | -3.90761900 |
| H | -5.55996200 | 2.17828000  | -5.07406600 |
| C | -2.48998900 | 3.81286200  | 0.08848900  |
| H | -3.51249400 | 4.12904200  | 0.31911700  |
| H | -1.93217200 | 3.79782100  | 1.02672600  |
| H | -2.03370500 | 4.57010900  | -0.55631200 |
| C | -0.74023000 | 0.38390600  | 4.45561300  |
| C | -1.63063000 | 1.31372600  | 5.01086500  |
| C | 0.55987300  | 0.31719400  | 4.98281500  |
| C | -1.23139200 | 2.15508800  | 6.05298700  |
| H | -2.64123200 | 1.38709000  | 4.62124900  |
| C | 0.96209300  | 1.15542100  | 6.02367700  |
| H | 1.26295300  | -0.40491400 | 4.57349300  |
| C | 0.06579500  | 2.08132200  | 6.56313100  |
| H | -1.93798200 | 2.87046300  | 6.46499100  |
| H | 1.97486600  | 1.08639800  | 6.41115900  |
| H | 0.37566100  | 2.73769800  | 7.37115800  |
| C | -1.55948800 | -1.93639000 | 4.03375600  |
| H | -1.85751900 | -2.67753600 | 3.29283900  |
| H | -0.70992200 | -2.32863200 | 4.60066700  |
| H | -2.38023400 | -1.79459800 | 4.74359200  |
| C | 3.39665000  | -3.13813600 | 0.95563100  |
| C | 4.56313400  | -3.81885600 | 1.33609000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2. 37750500  | -3. 87229000 | 0. 32958400  |
| C | 4. 71384400  | -5. 18631000 | 1. 08776300  |
| H | 5. 36656000  | -3. 28961100 | 1. 83797500  |
| C | 2. 52616300  | -5. 23801300 | 0. 08222300  |
| H | 1. 45829800  | -3. 37958400 | 0. 03293500  |
| C | 3. 69629200  | -5. 90246300 | 0. 45758300  |
| H | 5. 62733200  | -5. 68923700 | 1. 39356300  |
| H | 1. 72004300  | -5. 78357900 | -0. 40096700 |
| H | 3. 81033300  | -6. 96591500 | 0. 26708300  |
| C | 3. 99447400  | -1. 14186000 | 2. 43213500  |
| H | 3. 77340900  | -0. 09389500 | 2. 64553900  |
| H | 3. 74764800  | -1. 73445000 | 3. 31892600  |
| H | 5. 07358800  | -1. 20973500 | 2. 26540000  |
| C | 2. 91219900  | 3. 72262400  | -0. 89353600 |
| C | 4. 21407600  | 3. 92721400  | -0. 41525800 |
| C | 1. 94044400  | 4. 69546100  | -0. 61088200 |
| C | 4. 53248200  | 5. 06639200  | 0. 32860400  |
| H | 4. 98285700  | 3. 18764100  | -0. 61741900 |
| C | 2. 25522600  | 5. 83486000  | 0. 13153900  |
| H | 0. 92660300  | 4. 55803300  | -0. 98041300 |
| C | 3. 55527800  | 6. 02413700  | 0. 60594600  |
| H | 5. 54693100  | 5. 20293600  | 0. 69296000  |
| H | 1. 48507500  | 6. 57198900  | 0. 34108300  |
| H | 3. 80311800  | 6. 90769300  | 1. 18690500  |
| C | 2. 69031400  | 2. 92848300  | -3. 25506700 |
| H | 2. 01257700  | 3. 75721900  | -3. 47945200 |
| H | 3. 70446300  | 3. 27204800  | -3. 47871800 |
| H | 2. 45269400  | 2. 09910000  | -3. 92787500 |
| C | -6. 01357800 | -0. 07099900 | 2. 05672700  |
| C | 6. 44109100  | -0. 60971700 | -2. 53023600 |
| H | 7. 09878500  | -1. 25911800 | -1. 94580200 |
| H | 6. 19289300  | -1. 14321700 | -3. 45606800 |
| H | 7. 00484200  | 0. 28439600  | -2. 81391400 |
| H | -6. 68302900 | 0. 70099600  | 1. 66649300  |
| H | -6. 25458200 | -1. 00953600 | 1. 54136200  |
| H | -6. 23466000 | -0. 21606700 | 3. 11859300  |
| C | -4. 04844200 | -2. 84061300 | -0. 64647100 |
| C | 1. 73051900  | -1. 18559600 | -3. 94692300 |
| H | 1. 91019700  | -1. 21867900 | -5. 03163500 |
| H | 2. 35089400  | -0. 39144700 | -3. 52695500 |
| H | 2. 07545800  | -2. 14240000 | -3. 53946700 |
| F | -0. 82926700 | -2. 57244000 | 0. 99136700  |
| F | -3. 41002100 | -3. 16411900 | 1. 61482900  |
| F | -5. 32894100 | -3. 11303700 | -0. 30322100 |

|            |             |             |             |
|------------|-------------|-------------|-------------|
| H          | -4.46590300 | -2.61059500 | -2.71945900 |
| F          | 0.05876900  | -2.94235300 | -1.56605200 |
| <b>IM9</b> |             |             |             |
| C          | 1.92404000  | 2.33247900  | -3.11027100 |
| C          | 0.93707200  | 1.59095100  | -2.46826900 |
| C          | 1.13540800  | 0.29053900  | -2.03473000 |
| C          | 2.36723800  | -0.32674300 | -2.32126600 |
| C          | 3.37156600  | 0.40810300  | -2.97568300 |
| C          | 2.61948500  | -1.78609900 | -1.99868000 |
| H          | 2.09740600  | -2.04514300 | -1.07074500 |
| H          | 3.68805500  | -1.93912800 | -1.81701100 |
| C          | 2.13961700  | -2.71778100 | -3.12647900 |
| H          | 1.06759700  | -2.54098200 | -3.27975400 |
| H          | 2.62653300  | -2.42061300 | -4.06826200 |
| C          | 2.37123300  | -4.19937600 | -2.92186500 |
| C          | 2.98371600  | -4.72769200 | -1.85434400 |
| H          | 3.37339500  | -4.12039700 | -1.04366400 |
| H          | 3.12065900  | -5.80230700 | -1.76244300 |
| Ni         | -0.32525300 | -0.59318500 | -1.26287700 |
| C          | -0.38855000 | 0.11433300  | 0.51174100  |
| C          | -1.73235000 | 0.03802700  | 2.46042100  |
| C          | -0.49874400 | 0.91375600  | 2.71955200  |
| H          | -2.65398200 | 0.62755700  | 2.42933500  |
| H          | -1.84627200 | -0.76749900 | 3.18706300  |
| H          | -0.75066900 | 1.91309800  | 3.07379100  |
| H          | 0.19369200  | 0.44986000  | 3.42961500  |
| N          | 0.14794400  | 0.99286200  | 1.37633100  |
| N          | -1.42704700 | -0.50294900 | 1.11728500  |
| C          | 1.24396000  | 1.90985100  | 1.18555800  |
| C          | 0.96836600  | 3.22147700  | 0.72509500  |
| C          | 2.54197300  | 1.54232900  | 1.59921300  |
| C          | 2.03259600  | 4.12266000  | 0.63396200  |
| C          | 3.55806600  | 2.50644700  | 1.52546400  |
| C          | 3.33273800  | 3.78871800  | 1.02822500  |
| H          | 1.84724900  | 5.12361700  | 0.25978900  |
| H          | 4.55386500  | 2.24769500  | 1.87271100  |
| C          | -2.18248700 | -1.52223800 | 0.43036900  |
| C          | -3.34175600 | -1.17717200 | -0.30297400 |
| C          | -1.76095000 | -2.87566600 | 0.53494800  |
| C          | -4.05461500 | -2.19970000 | -0.93913500 |
| C          | -2.50217500 | -3.84696000 | -0.13935800 |
| C          | -3.64835400 | -3.53161900 | -0.88132900 |
| H          | -4.93913200 | -1.93689600 | -1.51212100 |
| H          | -2.18674900 | -4.88362100 | -0.09092200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.84694300  | 0.18739900  | 2.23112200  |
| C | -0.45068800 | 3.67063400  | 0.37112900  |
| C | -3.88427800 | 0.24918600  | -0.35732700 |
| C | -0.55470400 | -3.26345500 | 1.38923700  |
| H | 0.18066100  | -2.45955900 | 1.29253300  |
| H | 1.92665000  | -0.40313500 | 2.20225600  |
| H | -0.95135000 | 2.82050200  | -0.09573300 |
| H | -3.07700900 | 0.91768100  | -0.03721100 |
| C | 3.92122700  | -0.67290400 | 1.54505700  |
| C | 4.07784400  | -1.99683700 | 1.99398300  |
| C | 4.76980100  | -0.22888600 | 0.52357700  |
| C | 5.05768000  | -2.83563900 | 1.46549000  |
| H | 3.42400300  | -2.37916100 | 2.77399600  |
| C | 5.75937300  | -1.06468400 | -0.00550800 |
| H | 4.65686600  | 0.76846100  | 0.11720300  |
| C | 5.91422200  | -2.36760700 | 0.46477100  |
| H | 5.15363800  | -3.85235200 | 1.83616200  |
| H | 6.40650900  | -0.68950800 | -0.79349500 |
| H | 6.68371800  | -3.01416200 | 0.05334700  |
| C | 3.21352700  | 0.39190200  | 3.72610100  |
| H | 4.15201900  | 0.94499200  | 3.82562900  |
| H | 2.43343900  | 0.95731300  | 4.24546100  |
| H | 3.33659500  | -0.56805200 | 4.23478300  |
| C | -1.28191700 | 4.06527700  | 1.59614500  |
| C | -0.72963700 | 4.73828800  | 2.69562500  |
| C | -2.66201600 | 3.80956000  | 1.60096600  |
| C | -1.53056800 | 5.13486100  | 3.76976700  |
| H | 0.33580000  | 4.94781000  | 2.71639600  |
| C | -3.46591500 | 4.20581800  | 2.67161600  |
| H | -3.11203700 | 3.30533100  | 0.74885100  |
| C | -2.90137700 | 4.86902900  | 3.76365200  |
| H | -1.08055400 | 5.65258300  | 4.61244900  |
| H | -4.53185100 | 3.99603500  | 2.65244400  |
| H | -3.52297600 | 5.17576700  | 4.59983000  |
| C | -0.49243600 | 4.82036900  | -0.66129500 |
| H | 0.10578900  | 4.57979000  | -1.54264000 |
| H | -1.52599200 | 4.98012700  | -0.98185700 |
| H | -0.13743100 | 5.76385300  | -0.23542200 |
| C | -4.28784700 | 0.69596500  | -1.77121300 |
| C | -5.40844300 | 1.51149800  | -1.98773800 |
| C | -3.50250600 | 0.34458400  | -2.88446700 |
| C | -5.73468800 | 1.96935000  | -3.26778600 |
| H | -6.04457300 | 1.80123800  | -1.15870800 |
| C | -3.82918700 | 0.80347900  | -4.16149100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.63862500 | -0.30572600 | -2.77524300 |
| C | -4.94500900 | 1.61939300  | -4.36194500 |
| H | -6.61019900 | 2.59854200  | -3.40348700 |
| H | -3.20601000 | 0.51573900  | -5.00396000 |
| H | -5.19653800 | 1.97335400  | -5.35769900 |
| C | -5.02498700 | 0.38635100  | 0.67791300  |
| H | -4.71423700 | -0.01198900 | 1.64729200  |
| H | -5.31042000 | 1.43164500  | 0.82654100  |
| H | -5.91247100 | -0.16998800 | 0.36015900  |
| C | -0.90178600 | -3.37017900 | 2.87870900  |
| C | -2.11463500 | -3.91355400 | 3.32585600  |
| C | 0.03911800  | -2.97017800 | 3.83953800  |
| C | -2.37864200 | -4.04949800 | 4.69076300  |
| H | -2.86158200 | -4.22751700 | 2.60290200  |
| C | -0.22078500 | -3.10394100 | 5.20482400  |
| H | 0.98839400  | -2.55285300 | 3.51250700  |
| C | -1.43424800 | -3.64434600 | 5.63612300  |
| H | -3.32615800 | -4.47117700 | 5.01456000  |
| H | 0.52315600  | -2.78481000 | 5.92945800  |
| H | -1.64182300 | -3.74732800 | 6.69719200  |
| C | 0.14909800  | -4.55578500 | 0.92288000  |
| H | 1.06310800  | -4.70012700 | 1.50608400  |
| H | -0.47510800 | -5.44108900 | 1.07698400  |
| H | 0.42667300  | -4.49911100 | -0.13389600 |
| C | 4.45742500  | 4.78895700  | 0.90785700  |
| C | -4.40540200 | -4.60871200 | -1.61912100 |
| H | -3.94053700 | -4.80892200 | -2.59210500 |
| H | -4.40823600 | -5.54979500 | -1.06096100 |
| H | -5.44159500 | -4.31356100 | -1.80496800 |
| H | 5.27840400  | 4.55253300  | 1.59063100  |
| H | 4.86752400  | 4.79460800  | -0.10947100 |
| H | 4.11339200  | 5.80521800  | 1.12282100  |
| C | 3.14994900  | 1.72465300  | -3.35455200 |
| C | 1.84640200  | -5.07225900 | -4.03795800 |
| H | 2.31205800  | -4.80668600 | -4.99597600 |
| H | 2.03389300  | -6.13307900 | -3.84934300 |
| H | 0.76614100  | -4.93039800 | -4.16948500 |
| F | -0.26416500 | 2.20320900  | -2.28327800 |
| F | 1.69731800  | 3.60959700  | -3.48234500 |
| F | 4.11630100  | 2.43867600  | -3.97183200 |
| H | 4.33437000  | -0.04096900 | -3.19961000 |
| F | -0.75326800 | -1.47012900 | -2.75300400 |

**IM10**

|   |             |            |            |
|---|-------------|------------|------------|
| C | -3.67594700 | 1.72510100 | 1.50500600 |
|---|-------------|------------|------------|

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.44781900 | 1.13967800  | 1.21341000  |
| C  | -1.64574800 | 0.43748400  | 2.11486900  |
| C  | -2.27663200 | 0.21438900  | 3.37297000  |
| C  | -3.55303700 | 0.72967700  | 3.66771300  |
| C  | -1.66861000 | -0.56075800 | 4.54011500  |
| H  | -1.51337200 | 0.13290500  | 5.37851700  |
| H  | -2.42446100 | -1.27294500 | 4.89200500  |
| C  | -0.37610700 | -1.33077700 | 4.31124000  |
| H  | -0.50895000 | -2.07587100 | 3.51322000  |
| H  | -0.15238200 | -1.91439600 | 5.21511000  |
| C  | 0.84070500  | -0.49859700 | 3.98789600  |
| C  | 0.79855900  | 0.84569600  | 3.77402800  |
| H  | -0.09562700 | 1.43658400  | 3.92219800  |
| H  | 1.72034800  | 1.39095200  | 3.59517200  |
| Ni | 0.26258600  | 0.03347000  | 1.73159200  |
| C  | 0.23687300  | 0.00095800  | -0.18989400 |
| C  | 0.66043800  | 0.73363300  | -2.36037400 |
| C  | 0.15542900  | -0.70162800 | -2.42122200 |
| H  | 1.53889500  | 0.90334700  | -2.97698400 |
| H  | -0.11241400 | 1.45811200  | -2.64392500 |
| H  | 0.94965000  | -1.42370000 | -2.63992700 |
| H  | -0.64582300 | -0.82610700 | -3.14405000 |
| N  | -0.32528600 | -0.90206100 | -1.02686400 |
| N  | 0.96584500  | 0.88489000  | -0.91757700 |
| C  | -1.07325800 | -2.07010200 | -0.61550200 |
| C  | -0.42641400 | -3.09140700 | 0.13246200  |
| C  | -2.43142200 | -2.22281000 | -0.99166800 |
| C  | -1.21025600 | -4.12474500 | 0.65610000  |
| C  | -3.15775300 | -3.28644300 | -0.44082200 |
| C  | -2.58447400 | -4.21862600 | 0.42071900  |
| H  | -0.73600600 | -4.89926000 | 1.24809400  |
| H  | -4.20842600 | -3.38259900 | -0.69161100 |
| C  | 1.92810100  | 1.87186600  | -0.46018000 |
| C  | 3.31611900  | 1.59095600  | -0.55826600 |
| C  | 1.50121800  | 3.14291500  | -0.00683800 |
| C  | 4.22926700  | 2.56310900  | -0.13602300 |
| C  | 2.46371700  | 4.06604400  | 0.42170300  |
| C  | 3.83171500  | 3.79762400  | 0.37579100  |
| H  | 5.28958700  | 2.33565200  | -0.20269500 |
| H  | 2.13529000  | 5.03360500  | 0.78721700  |
| C  | -3.09708300 | -1.38808600 | -2.10033200 |
| C  | 1.09748500  | -3.17569200 | 0.24898000  |
| C  | 3.89705800  | 0.31935700  | -1.18916200 |
| C  | 0.03645200  | 3.55628700  | -0.02590600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.54905900 | 2.64848900  | 0.06358300  |
| H | -2.57788300 | -0.42746100 | -2.15296800 |
| H | 1.49576300  | -2.18771100 | 0.49408200  |
| H | 3.12036900  | -0.44959900 | -1.15988500 |
| C | -4.57587500 | -1.06459500 | -1.86985000 |
| C | -5.61609800 | -1.94265400 | -2.21703000 |
| C | -4.92565300 | 0.17448700  | -1.31939500 |
| C | -6.95205100 | -1.60158300 | -1.99209200 |
| H | -5.39662200 | -2.90161900 | -2.67542500 |
| C | -6.25815100 | 0.51972700  | -1.08847700 |
| H | -4.14355200 | 0.88111300  | -1.07591900 |
| C | -7.28009200 | -0.37043700 | -1.42185800 |
| H | -7.73656100 | -2.30048600 | -2.26917600 |
| H | -6.48791200 | 1.48490200  | -0.64739600 |
| H | -8.31916200 | -0.10641200 | -1.24688000 |
| C | -2.90503200 | -2.12518100 | -3.45093600 |
| H | -1.85248000 | -2.33949400 | -3.65071800 |
| H | -3.30234800 | -1.52713400 | -4.27720100 |
| H | -3.42142400 | -3.08869700 | -3.44828000 |
| C | 1.74415700  | -3.62851400 | -1.06856300 |
| C | 1.07321900  | -4.40841600 | -2.02174200 |
| C | 3.08998100  | -3.30708900 | -1.30880700 |
| C | 1.72144100  | -4.83937900 | -3.18307400 |
| H | 0.03493100  | -4.68078700 | -1.86012400 |
| C | 3.74018700  | -3.73529100 | -2.46734700 |
| H | 3.63651400  | -2.71969600 | -0.57643100 |
| C | 3.05616500  | -4.50261700 | -3.41368200 |
| H | 1.17878400  | -5.44039700 | -3.90789500 |
| H | 4.78100400  | -3.46724500 | -2.62765800 |
| H | 3.55806300  | -4.83524400 | -4.31782000 |
| C | 1.58634400  | -4.11339200 | 1.37652400  |
| H | 1.12314100  | -3.86207300 | 2.33585800  |
| H | 2.66965400  | -4.01316300 | 1.48650500  |
| H | 1.37869300  | -5.16618300 | 1.16047200  |
| C | 5.10386000  | -0.23508700 | -0.41190300 |
| C | 4.92963500  | -0.67716000 | 0.91219900  |
| C | 6.38473800  | -0.34026400 | -0.97408200 |
| C | 5.99736200  | -1.20163400 | 1.64036200  |
| H | 3.94183600  | -0.60696200 | 1.35653400  |
| C | 7.45690900  | -0.86260800 | -0.24160100 |
| H | 6.56831600  | -0.01820600 | -1.99280000 |
| C | 7.26989100  | -1.29589900 | 1.06933000  |
| H | 5.83418300  | -1.53945900 | 2.66079400  |
| H | 8.43781600  | -0.92914700 | -0.70472000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 8.10109100  | -1.70326000 | 1.63817300  |
| C | 4.24936500  | 0.59233600  | -2.66852600 |
| H | 4.57658900  | -0.32361100 | -3.17032100 |
| H | 5.04677400  | 1.33688600  | -2.75306000 |
| H | 3.39535800  | 0.98788000  | -3.22019300 |
| C | -0.39315200 | 4.21756600  | -1.34375300 |
| C | 0.48852900  | 4.93112200  | -2.16721200 |
| C | -1.74524100 | 4.14915200  | -1.72267600 |
| C | 0.03532500  | 5.55941400  | -3.33080000 |
| H | 1.53916600  | 4.99463400  | -1.90244500 |
| C | -2.19942700 | 4.77643600  | -2.88334200 |
| H | -2.44591800 | 3.60088200  | -1.09986000 |
| C | -1.30968400 | 5.48566700  | -3.69443300 |
| H | 0.73857100  | 6.10585400  | -3.95367100 |
| H | -3.24922500 | 4.70820700  | -3.15571800 |
| H | -1.66126100 | 5.97252100  | -4.59969400 |
| C | -0.36833300 | 4.45393800  | 1.16631200  |
| H | -1.45437900 | 4.58447000  | 1.17577500  |
| H | 0.07615700  | 5.45187000  | 1.10641500  |
| H | -0.06998400 | 3.99851900  | 2.11621200  |
| C | -3.40972800 | -5.31227000 | 1.05482300  |
| C | 4.84517300  | 4.80242300  | 0.86937900  |
| H | 4.46377100  | 5.82512000  | 0.79561800  |
| H | 5.77775600  | 4.74199200  | 0.30031600  |
| H | 5.09623800  | 4.62272500  | 1.92217900  |
| H | -4.31350500 | -5.52017100 | 0.47502100  |
| H | -3.72844700 | -5.02690100 | 2.06511800  |
| H | -2.83948000 | -6.24194600 | 1.14704900  |
| C | -4.23915900 | 1.50253300  | 2.75070900  |
| C | 2.15578500  | -1.22871800 | 4.07134200  |
| H | 2.33640800  | -1.48424300 | 5.12448800  |
| H | 2.98224600  | -0.61952700 | 3.70938500  |
| H | 2.13937600  | -2.16408200 | 3.50785000  |
| F | -2.05812600 | 1.33414000  | -0.08671900 |
| F | -4.31405100 | 2.48939100  | 0.58825000  |
| F | -5.44197900 | 2.03796000  | 3.03968600  |
| F | 2.00845300  | -0.43212800 | 1.42164300  |
| H | -4.01448200 | 0.54463200  | 4.63358500  |

**TS6(R)**

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 3.46647200 | -1.14594600 | -2.61094100 |
| C | 2.24947600 | -0.61726800 | -2.19262200 |
| C | 1.03601100 | -1.28686200 | -2.27286700 |
| C | 1.07161900 | -2.58001700 | -2.85911000 |



|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.30272200  | -3.15025400 | -3.23621300 |
| C  | -0.14189400 | -3.42771900 | -3.27510900 |
| H  | -0.24983300 | -3.31393400 | -4.36328100 |
| H  | 0.13376300  | -4.47922200 | -3.13379900 |
| C  | -1.54372600 | -3.27322100 | -2.65816000 |
| H  | -1.53191100 | -3.49291400 | -1.58828500 |
| H  | -2.17446900 | -4.05099500 | -3.10844600 |
| C  | -2.25209900 | -1.94000000 | -2.83130200 |
| C  | -1.46061200 | -0.85123200 | -3.33148900 |
| H  | -0.71274900 | -1.10455300 | -4.07482000 |
| H  | -2.00975500 | 0.06347300  | -3.56688700 |
| Ni | -0.59476900 | -0.60712900 | -1.55897800 |
| C  | -0.19717900 | 0.13476000  | 0.27511800  |
| C  | -0.73399300 | 1.64840100  | 2.00553500  |
| C  | 0.10810400  | 0.52132700  | 2.57292700  |
| H  | -1.62369400 | 1.84009000  | 2.59925700  |
| H  | -0.17221800 | 2.58231900  | 1.89025000  |
| H  | -0.48976800 | -0.20191500 | 3.13761300  |
| H  | 0.91537800  | 0.87843700  | 3.20326100  |
| N  | 0.61001700  | -0.13317000 | 1.33314000  |
| N  | -1.07035700 | 1.10664600  | 0.66564200  |
| C  | 1.69294800  | -1.08468000 | 1.41283400  |
| C  | 1.44576200  | -2.47187700 | 1.24056400  |
| C  | 2.99117100  | -0.63372300 | 1.75827100  |
| C  | 2.52676200  | -3.35400000 | 1.31641900  |
| C  | 4.03002600  | -1.57167800 | 1.83285300  |
| C  | 3.83034500  | -2.92740000 | 1.59269000  |
| H  | 2.35569500  | -4.41446400 | 1.17059700  |
| H  | 5.02644900  | -1.21718100 | 2.08173500  |
| C  | -2.00820900 | 1.79487800  | -0.19236600 |
| C  | -3.39284700 | 1.75559300  | 0.10158500  |
| C  | -1.53525100 | 2.57328900  | -1.28259900 |
| C  | -4.28123200 | 2.41006100  | -0.76093300 |
| C  | -2.47401100 | 3.19037700  | -2.11575200 |
| C  | -3.85125700 | 3.10807600  | -1.88733100 |
| H  | -5.34398500 | 2.36179400  | -0.53945300 |
| H  | -2.12453700 | 3.77160600  | -2.96230400 |
| C  | 3.32018000  | 0.80099300  | 2.19495700  |
| C  | 0.02930400  | -3.01010100 | 1.03335400  |
| C  | -3.97637000 | 1.14506400  | 1.38262400  |
| C  | -0.04354100 | 2.82161900  | -1.50642000 |
| H  | 0.48242800  | 1.89155000  | -1.29876100 |
| H  | 2.50297300  | 1.45229000  | 1.86602400  |
| H  | -0.43112200 | -2.41781000 | 0.23879900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.23384600 | 0.45268300  | 1.79404100  |
| C | 4.59788300  | 1.37302400  | 1.56116500  |
| C | 5.52017500  | 2.13781300  | 2.29214000  |
| C | 4.84855900  | 1.18239800  | 0.19424600  |
| C | 6.64897700  | 2.68964500  | 1.67735400  |
| H | 5.37371700  | 2.31328200  | 3.35174900  |
| C | 5.97378500  | 1.72816000  | -0.42236200 |
| H | 4.15780200  | 0.59647700  | -0.39401600 |
| C | 6.88295400  | 2.48745100  | 0.31755600  |
| H | 7.34642300  | 3.27525100  | 2.27023500  |
| H | 6.13463700  | 1.55217100  | -1.48180500 |
| H | 7.76181600  | 2.91292900  | -0.15847700 |
| C | 3.38287900  | 0.83992600  | 3.74254300  |
| H | 2.54033200  | 0.30826100  | 4.18995200  |
| H | 3.37231200  | 1.86613200  | 4.12182800  |
| H | 4.29354000  | 0.35089500  | 4.10177400  |
| C | -0.85467100 | -2.84424300 | 2.27117700  |
| C | -0.39037000 | -3.14097300 | 3.56028300  |
| C | -2.19069900 | -2.44761300 | 2.11195500  |
| C | -1.23964700 | -3.03946200 | 4.66488700  |
| H | 0.64272500  | -3.44715100 | 3.70176200  |
| C | -3.04166300 | -2.34651700 | 3.21569000  |
| H | -2.54992800 | -2.20715700 | 1.11475100  |
| C | -2.56827400 | -2.64116800 | 4.49681700  |
| H | -0.86256500 | -3.27163000 | 5.65733400  |
| H | -4.07201000 | -2.03349800 | 3.07067200  |
| H | -3.22782300 | -2.56101600 | 5.35637300  |
| C | -0.02193600 | -4.48203300 | 0.57454600  |
| H | 0.56850300  | -4.63922600 | -0.33347300 |
| H | -1.05867900 | -4.76081200 | 0.36442500  |
| H | 0.34214200  | -5.16511600 | 1.34838400  |
| C | -5.24855500 | 0.31965200  | 1.13831400  |
| C | -5.19963600 | -0.76566100 | 0.24687900  |
| C | -6.46178700 | 0.58081700  | 1.79081800  |
| C | -6.32388800 | -1.55881300 | 0.01947300  |
| H | -4.27116300 | -0.97926900 | -0.27297500 |
| C | -7.59071500 | -0.21370300 | 1.56126200  |
| H | -6.54590000 | 1.40644700  | 2.48813300  |
| C | -7.52824100 | -1.28740000 | 0.67530200  |
| H | -6.26010700 | -2.39348000 | -0.67395500 |
| H | -8.51814400 | 0.01336700  | 2.08010600  |
| H | -8.40397000 | -1.90514200 | 0.49715400  |
| C | -4.20440000 | 2.27739200  | 2.41044400  |
| H | -4.48555900 | 1.87670900  | 3.38943900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.99650500 | 2.95430500  | 2.07574700  |
| H | -3.30674100 | 2.88567000  | 2.53869400  |
| C | 0.52133200  | 3.87695700  | -0.54879600 |
| C | -0.20744100 | 5.01122400  | -0.16323000 |
| C | 1.83628300  | 3.74015600  | -0.07654500 |
| C | 0.35923100  | 5.97663000  | 0.67298600  |
| H | -1.22785100 | 5.13870500  | -0.51291000 |
| C | 2.40504000  | 4.70236200  | 0.76082700  |
| H | 2.42151800  | 2.87395100  | -0.37185700 |
| C | 1.66633400  | 5.82552200  | 1.14063600  |
| H | -0.22435500 | 6.84711100  | 0.96069400  |
| H | 3.42286700  | 4.56851300  | 1.11664300  |
| H | 2.10445300  | 6.57489400  | 1.79379000  |
| C | 0.32409300  | 3.19039100  | -2.95963700 |
| H | 1.41263700  | 3.20168300  | -3.06234300 |
| H | -0.04146900 | 4.18243200  | -3.24231800 |
| H | -0.07699300 | 2.45603600  | -3.66568100 |
| C | 4.97666800  | -3.90945500 | 1.62800300  |
| C | -4.83537600 | 3.75977700  | -2.82930800 |
| H | -4.43351100 | 4.68712600  | -3.24905800 |
| H | -5.77811700 | 3.99140100  | -2.32547800 |
| H | -5.06962000 | 3.09804800  | -3.67244500 |
| H | 5.81382400  | -3.52604600 | 2.21813900  |
| H | 5.35290500  | -4.10934700 | 0.61707000  |
| H | 4.66849300  | -4.86978400 | 2.05338300  |
| C | 3.48427400  | -2.43909700 | -3.11430000 |
| C | -3.73593400 | -2.00699100 | -3.06529000 |
| H | -3.89083300 | -2.35673900 | -4.09501800 |
| H | -4.19851200 | -1.02416300 | -2.96406900 |
| H | -4.22428000 | -2.71298200 | -2.38827200 |
| F | 2.30501900  | 0.64726700  | -1.68163300 |
| F | 4.60952300  | -0.43133400 | -2.52630300 |
| F | 4.66163000  | -2.97533800 | -3.50134800 |
| F | -2.43849300 | -1.37019800 | -1.08479600 |
| H | 2.34845700  | -4.14655000 | -3.66715400 |

**IM11(R)**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.64836100 | -3.30276200 | -2.64591600 |
| C | -0.80346400 | -2.35136400 | -2.07820700 |
| C | -0.95845300 | -0.98328200 | -2.26050200 |
| C | -2.01913200 | -0.56901100 | -3.09810000 |
| C | -2.88869600 | -1.51297900 | -3.66700200 |
| C | -2.23238400 | 0.89481800  | -3.42242800 |
| H | -2.24454100 | 1.48293700  | -2.50170200 |
| H | -3.22049000 | 1.01355000  | -3.88125000 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.19457000 | 1.51280700  | -4.38114200 |
| H  | -1.05336600 | 0.85783900  | -5.24972200 |
| H  | -1.60017800 | 2.45791200  | -4.76355900 |
| C  | 0.18422400  | 1.81606900  | -3.78055300 |
| C  | 0.89379600  | 0.61360400  | -3.19034600 |
| H  | 0.96947900  | -0.18622400 | -3.93273300 |
| H  | 1.92270200  | 0.89885800  | -2.89390400 |
| Ni | 0.29021700  | 0.15210300  | -1.43720300 |
| C  | 0.25456600  | -0.00358700 | 0.57661400  |
| C  | -0.06578700 | -0.03338600 | 2.91954800  |
| C  | 1.43121400  | 0.10531800  | 2.63470800  |
| H  | -0.48955000 | 0.88979300  | 3.32799900  |
| H  | -0.29921700 | -0.85652300 | 3.59334500  |
| H  | 1.88748400  | 0.96183900  | 3.13337800  |
| H  | 1.98082600  | -0.80154000 | 2.90636200  |
| N  | 1.44182200  | 0.28339400  | 1.16181400  |
| N  | -0.62568100 | -0.28360800 | 1.56166900  |
| C  | 2.60755700  | 0.72621600  | 0.44202900  |
| C  | 2.76344600  | 2.11185600  | 0.17624500  |
| C  | 3.60162400  | -0.19803000 | 0.05210400  |
| C  | 3.91000300  | 2.52920600  | -0.50574300 |
| C  | 4.73459200  | 0.28153400  | -0.61638500 |
| C  | 4.90675400  | 1.63349800  | -0.91042700 |
| H  | 4.04011700  | 3.58323300  | -0.72754000 |
| H  | 5.49509700  | -0.43050000 | -0.92470200 |
| C  | -2.02130000 | -0.59277000 | 1.38262400  |
| C  | -2.97423800 | 0.44613100  | 1.34941700  |
| C  | -2.42345100 | -1.94967600 | 1.30295300  |
| C  | -4.31800600 | 0.11298200  | 1.13532100  |
| C  | -3.77848600 | -2.22240000 | 1.09923400  |
| C  | -4.73811400 | -1.20770100 | 0.99031800  |
| H  | -5.05266000 | 0.91150300  | 1.08114800  |
| H  | -4.10596600 | -3.25296700 | 1.01691000  |
| C  | 3.52353600  | -1.69103100 | 0.38191100  |
| C  | 1.73318300  | 3.13652800  | 0.65161600  |
| C  | -2.61293500 | 1.90374000  | 1.66300700  |
| C  | -1.41238900 | -3.08703900 | 1.47098700  |
| H  | -0.52573300 | -2.81775600 | 0.89323600  |
| H  | 2.47702000  | -1.92270300 | 0.60911300  |
| H  | 0.75436300  | 2.65084300  | 0.61317400  |
| H  | -1.52408300 | 1.98571700  | 1.62203600  |
| C  | 3.91910100  | -2.56379700 | -0.81605400 |
| C  | 4.94130900  | -3.51959700 | -0.75603600 |
| C  | 3.22415900  | -2.41666100 | -2.02842300 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 5. 26028500  | -4. 30458800 | -1. 86999600 |
| H | 5. 50164500  | -3. 66678300 | 0. 16058000  |
| C | 3. 53826000  | -3. 19731800 | -3. 13883700 |
| H | 2. 42751900  | -1. 68275600 | -2. 09760100 |
| C | 4. 56166600  | -4. 14749900 | -3. 06533200 |
| H | 6. 05807500  | -5. 03862100 | -1. 79613300 |
| H | 2. 98192200  | -3. 06562600 | -4. 06297100 |
| H | 4. 80797600  | -4. 75704000 | -3. 93006200 |
| C | 4. 35304800  | -1. 98371900 | 1. 64989600  |
| H | 5. 41786600  | -1. 79557100 | 1. 47939000  |
| H | 4. 03842200  | -1. 34027500 | 2. 47484300  |
| H | 4. 23472600  | -3. 02383800 | 1. 96922400  |
| C | 1. 94470200  | 3. 57369200  | 2. 10655500  |
| C | 3. 20933200  | 3. 61984000  | 2. 70924400  |
| C | 0. 83681400  | 3. 99874500  | 2. 85741100  |
| C | 3. 36083500  | 4. 07219700  | 4. 02316600  |
| H | 4. 08269400  | 3. 29554200  | 2. 15183000  |
| C | 0. 98435100  | 4. 45082300  | 4. 16939200  |
| H | -0. 15118900 | 3. 98486800  | 2. 40303100  |
| C | 2. 25029900  | 4. 48766300  | 4. 75933300  |
| H | 4. 35071300  | 4. 09747900  | 4. 47053200  |
| H | 0. 11105900  | 4. 77192300  | 4. 73035500  |
| H | 2. 36879400  | 4. 83584100  | 5. 78128900  |
| C | 1. 62954400  | 4. 37795900  | -0. 26203400 |
| H | 1. 43546100  | 4. 07959500  | -1. 29525400 |
| H | 0. 79870900  | 5. 00581400  | 0. 07270100  |
| H | 2. 53381900  | 4. 99261400  | -0. 22542500 |
| C | -3. 14781500 | 2. 91447900  | 0. 64749200  |
| C | -2. 37022100 | 3. 22673300  | -0. 47699900 |
| C | -4. 37760400 | 3. 57242800  | 0. 79931700  |
| C | -2. 80258900 | 4. 15625800  | -1. 42378700 |
| H | -1. 41457000 | 2. 73399800  | -0. 62697500 |
| C | -4. 81695800 | 4. 50195200  | -0. 14772900 |
| H | -5. 00093600 | 3. 37576100  | 1. 66596800  |
| C | -4. 03187400 | 4. 79898900  | -1. 26289700 |
| H | -2. 17052300 | 4. 36482500  | -2. 28140400 |
| H | -5. 77312500 | 4. 99851800  | -0. 00673800 |
| H | -4. 37257300 | 5. 52547700  | -1. 99513000 |
| C | -3. 04643200 | 2. 23538600  | 3. 10942700  |
| H | -2. 56933800 | 1. 55747200  | 3. 82259100  |
| H | -2. 77265200 | 3. 26228700  | 3. 37214700  |
| H | -4. 12675700 | 2. 12607400  | 3. 24056300  |
| C | -0. 96445700 | -3. 27768900 | 2. 92284900  |
| C | -1. 86273100 | -3. 19307500 | 3. 99647500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.36934500  | -3.61478300 | 3.19832400  |
| C | -1.43785400 | -3.42768000 | 5.30640600  |
| H | -2.89983100 | -2.93114000 | 3.80699800  |
| C | 0.79801900  | -3.85040000 | 4.50643300  |
| H | 1.07777300  | -3.69566500 | 2.37700400  |
| C | -0.10533700 | -3.75508400 | 5.56750200  |
| H | -2.14972900 | -3.35287500 | 6.12394800  |
| H | 1.83692600  | -4.10622500 | 4.69589800  |
| H | 0.22530700  | -3.93437600 | 6.58647500  |
| C | -1.89430800 | -4.44945100 | 0.92750800  |
| H | -1.07733900 | -5.17321300 | 0.99924600  |
| H | -2.73007000 | -4.84710300 | 1.51165500  |
| H | -2.19473700 | -4.38837100 | -0.12009200 |
| C | 6.12241000  | 2.11993800  | -1.66304700 |
| C | -6.18566500 | -1.54255200 | 0.71885900  |
| H | -6.84954500 | -0.73090400 | 1.02953200  |
| H | -6.35417100 | -1.71339300 | -0.35149800 |
| H | -6.49016400 | -2.45416000 | 1.24247100  |
| H | 6.95215900  | 1.41255700  | -1.58120200 |
| H | 5.89944300  | 2.24250800  | -2.72999200 |
| H | 6.46092800  | 3.09164200  | -1.29034100 |
| C | -2.70147400 | -2.86912000 | -3.43880500 |
| F | -1.46295300 | -4.62096700 | -2.41407500 |
| F | -3.53109800 | -3.78703700 | -3.98347100 |
| F | 0.21106400  | -2.83831800 | -1.30496900 |
| C | 1.04707400  | 2.60092700  | -4.76959800 |
| F | -0.05088600 | 2.74094700  | -2.68570600 |
| H | 1.98993100  | 2.89451300  | -4.29882900 |
| H | 1.27937100  | 1.98449700  | -5.64353500 |
| H | 0.52974600  | 3.50401500  | -5.11169600 |
| H | -3.71501100 | -1.20322600 | -4.29999100 |

**TS7(R)**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.76544100 | -2.74908900 | -2.25128100 |
| C | -1.48477900 | -2.23259200 | -2.14806200 |
| C | -1.17475900 | -0.88877600 | -2.40688800 |
| C | -2.21474300 | -0.10155000 | -2.96967000 |
| C | -3.51215100 | -0.61639900 | -3.09100300 |
| C | -1.87246900 | 1.25801400  | -3.53388100 |
| H | -1.47277500 | 1.91861100  | -2.75598400 |
| H | -2.77231700 | 1.73336900  | -3.93608000 |
| C | -0.81443500 | 1.13903300  | -4.64321900 |
| H | -1.15318500 | 0.42823200  | -5.40656100 |
| H | -0.67669100 | 2.10706400  | -5.13911400 |
| C | 0.55296400  | 0.68802400  | -4.11960800 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.52196900  | -0.57909000 | -3.27007600 |
| H  | 0.39749600  | -1.45935300 | -3.90143700 |
| H  | 1.51135900  | -0.70560900 | -2.77843500 |
| Ni | 0.20195600  | -0.23008300 | -1.32169900 |
| C  | 0.37217100  | 0.13214900  | 0.55944900  |
| C  | 0.10058400  | 0.30802000  | 2.91481500  |
| C  | 1.50112500  | 0.81229500  | 2.54232900  |
| H  | -0.52635000 | 1.11303600  | 3.30761300  |
| H  | 0.11972900  | -0.50451000 | 3.64251900  |
| H  | 1.68905400  | 1.83511000  | 2.87537900  |
| H  | 2.28806400  | 0.16465600  | 2.94203700  |
| N  | 1.47735200  | 0.74218900  | 1.06277400  |
| N  | -0.43087800 | -0.17161500 | 1.61260900  |
| C  | 2.57072000  | 1.23173600  | 0.26787800  |
| C  | 2.48151200  | 2.51926000  | -0.31977300 |
| C  | 3.73399400  | 0.45103800  | 0.11499200  |
| C  | 3.56501300  | 2.97877200  | -1.07082400 |
| C  | 4.79020500  | 0.96186300  | -0.65122800 |
| C  | 4.72661100  | 2.21679300  | -1.25288200 |
| H  | 3.51045100  | 3.95650100  | -1.53803000 |
| H  | 5.68074900  | 0.35376100  | -0.78697400 |
| C  | -1.71558600 | -0.81456300 | 1.51128700  |
| C  | -2.89447100 | -0.04019100 | 1.53437000  |
| C  | -1.78841300 | -2.22791100 | 1.41747000  |
| C  | -4.12666200 | -0.68158700 | 1.35338700  |
| C  | -3.04483300 | -2.81455500 | 1.24606900  |
| C  | -4.22193600 | -2.05979900 | 1.17559700  |
| H  | -5.03088500 | -0.07917900 | 1.33151000  |
| H  | -3.11779600 | -3.89051100 | 1.13763200  |
| C  | 3.90401000  | -0.91254400 | 0.79239100  |
| C  | 1.23731300  | 3.38550200  | -0.12951100 |
| C  | -2.88755600 | 1.46175900  | 1.84072200  |
| C  | -0.53219300 | -3.09728000 | 1.50827000  |
| H  | 0.21235900  | -2.64921300 | 0.84363400  |
| H  | 2.93632700  | -1.18413400 | 1.22091600  |
| H  | 0.37784800  | 2.70927600  | -0.16336000 |
| H  | -1.86030500 | 1.81541400  | 1.72141300  |
| C  | 4.25065200  | -2.01705700 | -0.20933500 |
| C  | 5.55424300  | -2.49724400 | -0.39454600 |
| C  | 3.22239600  | -2.58313100 | -0.98099200 |
| C  | 5.82391700  | -3.50388100 | -1.32706000 |
| H  | 6.37280600  | -2.09578400 | 0.19420500  |
| C  | 3.48705200  | -3.59008700 | -1.90945800 |
| H  | 2.20289300  | -2.22461700 | -0.85698000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 4.79297100  | -4.05467300 | -2.08827500 |
| H | 6.84303700  | -3.85972200 | -1.45149300 |
| H | 2.67093500  | -4.01569700 | -2.48709200 |
| H | 5.00222900  | -4.84066600 | -2.80819700 |
| C | 4.90938700  | -0.80604000 | 1.95760700  |
| H | 5.89603900  | -0.48006900 | 1.61540600  |
| H | 4.56691000  | -0.07128400 | 2.69188400  |
| H | 5.02444800  | -1.76989100 | 2.46377200  |
| C | 1.19717800  | 4.09178000  | 1.22919800  |
| C | 2.35753500  | 4.53174700  | 1.88161200  |
| C | -0.04350500 | 4.37125300  | 1.82384900  |
| C | 2.28107100  | 5.22154700  | 3.09476700  |
| H | 3.32908400  | 4.32824600  | 1.44116500  |
| C | -0.12386900 | 5.05963100  | 3.03556600  |
| H | -0.95684900 | 4.05515400  | 1.32535500  |
| C | 1.04081900  | 5.48628200  | 3.67844600  |
| H | 3.19400400  | 5.55079800  | 3.58359800  |
| H | -1.09599100 | 5.26177700  | 3.47700600  |
| H | 0.98167400  | 6.01967500  | 4.62281800  |
| C | 1.01906700  | 4.41912600  | -1.25615400 |
| H | 1.02247300  | 3.93121600  | -2.23405200 |
| H | 0.05079400  | 4.90884400  | -1.11592400 |
| H | 1.78135300  | 5.20435000  | -1.24610200 |
| C | -3.73267500 | 2.28556300  | 0.86788700  |
| C | -3.19286700 | 2.62367400  | -0.38284200 |
| C | -5.02241200 | 2.74262600  | 1.17354000  |
| C | -3.91250000 | 3.39414200  | -1.29611800 |
| H | -2.19807600 | 2.26897400  | -0.63948500 |
| C | -5.75088600 | 3.50739600  | 0.25747300  |
| H | -5.46873300 | 2.51323500  | 2.13538500  |
| C | -5.19871100 | 3.83910100  | -0.97946600 |
| H | -3.46743000 | 3.65024300  | -2.25311600 |
| H | -6.74881000 | 3.84898200  | 0.51827400  |
| H | -5.76086500 | 4.44045800  | -1.68810400 |
| C | -3.28959300 | 1.68459900  | 3.31558900  |
| H | -2.60818200 | 1.15500900  | 3.98659200  |
| H | -3.26724100 | 2.74884300  | 3.57138900  |
| H | -4.29455200 | 1.30327600  | 3.51869900  |
| C | 0.07154200  | -3.12718900 | 2.91423000  |
| C | -0.72902100 | -3.15615200 | 4.06543900  |
| C | 1.46323100  | -3.20497000 | 3.07246900  |
| C | -0.15518300 | -3.24488800 | 5.33609900  |
| H | -1.80940100 | -3.10129500 | 3.96625600  |
| C | 2.04104700  | -3.29311400 | 4.34088600  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.09907500  | -3.20733100 | 2.19028600  |
| C | 1.23261500  | -3.30979600 | 5.47981000  |
| H | -0.79452700 | -3.26274400 | 6.21460700  |
| H | 3.12184500  | -3.34890800 | 4.43839200  |
| H | 1.67886500  | -3.37540300 | 6.46794000  |
| C | -0.73814500 | -4.55211900 | 1.03237700  |
| H | 0.22786600  | -5.06512700 | 1.01426600  |
| H | -1.38910600 | -5.10988000 | 1.71329200  |
| H | -1.16447800 | -4.58471000 | 0.02832800  |
| C | 5.86616500  | 2.74163200  | -2.09451000 |
| C | -5.54314000 | -2.72343700 | 0.86883700  |
| H | -6.38776400 | -2.11624600 | 1.20693000  |
| H | -5.65021400 | -2.86776800 | -0.21325000 |
| H | -5.61761300 | -3.70935700 | 1.33826000  |
| H | 6.77704700  | 2.15581500  | -1.94409700 |
| H | 5.61896700  | 2.70128200  | -3.16225400 |
| H | 6.08952900  | 3.78691100  | -1.85650100 |
| C | -3.78823000 | -1.92145600 | -2.70776000 |
| F | -3.02752200 | -4.02014100 | -1.88058400 |
| F | -5.04585000 | -2.42086800 | -2.77217600 |
| F | -0.49812500 | -3.07706400 | -1.73718100 |
| C | 1.58254700  | 0.58650200  | -5.24422000 |
| F | 1.01052100  | 1.74059900  | -3.26502400 |
| H | 2.56846600  | 0.34290400  | -4.83786800 |
| H | 1.29893300  | -0.19444300 | -5.95587400 |
| H | 1.65112300  | 1.53689800  | -5.78308400 |
| H | -4.31776500 | -0.00709000 | -3.48913500 |

**5(R)<sup>C-F</sup><sub>endo</sub>**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.35234800  | 0.52808100  | 0.00612600  |
| C | 1.09078800  | 1.10590400  | -0.06068500 |
| C | -0.07969000 | 0.34714800  | -0.10661500 |
| C | 0.03722100  | -1.05349600 | -0.09051300 |
| C | 1.30542500  | -1.64791700 | -0.02660500 |
| C | -1.20412000 | -1.92216600 | -0.10282400 |
| H | -1.42234800 | -2.23711500 | 0.92497900  |
| H | -1.01213300 | -2.83563600 | -0.67510000 |
| C | -2.43320600 | -1.19497900 | -0.65971600 |
| H | -2.32351200 | -1.02597000 | -1.73776600 |
| H | -3.32935900 | -1.80746000 | -0.51539700 |
| C | -2.62193500 | 0.15788500  | 0.02745100  |
| C | -1.41103900 | 1.06435400  | -0.20318300 |
| H | -1.50128100 | 1.52921300  | -1.19338900 |
| H | -1.45136000 | 1.88445600  | 0.52142600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.44503600  | -0.86126000 | 0.02203600  |
| F | 3.45541400  | 1.29253400  | 0.04810200  |
| F | 3.66709300  | -1.42199000 | 0.08044200  |
| F | 1.01149100  | 2.45268400  | -0.08392700 |
| F | -2.67804600 | -0.10281800 | 1.42292300  |
| C | -3.93048600 | 0.84277100  | -0.34215400 |
| H | -4.02196200 | 1.80171500  | 0.17669600  |
| H | -3.98474000 | 1.02545100  | -1.41938600 |
| H | -4.77576100 | 0.21101700  | -0.05493700 |
| H | 1.41683100  | -2.72731300 | -0.01489400 |

**TS6(S)**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.46635300 | -1.14621200 | -2.61066800 |
| C  | -2.24932500 | -0.61746900 | -2.19252500 |
| C  | -1.03586000 | -1.28705300 | -2.27277300 |
| C  | -1.07148300 | -2.58026900 | -2.85887600 |
| C  | -2.30260800 | -3.15057000 | -3.23581100 |
| C  | 0.14202600  | -3.42796900 | -3.27488600 |
| H  | 0.24995400  | -3.31418600 | -4.36306000 |
| H  | -0.13362200 | -4.47947200 | -3.13356900 |
| C  | 1.54386100  | -3.27345100 | -2.65794900 |
| H  | 1.53205100  | -3.49310800 | -1.58806600 |
| H  | 2.17460300  | -4.05124100 | -3.10821200 |
| C  | 2.25223700  | -1.94023700 | -2.83113600 |
| C  | 1.46077300  | -0.85149000 | -3.33140900 |
| H  | 0.71290800  | -1.10485100 | -4.07472500 |
| H  | 2.00993300  | 0.06318900  | -3.56687000 |
| Ni | 0.59489500  | -0.60722900 | -1.55892900 |
| C  | 0.19722200  | 0.13476500  | 0.27510400  |
| C  | 0.73398500  | 1.64848700  | 2.00546300  |
| C  | -0.10821500 | 0.52149400  | 2.57286300  |
| H  | 1.62365200  | 1.84016600  | 2.59924000  |
| H  | 0.17226700  | 2.58242800  | 1.89007700  |
| H  | 0.48957600  | -0.20173900 | 3.13764500  |
| H  | -0.91551500 | 0.87869500  | 3.20311000  |
| N  | -0.61006700 | -0.13306200 | 1.33308300  |
| N  | 1.07042300  | 1.10662800  | 0.66563200  |
| C  | -1.69306000 | -1.08451100 | 1.41270300  |
| C  | -1.44593500 | -2.47171900 | 1.24041200  |
| C  | -2.99130000 | -0.63349600 | 1.75800700  |
| C  | -2.52700500 | -3.35377400 | 1.31603800  |
| C  | -4.03022900 | -1.57138800 | 1.83235500  |
| C  | -3.83060600 | -2.92710300 | 1.59211700  |
| H  | -2.35598400 | -4.41424100 | 1.17018500  |
| H  | -5.02666300 | -1.21684000 | 2.08111700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.00831500  | 1.79480200  | -0.19237700 |
| C | 3.39294200  | 1.75549900  | 0.10162200  |
| C | 1.53540900  | 2.57318200  | -1.28265400 |
| C | 4.28137000  | 2.40991100  | -0.76089300 |
| C | 2.47421000  | 3.19021600  | -2.11580100 |
| C | 3.85144700  | 3.10789500  | -1.88733100 |
| H | 5.34411400  | 2.36163100  | -0.53937700 |
| H | 2.12477400  | 3.77142300  | -2.96238400 |
| C | -3.32028900 | 0.80120100  | 2.19479700  |
| C | -0.02947800 | -3.01002900 | 1.03340200  |
| C | 3.97640100  | 1.14501400  | 1.38271200  |
| C | 0.04371300  | 2.82154700  | -1.50653500 |
| H | -0.48230600 | 1.89154300  | -1.29871800 |
| H | -2.50308900 | 1.45252000  | 1.86588500  |
| H | 0.43106100  | -2.41783100 | 0.23884200  |
| H | 3.23384200  | 0.45267300  | 1.79413500  |
| C | -4.59801400 | 1.37325500  | 1.56106800  |
| C | -5.52068300 | 2.13739000  | 2.29224400  |
| C | -4.84834900 | 1.18326000  | 0.19399400  |
| C | -6.64952700 | 2.68919600  | 1.67750800  |
| H | -5.37449200 | 2.31237200  | 3.35196900  |
| C | -5.97362000 | 1.72898400  | -0.42256000 |
| H | -4.15728500 | 0.59786300  | -0.39443400 |
| C | -6.88317400 | 2.48761800  | 0.31756300  |
| H | -7.34726600 | 3.27429500  | 2.27054500  |
| H | -6.13421900 | 1.55347000  | -1.48212200 |
| H | -7.76207300 | 2.91306600  | -0.15842800 |
| C | -3.38296000 | 0.84001800  | 3.74238200  |
| H | -2.54033100 | 0.30844600  | 4.18974300  |
| H | -3.37254900 | 1.86620400  | 4.12173100  |
| H | -4.29353500 | 0.35081800  | 4.10159700  |
| C | 0.85436900  | -2.84410300 | 2.27130700  |
| C | 0.38992100  | -3.14074700 | 3.56038000  |
| C | 2.19041900  | -2.44750200 | 2.11220700  |
| C | 1.23907700  | -3.03917600 | 4.66507200  |
| H | -0.64319300 | -3.44690500 | 3.70176300  |
| C | 3.04126100  | -2.34634500 | 3.21603200  |
| H | 2.54976400  | -2.20711300 | 1.11502900  |
| C | 2.56772800  | -2.64090900 | 4.49712400  |
| H | 0.86188200  | -3.27127900 | 5.65749100  |
| H | 4.07162900  | -2.03334800 | 3.07110800  |
| H | 3.22718200  | -2.56071000 | 5.35674900  |
| C | 0.02175000  | -4.48200500 | 0.57473200  |
| H | -0.56855600 | -4.63924700 | -0.33336500 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 1. 05850900  | -4. 76085900 | 0. 36479400  |
| H | -0. 34248800 | -5. 16499600 | 1. 34857600  |
| C | 5. 24857700  | 0. 31956300  | 1. 13849000  |
| C | 5. 19966700  | -0. 76579800 | 0. 24711200  |
| C | 6. 46179300  | 0. 58074200  | 1. 79101800  |
| C | 6. 32391300  | -1. 55898100 | 0. 01978400  |
| H | 4. 27120700  | -0. 97942000 | -0. 27275900 |
| C | 7. 59071500  | -0. 21381000 | 1. 56154100  |
| H | 6. 54589800  | 1. 40640700  | 2. 48829200  |
| C | 7. 52825100  | -1. 28755300 | 0. 67563600  |
| H | 6. 26014000  | -2. 39368400 | -0. 67360200 |
| H | 8. 51813200  | 0. 01327200  | 2. 08040100  |
| H | 8. 40397400  | -1. 90531900 | 0. 49754700  |
| C | 4. 20441700  | 2. 27738500  | 2. 41048800  |
| H | 4. 48554100  | 1. 87674100  | 3. 38950900  |
| H | 4. 99654100  | 2. 95427300  | 2. 07578400  |
| H | 3. 30676200  | 2. 88568000  | 2. 53868400  |
| C | -0. 52112300 | 3. 87708200  | -0. 54910500 |
| C | 0. 20769600  | 5. 01137800  | -0. 16371100 |
| C | -1. 83609100 | 3. 74042700  | -0. 07686100 |
| C | -0. 35894800 | 5. 97695200  | 0. 67232900  |
| H | 1. 22812200  | 5. 13874700  | -0. 51338400 |
| C | -2. 40482200 | 4. 70280100  | 0. 76033500  |
| H | -2. 42136800 | 2. 87420700  | -0. 37204800 |
| C | -1. 66607000 | 5. 82598700  | 1. 13997500  |
| H | 0. 22467400  | 6. 84745200  | 0. 95990600  |
| H | -3. 42266500 | 4. 56906600  | 1. 11614800  |
| H | -2. 10416700 | 6. 57549000  | 1. 79299300  |
| C | -0. 32387800 | 3. 19007300  | -2. 95982600 |
| H | -1. 41241900 | 3. 20139400  | -3. 06255700 |
| H | 0. 04173200  | 4. 18204500  | -3. 24268400 |
| H | 0. 07719200  | 2. 45556900  | -3. 66572200 |
| C | -4. 97699300 | -3. 90909100 | 1. 62716800  |
| C | 4. 83560700  | 3. 75955900  | -2. 82929100 |
| H | 5. 77843400  | 3. 99093600  | -2. 32550800 |
| H | 5. 06965300  | 3. 09792300  | -3. 67255600 |
| H | 4. 43387100  | 4. 68704800  | -3. 24885900 |
| H | -4. 66903900 | -4. 86935300 | 2. 05286500  |
| H | -5. 81435900 | -3. 52551900 | 2. 21689700  |
| H | -5. 35283600 | -4. 10917300 | 0. 61612600  |
| C | -3. 48416600 | -2. 43942500 | -3. 11387300 |
| C | 3. 73608000  | -2. 00723500 | -3. 06508200 |
| H | 3. 89101000  | -2. 35702300 | -4. 09479200 |
| H | 4. 19865100  | -1. 02440100 | -2. 96388600 |

|               |             |             |             |
|---------------|-------------|-------------|-------------|
| H             | 4.22440900  | -2.71319600 | -2.38802200 |
| F             | -2.30483200 | 0.64713500  | -1.68168600 |
| F             | -4.60940400 | -0.43160800 | -2.52601800 |
| F             | -4.66154300 | -2.97573900 | -3.50075500 |
| F             | 2.43858500  | -1.37036700 | -1.08465800 |
| H             | -2.34836000 | -4.14691400 | -3.66663900 |
| <b>IM6(S)</b> |             |             |             |
| C             | -2.95430500 | -2.22753900 | -2.31279100 |
| C             | -1.69131400 | -1.75391900 | -1.97035800 |
| C             | -1.25750300 | -0.46476500 | -2.24368800 |
| C             | -2.11400500 | 0.34359000  | -3.02246700 |
| C             | -3.39574700 | -0.11130300 | -3.37162500 |
| C             | -1.64106400 | 1.67361700  | -3.56881200 |
| H             | -1.26786800 | 2.30579000  | -2.75725500 |
| H             | -2.49473600 | 2.20538200  | -4.00270400 |
| C             | -0.55246800 | 1.52613900  | -4.65455300 |
| H             | -0.81079600 | 0.69237000  | -5.31751800 |
| H             | -0.53801500 | 2.43036400  | -5.27551800 |
| C             | 0.87856500  | 1.30373100  | -4.14522900 |
| C             | 1.06700400  | 0.05290700  | -3.31268200 |
| H             | 0.80018700  | -0.82907800 | -3.90306200 |
| H             | 2.13291600  | -0.04119900 | -3.02771700 |
| Ni            | 0.39142100  | 0.04157800  | -1.51469900 |
| C             | 0.32203300  | 0.04834600  | 0.52175800  |
| C             | -0.01173900 | 0.09026300  | 2.86203000  |
| C             | 1.48932700  | 0.10569400  | 2.58661600  |
| H             | -0.36434200 | 1.06267400  | 3.22181100  |
| H             | -0.31353800 | -0.68158200 | 3.56836200  |
| H             | 2.01485900  | 0.90900400  | 3.10284900  |
| H             | 1.95953700  | -0.85131100 | 2.83897800  |
| N             | 1.51298300  | 0.30934800  | 1.11713000  |
| N             | -0.57489000 | -0.17698100 | 1.50924300  |
| C             | 2.72318100  | 0.59398900  | 0.39278800  |
| C             | 3.05163100  | 1.94652900  | 0.11119600  |
| C             | 3.58921500  | -0.45466800 | 0.01113500  |
| C             | 4.23056000  | 2.20656700  | -0.59127400 |
| C             | 4.75504300  | -0.13151300 | -0.69539100 |
| C             | 5.08999100  | 1.18361800  | -1.01259500 |
| H             | 4.49603100  | 3.23205200  | -0.82471800 |
| H             | 5.41435000  | -0.93507600 | -1.01061100 |
| C             | -1.96748000 | -0.50169700 | 1.33059100  |
| C             | -2.92256900 | 0.52929600  | 1.20173200  |
| C             | -2.36360700 | -1.86206100 | 1.32902400  |
| C             | -4.24563100 | 0.17600500  | 0.90952400  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -3. 70256200 | -2. 15395900 | 1. 05551800  |
| C | -4. 64692100 | -1. 15451600 | 0. 79449500  |
| H | -4. 97869500 | 0. 96160700  | 0. 75669700  |
| H | -4. 02080200 | -3. 18926400 | 1. 00855100  |
| C | 3. 34669700  | -1. 91513900 | 0. 41330900  |
| C | 2. 15684700  | 3. 09337000  | 0. 58678900  |
| C | -2. 57281400 | 1. 99010200  | 1. 51633200  |
| C | -1. 37022500 | -2. 98682800 | 1. 63300800  |
| H | -0. 43779700 | -2. 73574700 | 1. 12156200  |
| H | 2. 30400800  | -1. 99887100 | 0. 73221600  |
| H | 1. 12144100  | 2. 77659400  | 0. 42540600  |
| H | -1. 48542600 | 2. 08091400  | 1. 45784300  |
| C | 3. 52173500  | -2. 88762700 | -0. 75575100 |
| C | 4. 71960600  | -3. 57574900 | -0. 99671700 |
| C | 2. 44511300  | -3. 10882000 | -1. 62851800 |
| C | 4. 84274300  | -4. 44622400 | -2. 08365800 |
| H | 5. 56817100  | -3. 44654100 | -0. 33251700 |
| C | 2. 56427200  | -3. 97874000 | -2. 71289300 |
| H | 1. 49968700  | -2. 60352400 | -1. 45504300 |
| C | 3. 76685900  | -4. 64998300 | -2. 94787000 |
| H | 5. 78137100  | -4. 96813400 | -2. 24864100 |
| H | 1. 71399600  | -4. 13517600 | -3. 37098100 |
| H | 3. 86104700  | -5. 32868000 | -3. 79065800 |
| C | 4. 23345500  | -2. 27126600 | 1. 62751100  |
| H | 5. 29635100  | -2. 14650800 | 1. 40116300  |
| H | 4. 00981000  | -1. 62000600 | 2. 47685400  |
| H | 4. 06854900  | -3. 30847000 | 1. 93585400  |
| C | 2. 29939200  | 3. 38725300  | 2. 08360000  |
| C | 3. 53526100  | 3. 31542100  | 2. 74190800  |
| C | 1. 17930000  | 3. 80966300  | 2. 81541400  |
| C | 3. 64500100  | 3. 64504900  | 4. 09517900  |
| H | 4. 41643900  | 2. 99167300  | 2. 19551200  |
| C | 1. 28539700  | 4. 14002600  | 4. 16791100  |
| H | 0. 21531700  | 3. 88692900  | 2. 31758300  |
| C | 2. 52072400  | 4. 05584900  | 4. 81434900  |
| H | 4. 61139600  | 3. 57909000  | 4. 58733100  |
| H | 0. 40362200  | 4. 46090100  | 4. 71546700  |
| H | 2. 60624000  | 4. 30867000  | 5. 86712300  |
| C | 2. 35103800  | 4. 40975600  | -0. 19660000 |
| H | 2. 26026400  | 4. 25413500  | -1. 27484700 |
| H | 1. 58836000  | 5. 13032100  | 0. 11196300  |
| H | 3. 32551100  | 4. 86302900  | 0. 00865100  |
| C | -3. 13505000 | 3. 03167900  | 0. 54987500  |
| C | -2. 30352800 | 3. 56289300  | -0. 44625600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.44355400 | 3.53197600  | 0.64556500  |
| C | -2.75938000 | 4.54579100  | -1.32675300 |
| H | -1.28160700 | 3.20213400  | -0.52900600 |
| C | -4.90788100 | 4.50936700  | -0.23757500 |
| H | -5.11032500 | 3.17285100  | 1.42318200  |
| C | -4.06822800 | 5.02081000  | -1.22849500 |
| H | -2.09027900 | 4.94174200  | -2.08553400 |
| H | -5.92568500 | 4.87734100  | -0.14268700 |
| H | -4.42709400 | 5.78621900  | -1.91037000 |
| C | -2.98459600 | 2.29609700  | 2.97780900  |
| H | -2.50704200 | 1.59894100  | 3.67171700  |
| H | -2.69690300 | 3.31518600  | 3.25570100  |
| H | -4.06481500 | 2.19645000  | 3.11688000  |
| C | -1.04770000 | -3.11686400 | 3.12486400  |
| C | -2.02013500 | -2.93183600 | 4.11824700  |
| C | 0.24144500  | -3.50336000 | 3.52305600  |
| C | -1.71070400 | -3.11785000 | 5.46780400  |
| H | -3.02450400 | -2.63170100 | 3.83382100  |
| C | 0.55459600  | -3.69075100 | 4.87085300  |
| H | 1.00661100  | -3.66277000 | 2.76648300  |
| C | -0.42203600 | -3.49631300 | 5.85039200  |
| H | -2.47896200 | -2.96546800 | 6.22098800  |
| H | 1.56078100  | -3.98669200 | 5.15486400  |
| H | -0.18126100 | -3.63810100 | 6.89999700  |
| C | -1.80905800 | -4.37115200 | 1.10518400  |
| H | -0.98877300 | -5.08341400 | 1.23467200  |
| H | -2.66593400 | -4.76208800 | 1.66283400  |
| H | -2.06683100 | -4.32588800 | 0.04613200  |
| C | 6.33518000  | 1.50291400  | -1.80488300 |
| C | -6.04952700 | -1.51635700 | 0.36846900  |
| H | -6.75113000 | -0.69763900 | 0.55182500  |
| H | -6.07285100 | -1.73911800 | -0.70562400 |
| H | -6.41302700 | -2.40575200 | 0.89265400  |
| H | 7.07632200  | 0.70299900  | -1.72503200 |
| H | 6.09937300  | 1.62686800  | -2.86883400 |
| H | 6.79652100  | 2.43511700  | -1.46481600 |
| C | -3.81414200 | -1.38062400 | -2.99750700 |
| F | -3.34837300 | -3.47245800 | -1.96770300 |
| F | -5.06255600 | -1.81811800 | -3.28766500 |
| F | -0.87460200 | -2.63012400 | -1.31542400 |
| F | 1.65097700  | 1.14200400  | -5.35304300 |
| C | 1.45869000  | 2.55486500  | -3.48912200 |
| H | 2.49944900  | 2.38145000  | -3.20081000 |
| H | 1.42444900  | 3.40073400  | -4.18345400 |

|                |             |             |             |
|----------------|-------------|-------------|-------------|
| H              | 0.89933500  | 2.82259300  | -2.58859700 |
| H              | -4.07528100 | 0.51271400  | -3.94414500 |
| <b>IM11(S)</b> |             |             |             |
| C              | -2.95430500 | -2.22753900 | -2.31279100 |
| C              | -1.69131400 | -1.75391900 | -1.97035800 |
| C              | -1.25750300 | -0.46476500 | -2.24368800 |
| C              | -2.11400500 | 0.34359000  | -3.02246700 |
| C              | -3.39574700 | -0.11130300 | -3.37162500 |
| C              | -1.64106400 | 1.67361700  | -3.56881200 |
| H              | -1.26786800 | 2.30579000  | -2.75725500 |
| H              | -2.49473600 | 2.20538200  | -4.00270400 |
| C              | -0.55246800 | 1.52613900  | -4.65455300 |
| H              | -0.81079600 | 0.69237000  | -5.31751800 |
| H              | -0.53801500 | 2.43036400  | -5.27551800 |
| C              | 0.87856500  | 1.30373100  | -4.14522900 |
| C              | 1.06700400  | 0.05290700  | -3.31268200 |
| H              | 0.80018700  | -0.82907800 | -3.90306200 |
| H              | 2.13291600  | -0.04119900 | -3.02771700 |
| Ni             | 0.39142100  | 0.04157800  | -1.51469900 |
| C              | 0.32203300  | 0.04834600  | 0.52175800  |
| C              | -0.01173900 | 0.09026300  | 2.86203000  |
| C              | 1.48932700  | 0.10569400  | 2.58661600  |
| H              | -0.36434200 | 1.06267400  | 3.22181100  |
| H              | -0.31353800 | -0.68158200 | 3.56836200  |
| H              | 2.01485900  | 0.90900400  | 3.10284900  |
| H              | 1.95953700  | -0.85131100 | 2.83897800  |
| N              | 1.51298300  | 0.30934800  | 1.11713000  |
| N              | -0.57489000 | -0.17698100 | 1.50924300  |
| C              | 2.72318100  | 0.59398900  | 0.39278800  |
| C              | 3.05163100  | 1.94652900  | 0.11119600  |
| C              | 3.58921500  | -0.45466800 | 0.01113500  |
| C              | 4.23056000  | 2.20656700  | -0.59127400 |
| C              | 4.75504300  | -0.13151200 | -0.69539100 |
| C              | 5.08999100  | 1.18361900  | -1.01259500 |
| H              | 4.49603100  | 3.23205300  | -0.82471800 |
| H              | 5.41435000  | -0.93507500 | -1.01061100 |
| C              | -1.96748000 | -0.50169700 | 1.33059100  |
| C              | -2.92256900 | 0.52929600  | 1.20173200  |
| C              | -2.36360700 | -1.86206100 | 1.32902400  |
| C              | -4.24563100 | 0.17600400  | 0.90952400  |
| C              | -3.70256200 | -2.15396000 | 1.05551800  |
| C              | -4.64692100 | -1.15451700 | 0.79449500  |
| H              | -4.97869500 | 0.96160600  | 0.75669700  |
| H              | -4.02080200 | -3.18926500 | 1.00855100  |



|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 3. 34669700  | -1. 91513900 | 0. 41330900  |
| C | 2. 15684700  | 3. 09337000  | 0. 58678900  |
| C | -2. 57281400 | 1. 99010200  | 1. 51633200  |
| C | -1. 37022500 | -2. 98682800 | 1. 63300800  |
| H | -0. 43779700 | -2. 73574700 | 1. 12156200  |
| H | 2. 30400800  | -1. 99887100 | 0. 73221600  |
| H | 1. 12144100  | 2. 77659400  | 0. 42540600  |
| H | -1. 48542600 | 2. 08091400  | 1. 45784300  |
| C | 3. 52173500  | -2. 88762700 | -0. 75575100 |
| C | 4. 71960600  | -3. 57574800 | -0. 99671700 |
| C | 2. 44511300  | -3. 10882000 | -1. 62851800 |
| C | 4. 84274400  | -4. 44622300 | -2. 08365800 |
| H | 5. 56817100  | -3. 44654000 | -0. 33251700 |
| C | 2. 56427200  | -3. 97874000 | -2. 71289300 |
| H | 1. 49968700  | -2. 60352400 | -1. 45504300 |
| C | 3. 76686000  | -4. 64998300 | -2. 94787000 |
| H | 5. 78137200  | -4. 96813300 | -2. 24864100 |
| H | 1. 71399700  | -4. 13517600 | -3. 37098100 |
| H | 3. 86104800  | -5. 32868000 | -3. 79065800 |
| C | 4. 23345500  | -2. 27126600 | 1. 62751100  |
| H | 5. 29635100  | -2. 14650700 | 1. 40116300  |
| H | 4. 00981000  | -1. 62000600 | 2. 47685400  |
| H | 4. 06854900  | -3. 30847000 | 1. 93585400  |
| C | 2. 29939200  | 3. 38725300  | 2. 08360000  |
| C | 3. 53526100  | 3. 31542100  | 2. 74190800  |
| C | 1. 17930000  | 3. 80966300  | 2. 81541400  |
| C | 3. 64500100  | 3. 64504900  | 4. 09517900  |
| H | 4. 41643900  | 2. 99167300  | 2. 19551200  |
| C | 1. 28539600  | 4. 14002600  | 4. 16791100  |
| H | 0. 21531700  | 3. 88692900  | 2. 31758300  |
| C | 2. 52072300  | 4. 05584900  | 4. 81434900  |
| H | 4. 61139600  | 3. 57909100  | 4. 58733100  |
| H | 0. 40362100  | 4. 46090100  | 4. 71546700  |
| H | 2. 60623900  | 4. 30867000  | 5. 86712300  |
| C | 2. 35103700  | 4. 40975600  | -0. 19660000 |
| H | 2. 26026300  | 4. 25413500  | -1. 27484700 |
| H | 1. 58835900  | 5. 13032100  | 0. 11196300  |
| H | 3. 32551000  | 4. 86302900  | 0. 00865100  |
| C | -3. 13505000 | 3. 03167900  | 0. 54987500  |
| C | -2. 30352800 | 3. 56289300  | -0. 44625600 |
| C | -4. 44355400 | 3. 53197500  | 0. 64556500  |
| C | -2. 75938100 | 4. 54579100  | -1. 32675300 |
| H | -1. 28160700 | 3. 20213400  | -0. 52900600 |
| C | -4. 90788200 | 4. 50936600  | -0. 23757500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.11032500 | 3.17285000  | 1.42318200  |
| C | -4.06822900 | 5.02080900  | -1.22849500 |
| H | -2.09028000 | 4.94174200  | -2.08553400 |
| H | -5.92568600 | 4.87734000  | -0.14268700 |
| H | -4.42709500 | 5.78621800  | -1.91037000 |
| C | -2.98459600 | 2.29609700  | 2.97780900  |
| H | -2.50704200 | 1.59894100  | 3.67171700  |
| H | -2.69690300 | 3.31518600  | 3.25570100  |
| H | -4.06481500 | 2.19644900  | 3.11688000  |
| C | -1.04770000 | -3.11686400 | 3.12486400  |
| C | -2.02013500 | -2.93183600 | 4.11824700  |
| C | 0.24144500  | -3.50336000 | 3.52305600  |
| C | -1.71070400 | -3.11785000 | 5.46780400  |
| H | -3.02450400 | -2.63170100 | 3.83382100  |
| C | 0.55459600  | -3.69075100 | 4.87085300  |
| H | 1.00661100  | -3.66277000 | 2.76648300  |
| C | -0.42203600 | -3.49631300 | 5.85039200  |
| H | -2.47896200 | -2.96546800 | 6.22098800  |
| H | 1.56078100  | -3.98669200 | 5.15486400  |
| H | -0.18126100 | -3.63810100 | 6.89999700  |
| C | -1.80905700 | -4.37115200 | 1.10518400  |
| H | -0.98877200 | -5.08341400 | 1.23467200  |
| H | -2.66593300 | -4.76208800 | 1.66283400  |
| H | -2.06683000 | -4.32588800 | 0.04613200  |
| C | 6.33518000  | 1.50291500  | -1.80488300 |
| C | -6.04952700 | -1.51635800 | 0.36846900  |
| H | -6.75113000 | -0.69764000 | 0.55182500  |
| H | -6.07285100 | -1.73911900 | -0.70562400 |
| H | -6.41302700 | -2.40575300 | 0.89265400  |
| H | 7.07632200  | 0.70300000  | -1.72503200 |
| H | 6.09937300  | 1.62686900  | -2.86883400 |
| H | 6.79652100  | 2.43511800  | -1.46481600 |
| C | -3.81414200 | -1.38062500 | -2.99750700 |
| F | -3.34837300 | -3.47245800 | -1.96770300 |
| F | -5.06255600 | -1.81811900 | -3.28766500 |
| F | -0.87460200 | -2.63012400 | -1.31542400 |
| F | 1.65097700  | 1.14200400  | -5.35304300 |
| C | 1.45869000  | 2.55486500  | -3.48912200 |
| H | 2.49944900  | 2.38145000  | -3.20081000 |
| H | 1.42444900  | 3.40073400  | -4.18345400 |
| H | 0.89933500  | 2.82259300  | -2.58859700 |
| H | -4.07528100 | 0.51271300  | -3.94414500 |

**TS7(S)**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.08150100 | -2.92856500 | -1.43614900 |
| C  | -1.76877300 | -2.49314700 | -1.50245900 |
| C  | -1.38405000 | -1.29832400 | -2.13216200 |
| C  | -2.39657800 | -0.62134500 | -2.86310600 |
| C  | -3.72733100 | -1.05596900 | -2.80770300 |
| C  | -2.00057000 | 0.48725200  | -3.81035500 |
| H  | -1.55136900 | 1.32667400  | -3.26717500 |
| H  | -2.88820000 | 0.87897800  | -4.31639600 |
| C  | -1.00332400 | -0.04045100 | -4.85747400 |
| H  | -1.41490300 | -0.94109200 | -5.32749700 |
| H  | -0.85276200 | 0.70052400  | -5.65125000 |
| C  | 0.36379800  | -0.39684000 | -4.26301300 |
| C  | 0.28830300  | -1.36583800 | -3.08246400 |
| H  | 0.06182900  | -2.36566800 | -3.45294200 |
| H  | 1.28257800  | -1.44796200 | -2.59425500 |
| Ni | 0.08303500  | -0.50378000 | -1.27352000 |
| C  | 0.39235100  | 0.26264500  | 0.46777400  |
| C  | 0.21285700  | 1.00096200  | 2.71666300  |
| C  | 1.67511700  | 1.10875900  | 2.28142800  |
| H  | -0.24232000 | 1.98847600  | 2.84151500  |
| H  | 0.08041700  | 0.43232900  | 3.63716800  |
| H  | 2.09889500  | 2.10019900  | 2.44675400  |
| H  | 2.30381900  | 0.36570800  | 2.78400600  |
| N  | 1.58575600  | 0.80669700  | 0.83256800  |
| N  | -0.40776400 | 0.29474500  | 1.56635000  |
| C  | 2.72150300  | 0.95886700  | -0.03570600 |
| C  | 2.85890100  | 2.15513600  | -0.78487500 |
| C  | 3.70945000  | -0.04539600 | -0.09879300 |
| C  | 3.97517500  | 2.29422300  | -1.61249700 |
| C  | 4.80592000  | 0.14571700  | -0.95025800 |
| C  | 4.95633500  | 1.29935100  | -1.71712000 |
| H  | 4.09135000  | 3.19835300  | -2.20091300 |
| H  | 5.55804700  | -0.63542200 | -1.01692200 |
| C  | -1.76519300 | -0.18209600 | 1.62166800  |
| C  | -2.83761800 | 0.71204500  | 1.42122400  |
| C  | -2.01167800 | -1.54581100 | 1.92182000  |
| C  | -4.14332900 | 0.20475200  | 1.41947900  |
| C  | -3.33476000 | -1.99478100 | 1.91515300  |
| C  | -4.41179600 | -1.14555200 | 1.63443700  |
| H  | -4.96895000 | 0.88413100  | 1.22741200  |
| H  | -3.54151600 | -3.04099200 | 2.10907600  |
| C  | 3.66405700  | -1.30006500 | 0.78126700  |
| C  | 1.81923300  | 3.27096700  | -0.67909900 |
| C  | -2.62857300 | 2.22729900  | 1.30824600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.86780900 | -2.50438000 | 2.26244900  |
| H | -0.07856800 | -2.33285100 | 1.52495600  |
| H | 2.66794100  | -1.34519200 | 1.22852300  |
| H | 0.84092900  | 2.78399700  | -0.61636700 |
| H | -1.56911000 | 2.39418900  | 1.09866800  |
| C | 3.83240800  | -2.59419000 | -0.01851900 |
| C | 5.06926200  | -3.23501200 | -0.17978700 |
| C | 2.70439100  | -3.17878700 | -0.61538000 |
| C | 5.17715100  | -4.41202200 | -0.92649600 |
| H | 5.96141500  | -2.82700300 | 0.28480100  |
| C | 2.80740900  | -4.35456600 | -1.35947800 |
| H | 1.73299200  | -2.70635600 | -0.49819400 |
| C | 4.04806800  | -4.97620200 | -1.52109000 |
| H | 6.14692200  | -4.88960400 | -1.03653300 |
| H | 1.91562600  | -4.78569200 | -1.80597800 |
| H | 4.13193000  | -5.89289900 | -2.09764400 |
| C | 4.68412400  | -1.16827000 | 1.93309300  |
| H | 5.70551400  | -1.05426000 | 1.55842300  |
| H | 4.46652000  | -0.28579600 | 2.54127700  |
| H | 4.65501600  | -2.04977100 | 2.58151600  |
| C | 1.97337500  | 4.12090000  | 0.58659700  |
| C | 3.22890700  | 4.43191000  | 1.12748800  |
| C | 0.83354300  | 4.66883600  | 1.19472300  |
| C | 3.34086200  | 5.25795200  | 2.24884300  |
| H | 4.12495700  | 4.01946100  | 0.67310700  |
| C | 0.94162800  | 5.49453000  | 2.31539500  |
| H | -0.14806700 | 4.45254600  | 0.77935900  |
| C | 2.19816000  | 5.79068600  | 2.84893100  |
| H | 4.32358900  | 5.48346400  | 2.65383700  |
| H | 0.04482400  | 5.90458600  | 2.77156600  |
| H | 2.28540500  | 6.42974900  | 3.72281700  |
| C | 1.77506600  | 4.20540100  | -1.90814000 |
| H | 1.66623800  | 3.63904800  | -2.83771100 |
| H | 0.92278700  | 4.88514400  | -1.81899600 |
| H | 2.67499000  | 4.82344400  | -1.98346600 |
| C | -3.39234100 | 2.87670300  | 0.15387100  |
| C | -2.78702700 | 2.95130700  | -1.10954100 |
| C | -4.67028100 | 3.43533100  | 0.30383700  |
| C | -3.43287000 | 3.55778500  | -2.18760800 |
| H | -1.79591700 | 2.52539500  | -1.24430600 |
| C | -5.32458700 | 4.03685300  | -0.77462700 |
| H | -5.16428800 | 3.41708200  | 1.27000000  |
| C | -4.70880000 | 4.10244100  | -2.02473000 |
| H | -2.93759300 | 3.60920200  | -3.15307700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -6.31428800 | 4.46175500  | -0.63163500 |
| H | -5.21353700 | 4.57747900  | -2.86097100 |
| C | -2.94578500 | 2.89103100  | 2.66802700  |
| H | -2.31279800 | 2.47908700  | 3.45852600  |
| H | -2.78104900 | 3.97234900  | 2.62153500  |
| H | -3.98296000 | 2.71528300  | 2.96749000  |
| C | -0.26358200 | -2.24298100 | 3.64430900  |
| C | -1.05651000 | -1.89570500 | 4.74787300  |
| C | 1.11221400  | -2.42511200 | 3.84823100  |
| C | -0.48871700 | -1.72178800 | 6.01242000  |
| H | -2.12504200 | -1.75253300 | 4.61439700  |
| C | 1.68427300  | -2.25180400 | 5.11046000  |
| H | 1.73959800  | -2.71608200 | 3.00903700  |
| C | 0.88471000  | -1.89526300 | 6.19871900  |
| H | -1.12147500 | -1.44945400 | 6.85280300  |
| H | 2.75322000  | -2.39525700 | 5.24250200  |
| H | 1.32632300  | -1.75665900 | 7.18134100  |
| C | -1.24882600 | -3.99798400 | 2.16794100  |
| H | -0.35066500 | -4.60828000 | 2.30061200  |
| H | -1.95386100 | -4.28451400 | 2.95475200  |
| H | -1.68709300 | -4.23546900 | 1.19734400  |
| C | 6.13271400  | 1.47293600  | -2.64865200 |
| C | -5.81552900 | -1.69257800 | 1.52947100  |
| H | -6.56503300 | -0.91133700 | 1.68545500  |
| H | -5.98239700 | -2.11831400 | 0.53259100  |
| H | -5.99245000 | -2.48978700 | 2.25824300  |
| H | 6.93741000  | 0.77195000  | -2.41088600 |
| H | 5.83884600  | 1.29679100  | -3.69054400 |
| H | 6.53742400  | 2.48885700  | -2.59611800 |
| C | -4.06848700 | -2.18534900 | -2.07799500 |
| F | -3.40635200 | -4.03596900 | -0.73676600 |
| F | -5.35593400 | -2.59327800 | -1.97846500 |
| F | -0.82271800 | -3.26347100 | -0.89585900 |
| F | 1.05693600  | -1.09677000 | -5.29834400 |
| C | 1.20871500  | 0.83912900  | -3.97383100 |
| H | 2.20358400  | 0.55039800  | -3.62571000 |
| H | 1.31430400  | 1.43990300  | -4.88302800 |
| H | 0.74861300  | 1.45384700  | -3.19611300 |
| H | -4.50847800 | -0.52418700 | -3.34213900 |

**5(S)<sup>C-F</sup><sub>endo</sub>**

|   |             |            |             |
|---|-------------|------------|-------------|
| C | 2.34464600  | 0.51493200 | 0.01903200  |
| C | 1.08871600  | 1.09857000 | -0.08681600 |
| C | -0.08471200 | 0.34457900 | -0.15952400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.02597300  | -1.05705700 | -0.12726600 |
| C | 1.28942200  | -1.65660700 | -0.02278100 |
| C | -1.21431500 | -1.93089900 | -0.16577600 |
| H | -1.38683300 | -2.34106600 | 0.83838900  |
| H | -1.03313500 | -2.79653100 | -0.81204600 |
| C | -2.46745500 | -1.18328000 | -0.63990600 |
| H | -2.41359400 | -1.00630600 | -1.72052100 |
| H | -3.36308600 | -1.78461600 | -0.45328800 |
| C | -2.60930900 | 0.17413800  | 0.04869800  |
| C | -1.41166800 | 1.06179300  | -0.30430800 |
| H | -1.54152800 | 1.38741700  | -1.34426900 |
| H | -1.41927100 | 1.97033700  | 0.30606300  |
| C | 2.43065600  | -0.87489200 | 0.04881800  |
| F | 3.44964300  | 1.27388800  | 0.08559200  |
| F | 3.64769900  | -1.44006700 | 0.14570700  |
| F | 1.01911900  | 2.44485000  | -0.12116600 |
| F | -3.74875800 | 0.80147900  | -0.50614000 |
| C | -2.85603200 | 0.07687900  | 1.55042100  |
| H | -3.07109000 | 1.07086800  | 1.95279500  |
| H | -3.71033200 | -0.57455300 | 1.75721100  |
| H | -1.98150500 | -0.31950900 | 2.07382300  |
| H | 1.39549700  | -2.73633200 | 0.00235200  |

**IM12**

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -6.45828800 | 0.10243000  | -0.09392100 |
| C | -5.44275400 | -0.32160800 | -0.09670800 |
| C | -4.89263300 | -0.31916400 | -1.55049800 |
| H | -5.55344400 | -1.35971000 | 0.23709100  |
| C | -4.56619100 | 0.38980300  | 0.91310600  |
| C | -3.38568900 | -0.48986000 | -1.63172400 |
| H | -5.37227400 | -1.13783200 | -2.09800200 |
| H | -5.19219100 | 0.59875200  | -2.06324900 |
| C | -3.85666300 | 1.54739800  | 0.71811400  |
| H | -4.62168000 | 0.00415200  | 1.92929900  |
| C | -2.45509700 | 0.52363600  | -1.65234400 |
| H | -3.03231700 | -1.48979700 | -1.87754900 |
| C | -3.85392700 | 2.39110000  | -0.54220700 |
| H | -3.36624200 | 1.98162800  | 1.58762900  |
| C | -2.72039700 | 2.01031100  | -1.53326100 |
| H | -1.43955400 | 0.26070400  | -1.94322300 |
| H | -3.72847600 | 3.44362000  | -0.26561000 |
| H | -4.82560200 | 2.32457400  | -1.03803800 |
| H | -1.78903400 | 2.48569300  | -1.20392600 |
| H | -2.94267900 | 2.44312600  | -2.52064100 |
| C | 5.22144000  | 0.46256900  | -0.48829400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.84147800  | -0.80226500 | -0.93056900 |
| C  | 3.68146600  | -1.40515100 | -0.46437600 |
| C  | 2.85877200  | -0.75515400 | 0.46675800  |
| C  | 3.25209200  | 0.51284700  | 0.89713900  |
| C  | 1.57323800  | -1.36672900 | 0.96965800  |
| H  | 1.48106700  | -1.19702100 | 2.04751200  |
| H  | 1.61483700  | -2.44906300 | 0.81496500  |
| C  | 0.31441900  | -0.77919600 | 0.27138500  |
| H  | 0.31065200  | 0.30320000  | 0.44208200  |
| H  | 0.41984700  | -0.92991000 | -0.81132800 |
| C  | -0.99283100 | -1.38788800 | 0.76299900  |
| C  | -1.59517400 | -0.87872800 | 1.94236200  |
| H  | -1.12683300 | -0.05672900 | 2.48513400  |
| H  | -2.23637900 | -1.51626200 | 2.55156100  |
| Ni | -2.56183700 | -0.20748900 | 0.35183500  |
| H  | 3.42473300  | -2.39340000 | -0.83041400 |
| C  | 4.41577800  | 1.12255900  | 0.43501400  |
| C  | -1.23934900 | -2.82865900 | 0.34275200  |
| H  | -0.47760500 | -3.51232600 | 0.74727000  |
| H  | -2.21157400 | -3.18651000 | 0.69625800  |
| H  | -1.21789200 | -2.94070300 | -0.74856100 |
| F  | 5.63012200  | -1.43056500 | -1.82151200 |
| F  | 6.34296100  | 1.04255600  | -0.93855400 |
| F  | 4.76398800  | 2.34007800  | 0.87367000  |
| F  | 2.49898300  | 1.18972400  | 1.78955700  |

### IM13

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.68361300  | -2.29710600 | 0.44950100  |
| C  | 1.45800500  | -1.33011500 | 1.41351800  |
| C  | 1.68975700  | 0.02827100  | 1.16204600  |
| C  | 2.20044700  | 0.44535700  | -0.09477200 |
| C  | 2.41180500  | -0.56092000 | -1.05959000 |
| C  | 2.79664500  | 1.82429200  | -0.32926900 |
| H  | 2.68502500  | 2.07786900  | -1.38673300 |
| H  | 3.87854200  | 1.78564500  | -0.14136500 |
| C  | 2.14234900  | 2.89058700  | 0.54853800  |
| H  | 2.41372400  | 2.71980000  | 1.59779000  |
| H  | 2.55990400  | 3.87577100  | 0.29734100  |
| C  | 0.62301300  | 2.90899700  | 0.42070900  |
| C  | -0.00237800 | 2.88120700  | -0.81793900 |
| H  | 0.57036900  | 2.82109600  | -1.74124000 |
| H  | -1.02304100 | 3.23374700  | -0.92849000 |
| Ni | -0.03006800 | 0.96151200  | -0.05527200 |
| H  | 1.64847700  | 0.70718200  | 2.00548100  |
| C  | 2.16324700  | -1.89961200 | -0.80386900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.12234000 | 3.40087800  | 1.64462700  |
| H | 0.09299600  | 2.78620400  | 2.52747200  |
| H | 0.18183000  | 4.42761300  | 1.89634500  |
| H | -1.20432700 | 3.40378500  | 1.48617100  |
| F | 1.00308600  | -1.71437900 | 2.61916000  |
| F | 1.42392300  | -3.59104500 | 0.68855000  |
| F | 2.37021200  | -2.82266600 | -1.75176200 |
| F | 2.90364900  | -0.22937500 | -2.27087700 |
| H | -5.22889700 | 1.09485600  | -0.71331400 |
| C | -4.35197500 | 0.56507900  | -1.11765400 |
| C | -3.07027200 | 1.17233500  | -0.49028600 |
| H | -4.34677700 | 0.80396400  | -2.18979500 |
| C | -4.56132800 | -0.92909100 | -0.99189500 |
| C | -1.81625900 | 0.45496400  | -0.94280900 |
| H | -3.02604900 | 2.22316000  | -0.80153900 |
| H | -3.14344200 | 1.18674500  | 0.59899200  |
| C | -4.11363300 | -1.77057800 | -0.05101900 |
| H | -5.16487900 | -1.36038200 | -1.79134800 |
| C | -1.25431400 | -0.67347600 | -0.34143300 |
| H | -1.58870800 | 0.59950700  | -2.00110000 |
| C | -3.28832100 | -1.41859000 | 1.16224300  |
| H | -4.36328800 | -2.82532100 | -0.16743300 |
| C | -1.74879800 | -1.36192300 | 0.93281100  |
| H | -0.66479300 | -1.31591900 | -0.99581700 |
| H | -3.47116600 | -2.16388900 | 1.94587700  |
| H | -3.62839100 | -0.46710800 | 1.57901000  |
| H | -1.36608000 | -2.38905400 | 0.91129200  |
| H | -1.31252200 | -0.91376800 | 1.83362200  |

**TS8(R)**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.51724000  | -1.93192000 | 0.60366000  |
| C | 1.30710300  | -1.25444600 | 0.73427300  |
| C | 1.06626000  | -0.03487800 | 0.12063800  |
| C | 2.12740900  | 0.57711900  | -0.59126400 |
| C | 3.34028000  | -0.09701500 | -0.71822800 |
| C | 1.95733900  | 1.98746500  | -1.12607700 |
| H | 1.19124100  | 2.00003100  | -1.91129700 |
| H | 2.88838700  | 2.32028700  | -1.59152200 |
| C | 1.57187000  | 3.00147100  | -0.01467500 |
| H | 2.37492200  | 3.00842000  | 0.73091200  |
| H | 1.53739700  | 4.00615400  | -0.45127500 |
| C | 0.23261500  | 2.73155800  | 0.70791300  |
| C | -1.00117200 | 2.91578900  | 0.00225400  |
| H | -0.98068200 | 3.26192900  | -1.02972300 |



|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -1.88113700 | 3.21363300  | 0.56697100  |
| Ni | -0.66492800 | 0.95483900  | -0.04713100 |
| H  | 0.49720800  | 1.29401900  | 0.83672300  |
| C  | 3.54056400  | -1.34802200 | -0.13616000 |
| C  | 0.24288200  | 3.04223400  | 2.20563300  |
| H  | 1.02336900  | 2.48578400  | 2.73474700  |
| H  | 0.44007800  | 4.11048900  | 2.35450800  |
| H  | -0.72034400 | 2.80807700  | 2.66653400  |
| F  | 0.34735300  | -1.85003700 | 1.48988400  |
| F  | 2.71291500  | -3.13121100 | 1.17853900  |
| F  | 4.71673000  | -1.98202400 | -0.27205000 |
| F  | 4.37654700  | 0.44740700  | -1.39628400 |
| H  | -5.67064500 | 0.28605600  | 0.69340500  |
| C  | -4.95090800 | 0.04202500  | -0.10298700 |
| C  | -3.58211300 | 0.62970900  | 0.29114800  |
| H  | -5.32474200 | 0.57660600  | -0.98915300 |
| C  | -5.04122900 | -1.43733800 | -0.37568400 |
| C  | -2.55846700 | 0.63531800  | -0.83095200 |
| H  | -3.74785400 | 1.66989500  | 0.59262400  |
| H  | -3.20198400 | 0.11978300  | 1.17848400  |
| C  | -4.13986300 | -2.41707400 | -0.22789600 |
| H  | -6.02238400 | -1.73979900 | -0.74528600 |
| C  | -1.72820200 | -0.40209000 | -1.24554600 |
| H  | -2.69174200 | 1.44999300  | -1.54017600 |
| C  | -2.69226800 | -2.36048500 | 0.21823500  |
| H  | -4.47734500 | -3.41437800 | -0.51128600 |
| C  | -1.73058600 | -1.87686300 | -0.88608300 |
| H  | -1.22941300 | -0.21959200 | -2.19944700 |
| H  | -2.38692800 | -3.37651200 | 0.49069200  |
| H  | -2.55372700 | -1.76273400 | 1.12215900  |
| H  | -1.98539300 | -2.41480300 | -1.81143200 |
| H  | -0.71472200 | -2.19139400 | -0.63750900 |

**IM14(R)**

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.93780000 | -3.49204600 | 0.46682600  |
| C | -2.46530700 | -2.63489200 | -0.03421300 |
| C | -3.56053200 | -1.77161800 | -0.70836900 |
| H | -1.81625400 | -3.05613000 | -0.80713300 |
| C | -1.57353500 | -1.89567400 | 0.93436100  |
| C | -3.09797000 | -0.38346400 | -1.11269100 |
| H | -3.90099000 | -2.29594700 | -1.60709100 |
| H | -4.43435300 | -1.69058600 | -0.05711800 |
| C | -1.91011500 | -0.88241600 | 1.77312500  |
| H | -0.56379100 | -2.28431300 | 1.01022800  |
| C | -3.17667500 | 0.74692200  | -0.34682200 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -2.84185100 | -0.25528400 | -2.16179400 |
| C  | -3.30346400 | -0.33283000 | 1.99718800  |
| H  | -1.12885100 | -0.50464400 | 2.42984800  |
| C  | -3.65815400 | 0.86434400  | 1.08177900  |
| H  | -3.02348300 | 1.69692800  | -0.85039000 |
| H  | -3.38543300 | -0.00351800 | 3.03821500  |
| H  | -4.03779100 | -1.13231900 | 1.87440600  |
| H  | -3.22573000 | 1.77778200  | 1.50395500  |
| H  | -4.74700800 | 1.01990600  | 1.09315400  |
| C  | 2.72901500  | -1.67889700 | -0.36555900 |
| C  | 1.38721800  | -1.33155600 | -0.48350800 |
| C  | 0.84501200  | -0.13940500 | -0.01556800 |
| C  | 1.74431600  | 0.79392900  | 0.54392800  |
| C  | 3.09233100  | 0.44346600  | 0.67230100  |
| H  | -1.42789500 | 3.22903900  | -0.84872100 |
| C  | 1.36730100  | 2.19585200  | 1.00003400  |
| H  | 2.11077600  | 2.89482300  | 0.59814100  |
| H  | 1.49022400  | 2.25736100  | 2.09064400  |
| C  | -0.03823700 | 2.69199700  | 0.65020800  |
| H  | -0.77749900 | 2.05217100  | 1.15078500  |
| H  | -0.14681600 | 3.68987300  | 1.09705700  |
| C  | -0.41966900 | 2.78945000  | -0.84819900 |
| C  | -0.51124100 | 1.42659700  | -1.56727100 |
| H  | 0.43308000  | 1.17036800  | -2.05127400 |
| H  | -1.28445900 | 1.44672900  | -2.34682900 |
| Ni | -1.05770800 | 0.06405800  | -0.28125400 |
| C  | 3.59820700  | -0.77402900 | 0.23189800  |
| C  | 0.48777600  | 3.76984600  | -1.61411600 |
| H  | 1.51844800  | 3.40188000  | -1.66674400 |
| H  | 0.13510300  | 3.90098900  | -2.64278100 |
| H  | 0.50635600  | 4.75766900  | -1.13723000 |
| F  | 0.58835700  | -2.25208100 | -1.10852700 |
| F  | 3.19343600  | -2.85683700 | -0.82300400 |
| F  | 4.90341800  | -1.07044000 | 0.36837800  |
| F  | 3.96859000  | 1.31712600  | 1.22625600  |

**TS9(R)**

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.93780000 | -3.49204600 | 0.46682600  |
| C | -2.46530700 | -2.63489200 | -0.03421300 |
| C | -3.56053200 | -1.77161800 | -0.70836900 |
| H | -1.81625400 | -3.05613000 | -0.80713300 |
| C | -1.57353500 | -1.89567400 | 0.93436100  |
| C | -3.09797000 | -0.38346400 | -1.11269100 |
| H | -3.90099000 | -2.29594700 | -1.60709100 |
| H | -4.43435300 | -1.69058600 | -0.05711800 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.91011500 | -0.88241600 | 1.77312500  |
| H  | -0.56379100 | -2.28431300 | 1.01022800  |
| C  | -3.17667500 | 0.74692200  | -0.34682200 |
| H  | -2.84185100 | -0.25528400 | -2.16179400 |
| C  | -3.30346400 | -0.33283000 | 1.99718800  |
| H  | -1.12885100 | -0.50464400 | 2.42984800  |
| C  | -3.65815400 | 0.86434400  | 1.08177900  |
| H  | -3.02348300 | 1.69692800  | -0.85039000 |
| H  | -3.38543300 | -0.00351800 | 3.03821500  |
| H  | -4.03779100 | -1.13231900 | 1.87440600  |
| H  | -3.22573000 | 1.77778200  | 1.50395500  |
| H  | -4.74700800 | 1.01990600  | 1.09315400  |
| C  | 2.72901500  | -1.67889700 | -0.36555900 |
| C  | 1.38721800  | -1.33155600 | -0.48350800 |
| C  | 0.84501200  | -0.13940500 | -0.01556800 |
| C  | 1.74431600  | 0.79392900  | 0.54392800  |
| C  | 3.09233100  | 0.44346600  | 0.67230100  |
| H  | -1.42789500 | 3.22903900  | -0.84872100 |
| C  | 1.36730100  | 2.19585200  | 1.00003400  |
| H  | 2.11077600  | 2.89482300  | 0.59814100  |
| H  | 1.49022400  | 2.25736100  | 2.09064400  |
| C  | -0.03823700 | 2.69199700  | 0.65020800  |
| H  | -0.77749900 | 2.05217100  | 1.15078500  |
| H  | -0.14681600 | 3.68987300  | 1.09705700  |
| C  | -0.41966900 | 2.78945000  | -0.84819900 |
| C  | -0.51124100 | 1.42659700  | -1.56727100 |
| H  | 0.43308000  | 1.17036800  | -2.05127400 |
| H  | -1.28445900 | 1.44672900  | -2.34682900 |
| Ni | -1.05770800 | 0.06405800  | -0.28125400 |
| C  | 3.59820700  | -0.77402900 | 0.23189800  |
| C  | 0.48777600  | 3.76984600  | -1.61411600 |
| H  | 1.51844800  | 3.40188000  | -1.66674400 |
| H  | 0.13510300  | 3.90098900  | -2.64278100 |
| H  | 0.50635600  | 4.75766900  | -1.13723000 |
| F  | 0.58835700  | -2.25208100 | -1.10852700 |
| F  | 3.19343600  | -2.85683700 | -0.82300400 |
| F  | 4.90341800  | -1.07044000 | 0.36837800  |
| F  | 3.96859000  | 1.31712600  | 1.22625600  |

### IM15

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.05523900  | -2.47659600 | -0.02248400 |
| C | -0.32157100 | -1.58886800 | -1.08104600 |
| C | 0.61276100  | -0.54281900 | -1.42613400 |
| C | 1.93515200  | -0.50076000 | -0.85064200 |
| C | 2.21210700  | -1.38935400 | 0.15664100  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 0.48139800  | -0.06534800 | -2.39542400 |
| C  | 2.99887000  | 0.40104200  | -1.44817400 |
| H  | 2.53221000  | 1.01159900  | -2.22755700 |
| H  | 3.73737900  | -0.22909600 | -1.96151000 |
| C  | 3.78100600  | 1.31392800  | -0.46995600 |
| H  | 4.28270200  | 0.69207600  | 0.27379100  |
| H  | 4.56812900  | 1.80464700  | -1.06032400 |
| C  | 2.96760900  | 2.38296000  | 0.22674600  |
| C  | 2.83585600  | 2.39712500  | 1.55947300  |
| H  | 3.28854600  | 1.63083700  | 2.18316400  |
| H  | 2.28209600  | 3.18064800  | 2.07064700  |
| Ni | -1.06058500 | 0.02776800  | -0.35396300 |
| C  | 1.26242300  | -2.34401300 | 0.60774900  |
| C  | 2.36375000  | 3.45734000  | -0.64536000 |
| H  | 3.14337200  | 3.97710600  | -1.21763600 |
| H  | 1.66875500  | 3.03651700  | -1.38203300 |
| H  | 1.82065700  | 4.19940100  | -0.05430100 |
| F  | -1.13661200 | -2.14833100 | -2.05914800 |
| F  | -0.82526200 | -3.41557500 | 0.38232100  |
| F  | 1.57250800  | -3.11872200 | 1.66459800  |
| F  | 3.42944000  | -1.43303300 | 0.75787900  |
| H  | -4.76139500 | 1.20122700  | -0.93942100 |
| C  | -3.67105900 | 1.11107100  | -1.05522400 |
| C  | -2.99025500 | 2.36568600  | -0.44126600 |
| H  | -3.48673400 | 1.10205600  | -2.13554100 |
| C  | -3.18960600 | -0.21426600 | -0.50164600 |
| C  | -1.50514100 | 2.18742200  | -0.18754500 |
| H  | -3.13338700 | 3.20375400  | -1.13182600 |
| H  | -3.49360100 | 2.65130900  | 0.48587300  |
| C  | -2.85452500 | -0.49707100 | 0.80065800  |
| H  | -3.24240300 | -1.05228100 | -1.19389600 |
| C  | -0.93141900 | 1.74174700  | 0.97405600  |
| H  | -0.83775300 | 2.59139400  | -0.94694500 |
| C  | -2.95093300 | 0.45977700  | 1.97302100  |
| H  | -2.64023600 | -1.53692400 | 1.04123800  |
| C  | -1.64833800 | 1.27162800  | 2.22268900  |
| H  | 0.14828700  | 1.84208500  | 1.06871000  |
| H  | -3.17284600 | -0.11216600 | 2.88014300  |
| H  | -3.79500300 | 1.13952600  | 1.83112300  |
| H  | -0.94699700 | 0.64985600  | 2.79025900  |
| H  | -1.87901800 | 2.12933600  | 2.87223900  |

## TS10

|   |            |             |            |
|---|------------|-------------|------------|
| C | 2.57547700 | -1.97485000 | 0.24350700 |
|---|------------|-------------|------------|

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.24336300  | -1.74048200 | -0.06470000 |
| C  | 0.75855300  | -0.51143900 | -0.52742600 |
| C  | 1.70700000  | 0.52530400  | -0.72881200 |
| C  | 3.04899200  | 0.27171600  | -0.43725000 |
| H  | -0.19104900 | -0.61810800 | -1.66120600 |
| C  | 1.32859100  | 1.86963300  | -1.31724200 |
| H  | 0.27684300  | 1.83007000  | -1.61902700 |
| H  | 1.91363600  | 2.02894200  | -2.23220500 |
| C  | 1.57995900  | 3.09707100  | -0.39501200 |
| H  | 2.60628200  | 3.04681700  | -0.02434000 |
| H  | 1.51462400  | 3.99474000  | -1.02458800 |
| C  | 0.61876500  | 3.24710600  | 0.76443200  |
| C  | 0.96450800  | 2.92116200  | 2.01638500  |
| H  | 1.95185000  | 2.53295600  | 2.25162900  |
| H  | 0.27640300  | 3.04296800  | 2.84930000  |
| Ni | -1.17540100 | -0.40461700 | -0.57349100 |
| C  | 3.49767700  | -0.95043000 | 0.05218100  |
| C  | -0.73559300 | 3.82503600  | 0.43451200  |
| H  | -0.63315300 | 4.83836300  | 0.02476100  |
| H  | -1.24664600 | 3.23103400  | -0.33250100 |
| H  | -1.38361900 | 3.87740000  | 1.31382400  |
| F  | 0.37912700  | -2.77807100 | 0.11291000  |
| F  | 2.98329600  | -3.16513900 | 0.71681100  |
| F  | 4.79901400  | -1.14798500 | 0.32392100  |
| F  | 3.98406300  | 1.22997600  | -0.64933100 |
| H  | -3.38961000 | -2.32119900 | 2.07990100  |
| C  | -2.77961300 | -2.10170200 | 1.19142900  |
| C  | -3.71655100 | -1.94729200 | -0.03944100 |
| H  | -2.13776700 | -2.97520300 | 1.04143800  |
| C  | -1.87158600 | -0.92149200 | 1.45962500  |
| C  | -3.06312000 | -1.26632700 | -1.22848300 |
| H  | -4.04200100 | -2.94757900 | -0.34346700 |
| H  | -4.62422200 | -1.40748500 | 0.24229900  |
| C  | -2.16697400 | 0.40275200  | 1.30416800  |
| H  | -0.91722600 | -1.16878500 | 1.91818700  |
| C  | -3.06879200 | 0.08141700  | -1.48893600 |
| H  | -2.70242300 | -1.92252900 | -2.01840100 |
| C  | -3.51273100 | 0.97150000  | 0.89959400  |
| H  | -1.40788200 | 1.11809100  | 1.61442500  |
| C  | -3.67621200 | 1.17105800  | -0.63226800 |
| H  | -2.74245400 | 0.39680700  | -2.47895900 |
| H  | -3.64379000 | 1.94468200  | 1.38459800  |
| H  | -4.31392900 | 0.33467200  | 1.28248000  |
| H  | -3.20763100 | 2.11853500  | -0.91921900 |

|             |             |             |             |
|-------------|-------------|-------------|-------------|
| H           | -4.74477800 | 1.28659200  | -0.86756800 |
| <b>IM16</b> |             |             |             |
| C           | 2.57497700  | -1.97760400 | 0.27445100  |
| C           | 1.22819900  | -1.74013300 | 0.02351700  |
| C           | 0.72775700  | -0.52769500 | -0.43844700 |
| C           | 1.65720300  | 0.50470300  | -0.69725200 |
| C           | 3.01410000  | 0.25689300  | -0.46411900 |
| H           | -0.65712700 | -0.70249800 | -2.03834600 |
| C           | 1.25895900  | 1.84561300  | -1.28442900 |
| H           | 0.19201400  | 1.80966000  | -1.52485100 |
| H           | 1.78944500  | 1.98107100  | -2.23596700 |
| C           | 1.57580000  | 3.08653100  | -0.40108800 |
| H           | 2.61224500  | 3.01809300  | -0.06335300 |
| H           | 1.51189700  | 3.97284400  | -1.04641000 |
| C           | 0.65668500  | 3.28450400  | 0.78556200  |
| C           | 1.01336300  | 2.92921000  | 2.02658100  |
| H           | 1.98331000  | 2.48569000  | 2.23444100  |
| H           | 0.35254000  | 3.08037500  | 2.87669700  |
| Ni          | -1.17424800 | -0.49610200 | -0.70612000 |
| C           | 3.48482200  | -0.95708600 | 0.02461000  |
| C           | -0.67170400 | 3.93884300  | 0.49364700  |
| H           | -0.52346700 | 4.95840400  | 0.11442000  |
| H           | -1.22050200 | 3.39814600  | -0.28707500 |
| H           | -1.30571000 | 3.99633400  | 1.38294900  |
| F           | 0.37591500  | -2.78401700 | 0.25432600  |
| F           | 3.00617700  | -3.16461000 | 0.73854800  |
| F           | 4.79848900  | -1.14889200 | 0.24016600  |
| F           | 3.94199000  | 1.20880900  | -0.73737100 |
| H           | -3.32568300 | -2.25824600 | 2.18422900  |
| C           | -2.78595400 | -2.06190600 | 1.24671200  |
| C           | -3.80864600 | -1.86782300 | 0.09753700  |
| H           | -2.19134200 | -2.95846500 | 1.04638200  |
| C           | -1.81418500 | -0.91987600 | 1.43840200  |
| C           | -3.20629200 | -1.25964200 | -1.15530200 |
| H           | -4.22195800 | -2.84870400 | -0.15819100 |
| H           | -4.65237200 | -1.26201100 | 0.43633500  |
| C           | -2.04098200 | 0.41069200  | 1.26405000  |
| H           | -0.84433600 | -1.20810400 | 1.83365300  |
| C           | -3.14344800 | 0.07296000  | -1.46294200 |
| H           | -2.93082900 | -1.95954100 | -1.94165300 |
| C           | -3.36692800 | 1.05678300  | 0.91667600  |
| H           | -1.21881100 | 1.08447900  | 1.49707700  |
| C           | -3.59068200 | 1.23615000  | -0.60711000 |
| H           | -2.86250500 | 0.33135300  | -2.48196400 |

|   |             |            |             |
|---|-------------|------------|-------------|
| H | -3.40531000 | 2.04595600 | 1.38426100  |
| H | -4.18704900 | 0.48296100 | 1.35396000  |
| H | -3.04456700 | 2.12304300 | -0.94563000 |
| H | -4.65235600 | 1.45170200 | -0.79696400 |

### IM17

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.80654800  | -1.65536500 | -0.16725800 |
| C  | 1.46429800  | -1.28194500 | -0.16667300 |
| C  | 1.00824000  | 0.02088000  | 0.02580100  |
| C  | 2.01589000  | 1.01228100  | 0.15463100  |
| C  | 3.36343400  | 0.63713800  | 0.15805400  |
| H  | -2.56448400 | 0.98367800  | 0.39556800  |
| C  | 1.77740600  | 2.51683900  | 0.19355000  |
| H  | 2.10002200  | 2.93604900  | -0.77061500 |
| H  | 2.45651600  | 2.95753300  | 0.93083300  |
| C  | 0.37258400  | 3.02833800  | 0.50013600  |
| H  | 0.06164600  | 2.70197700  | 1.50253400  |
| H  | 0.42514000  | 4.12581600  | 0.56350400  |
| C  | -0.74117400 | 2.69507200  | -0.47176900 |
| C  | -0.58651300 | 1.98163300  | -1.62751100 |
| H  | 0.37899100  | 1.62790300  | -1.96709400 |
| H  | -1.41097400 | 1.89997200  | -2.33025700 |
| Ni | -0.86929300 | 0.49195100  | 0.01415000  |
| C  | 3.77678600  | -0.68039600 | 0.01097500  |
| C  | -2.03618400 | 3.43045800  | -0.18994100 |
| H  | -1.88923600 | 4.49866900  | -0.39552400 |
| H  | -2.85724900 | 3.07803300  | -0.81947600 |
| H  | -2.33487700 | 3.35016800  | 0.86039900  |
| F  | 0.60045100  | -2.30826900 | -0.40843700 |
| F  | 3.17044200  | -2.93856300 | -0.35078500 |
| F  | 5.08252100  | -1.00201100 | 0.01756600  |
| F  | 4.33146000  | 1.57959600  | 0.28196700  |
| H  | -5.20469600 | -1.19592100 | -0.81385100 |
| C  | -4.35067500 | -0.52391700 | -0.64532800 |
| C  | -4.10942700 | -0.39700000 | 0.87834900  |
| H  | -4.67527100 | 0.45461700  | -1.02033400 |
| C  | -3.16569600 | -0.96493400 | -1.47918400 |
| C  | -2.75417600 | 0.24600000  | 1.25016400  |
| H  | -4.91320000 | 0.22246300  | 1.29186200  |
| H  | -4.19635000 | -1.36665700 | 1.37465200  |
| C  | -2.26420800 | -1.90547500 | -1.15634200 |
| H  | -3.04905700 | -0.45756700 | -2.43575700 |
| C  | -1.52602100 | -0.63034000 | 1.43603100  |
| H  | -2.86417500 | 0.92228300  | 2.10400700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.30475200 | -2.76027100 | 0.08787800  |
| H | -1.45258400 | -2.09512600 | -1.85344100 |
| C | -1.64108600 | -2.14578900 | 1.35851600  |
| H | -0.97380000 | -0.35511600 | 2.33862100  |
| H | -1.80996100 | -3.71313700 | -0.12604300 |
| H | -3.34798600 | -3.00902600 | 0.30761200  |
| H | -0.63476400 | -2.55224100 | 1.46419100  |
| H | -2.19894900 | -2.50500800 | 2.23913600  |

**TS11(R)**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.96467600  | -1.42922800 | -0.32037900 |
| C  | 1.59291700  | -1.21788100 | -0.43689700 |
| C  | 0.96162100  | -0.01660700 | -0.14961400 |
| C  | 1.79965500  | 1.07154700  | 0.20947500  |
| C  | 3.17634400  | 0.85838300  | 0.33877600  |
| H  | -2.11143500 | 1.28002400  | 0.12856600  |
| C  | 1.35658600  | 2.53080100  | 0.34444100  |
| H  | 1.74055200  | 3.06782400  | -0.53506600 |
| H  | 1.89115400  | 2.97612700  | 1.19033100  |
| C  | -0.12928000 | 2.90768900  | 0.51136700  |
| H  | -0.48586400 | 2.60606800  | 1.50419800  |
| H  | -0.17100100 | 4.00701300  | 0.51530300  |
| C  | -1.12715400 | 2.41170500  | -0.54295500 |
| C  | -0.64490400 | 1.65917500  | -1.64429200 |
| H  | 0.40572900  | 1.63625100  | -1.89360000 |
| H  | -1.32428900 | 1.46923300  | -2.47286500 |
| Ni | -0.96434000 | 0.36398400  | -0.12116200 |
| C  | 3.76943100  | -0.37431900 | 0.08817700  |
| C  | -2.36672100 | 3.28907300  | -0.69880700 |
| H  | -2.06294000 | 4.24986300  | -1.13395900 |
| H  | -3.10250100 | 2.83297600  | -1.36637100 |
| H  | -2.84668300 | 3.49729100  | 0.26247400  |
| F  | 0.87512200  | -2.29593500 | -0.87862800 |
| F  | 3.51900000  | -2.62460900 | -0.60088500 |
| F  | 5.09947500  | -0.53832900 | 0.21561300  |
| F  | 3.99999800  | 1.88070900  | 0.68465100  |
| H  | -5.07789500 | -0.98876600 | -0.33769900 |
| C  | -4.15837300 | -0.39779900 | -0.21516200 |
| C  | -3.75055400 | -0.43291200 | 1.28266200  |
| H  | -4.43302300 | 0.63073100  | -0.47150400 |
| C  | -3.11008500 | -0.85334800 | -1.20935400 |
| C  | -2.30541500 | -0.07226900 | 1.61275300  |
| H  | -4.40557900 | 0.25902900  | 1.82261500  |
| H  | -3.95756000 | -1.42297800 | 1.70015200  |
| C  | -2.27613100 | -1.90215700 | -1.08257200 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.07212100 | -0.28818800 | -2.13863000 |
| C | -1.24167000 | -0.95992500 | 1.58513100  |
| H | -2.17213900 | 0.81676200  | 2.22534000  |
| C | -2.25569800 | -2.85144300 | 0.09146700  |
| H | -1.57617700 | -2.10609100 | -1.88856900 |
| C | -1.29551300 | -2.43332100 | 1.23411600  |
| H | -0.36448600 | -0.67622000 | 2.16119300  |
| H | -1.94817500 | -3.84393200 | -0.25572100 |
| H | -3.27069300 | -2.97201900 | 0.48042400  |
| H | -0.28622200 | -2.75172600 | 0.97480900  |
| H | -1.56788100 | -2.99035500 | 2.14435900  |

TS1(R)-D3

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.38766700  | 1.51064500  | -0.07489400 |
| C  | 3.00483600  | 1.54205500  | -0.21679400 |
| C  | 2.31326700  | 0.65691600  | -1.03227600 |
| C  | 3.07244000  | -0.30004900 | -1.75634500 |
| C  | 4.45507400  | -0.33625000 | -1.60790400 |
| C  | 2.36469600  | -1.24305400 | -2.70033800 |
| H  | 1.68095000  | -1.87149900 | -2.12322500 |
| H  | 3.09058800  | -1.90812500 | -3.17451500 |
| C  | 1.55119600  | -0.52200600 | -3.80683300 |
| H  | 2.24071400  | 0.10569800  | -4.38325900 |
| H  | 1.16667600  | -1.28719300 | -4.49118300 |
| C  | 0.37975700  | 0.34069100  | -3.31969100 |
| C  | -0.77326200 | -0.26730100 | -2.75103100 |
| H  | -0.84992100 | -1.34762000 | -2.69932300 |
| H  | -1.71703900 | 0.26706500  | -2.81508500 |
| Ni | 0.36050000  | 0.32316300  | -1.22019000 |
| H  | 1.31670800  | 1.04137000  | -2.10696800 |
| C  | -0.52112300 | -0.15772900 | 0.36364800  |
| C  | -2.01672900 | 0.11975600  | 2.17479000  |
| C  | -1.24885600 | -1.18720300 | 2.36432700  |
| H  | -1.67934300 | 0.88520600  | 2.87870900  |
| H  | -3.09567400 | 0.00014100  | 2.25800100  |
| H  | -0.78202400 | -1.26777000 | 3.34391500  |
| H  | -1.88475500 | -2.06403500 | 2.19749300  |
| N  | -0.22305900 | -1.09158400 | 1.29731000  |
| N  | -1.62666600 | 0.49580600  | 0.79760800  |
| C  | 0.78915800  | -2.09607500 | 1.17832700  |
| C  | 2.06420100  | -1.85764600 | 1.73823300  |
| C  | 0.47708100  | -3.33298500 | 0.59003300  |
| C  | 3.00504800  | -2.88564400 | 1.70276600  |
| C  | 1.45127900  | -4.34122300 | 0.59816500  |
| C  | 2.71633700  | -4.13687400 | 1.14299700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.99115800  | -2.72167500 | 2.12229900  |
| H | 1.21468700  | -5.30840600 | 0.16500000  |
| C | -2.34610700 | 1.47152400  | 0.03882500  |
| C | -1.99201800 | 2.82610600  | 0.09987200  |
| C | -3.42941800 | 1.04310900  | -0.76335400 |
| C | -2.75970900 | 3.75593700  | -0.61355800 |
| C | -4.15411400 | 2.00285600  | -1.46813000 |
| C | -3.84435800 | 3.36807200  | -1.39420200 |
| H | -2.47678600 | 4.80365200  | -0.57294000 |
| H | -4.98096700 | 1.69229000  | -2.09757500 |
| C | -0.88751500 | -3.60413900 | -0.01795600 |
| C | 2.39442100  | -0.49165400 | 2.32277500  |
| C | -0.79581700 | 3.31336600  | 0.90706400  |
| C | -3.78968100 | -0.43389900 | -0.84169700 |
| H | -2.84658000 | -0.98771500 | -0.85331000 |
| H | -1.50803300 | -2.72974600 | 0.18490500  |
| H | 2.09476700  | 0.23261300  | 1.56652500  |
| H | -0.14587100 | 2.45064300  | 1.07716900  |
| C | -0.89887800 | -3.75995900 | -1.53959000 |
| C | -2.13371600 | -3.65531900 | -2.19894700 |
| C | 0.24141200  | -3.98473700 | -2.31651900 |
| C | -2.22764400 | -3.75197100 | -3.58502900 |
| H | -3.03462100 | -3.48201300 | -1.61895600 |
| C | 0.15424500  | -4.08075200 | -3.70864100 |
| H | 1.21080200  | -4.06746100 | -1.84171100 |
| C | -1.07730100 | -3.96121300 | -4.35014100 |
| H | -3.19545900 | -3.65274500 | -4.06726800 |
| H | 1.05788700  | -4.24299700 | -4.28872000 |
| H | -1.14255100 | -4.02922200 | -5.43163200 |
| C | -1.56667300 | -4.81451700 | 0.65982300  |
| H | -1.00801700 | -5.73607700 | 0.47528100  |
| H | -1.62999600 | -4.66358200 | 1.74179700  |
| H | -2.57865900 | -4.95921500 | 0.27084900  |
| C | 1.59565000  | -0.15744900 | 3.57092200  |
| C | 1.43561200  | -1.08242100 | 4.60942600  |
| C | 1.04196000  | 1.12008900  | 3.71225500  |
| C | 0.71562300  | -0.74465500 | 5.75659000  |
| H | 1.85887600  | -2.07771400 | 4.50512000  |
| C | 0.32228500  | 1.46201300  | 4.85796800  |
| H | 1.18065400  | 1.84291500  | 2.91333900  |
| C | 0.15048100  | 0.52715100  | 5.88137800  |
| H | 0.59057400  | -1.47526800 | 6.55051700  |
| H | -0.10900100 | 2.45452100  | 4.94773200  |
| H | -0.41522800 | 0.78819400  | 6.77060700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.89065900  | -0.28088900 | 2.60873900  |
| H | 4.50318600  | -0.54461200 | 1.74390200  |
| H | 4.07283100  | 0.77084200  | 2.84226200  |
| H | 4.22144600  | -0.87751700 | 3.46472100  |
| C | 0.01907900  | 4.31507800  | 0.09582000  |
| C | 0.34823400  | 5.59205900  | 0.55549500  |
| C | 0.46954900  | 3.93054800  | -1.17656600 |
| C | 1.11517300  | 6.46030400  | -0.23102500 |
| H | 0.01436900  | 5.92483600  | 1.53206000  |
| C | 1.23200000  | 4.78730300  | -1.96149600 |
| H | 0.22346800  | 2.93742900  | -1.53872400 |
| C | 1.56013200  | 6.06313600  | -1.48962000 |
| H | 1.36089300  | 7.44859000  | 0.14691700  |
| H | 1.57251200  | 4.46235600  | -2.94049200 |
| H | 2.15520800  | 6.73686100  | -2.09888900 |
| C | -1.25035600 | 3.84067700  | 2.27697900  |
| H | -1.81804100 | 3.07443100  | 2.80959800  |
| H | -0.39315400 | 4.11981600  | 2.89739500  |
| H | -1.89720600 | 4.71710100  | 2.16903800  |
| C | -4.57678300 | -0.89527100 | 0.38162500  |
| C | -5.51542400 | -0.06521600 | 1.00716200  |
| C | -4.38932600 | -2.18698700 | 0.88819300  |
| C | -6.23126400 | -0.50939200 | 2.12013500  |
| H | -5.66911300 | 0.94172700  | 0.63245200  |
| C | -5.09942300 | -2.63550000 | 2.00203800  |
| H | -3.67132300 | -2.84557300 | 0.41280800  |
| C | -6.02191000 | -1.79400100 | 2.62635200  |
| H | -6.94843000 | 0.15240200  | 2.59686700  |
| H | -4.92665800 | -3.63761800 | 2.38328400  |
| H | -6.57195000 | -2.13528500 | 3.49791700  |
| C | -4.55416000 | -0.81942000 | -2.12127600 |
| H | -4.69025400 | -1.90328900 | -2.15547500 |
| H | -5.54985800 | -0.36790000 | -2.14824100 |
| H | -4.00471100 | -0.51452500 | -3.01643000 |
| C | 3.76350600  | -5.22220800 | 1.11696500  |
| C | -4.67180000 | 4.38238100  | -2.14407700 |
| H | -4.17177100 | 5.35354300  | -2.18194300 |
| H | -4.86497000 | 4.05649000  | -3.17119200 |
| H | -5.64680500 | 4.52807700  | -1.66372800 |
| H | 4.55827400  | -4.98257300 | 0.40088000  |
| H | 4.23850300  | -5.33979000 | 2.09637700  |
| H | 3.33356500  | -6.18463400 | 0.82774000  |
| C | 5.12223300  | 0.56301600  | -0.77834300 |
| C | 0.19753900  | 1.65100700  | -4.07415900 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 1. 10803800  | 2. 26005200  | -4. 06868600 |
| H | -0. 05079600 | 1. 44386500  | -5. 12302900 |
| H | -0. 61563400 | 2. 24361500  | -3. 64675400 |
| F | 2. 34137000  | 2. 43618500  | 0. 56549800  |
| F | 5. 01611600  | 2. 33895300  | 0. 78027800  |
| F | 6. 45802000  | 0. 50356300  | -0. 63537700 |
| F | 5. 20639800  | -1. 24560800 | -2. 27249400 |

TS1(S)-D3

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | 3. 18195400  | -3. 16600000 | -1. 19107500 |
| C  | 1. 87859800  | -2. 68129400 | -1. 23063400 |
| C  | 1. 57819300  | -1. 39195700 | -1. 63742100 |
| C  | 2. 62766800  | -0. 59118500 | -2. 15483200 |
| C  | 3. 92389600  | -1. 09059100 | -2. 15994600 |
| C  | 2. 28448300  | 0. 74645600  | -2. 76496400 |
| H  | 1. 87832200  | 1. 40783800  | -1. 99204400 |
| H  | 3. 18803000  | 1. 22311100  | -3. 15271900 |
| C  | 1. 25128800  | 0. 60894400  | -3. 91797100 |
| H  | 1. 70509700  | -0. 00572100 | -4. 70338400 |
| H  | 1. 08780900  | 1. 60342700  | -4. 34840000 |
| C  | -0. 11236100 | 0. 00141400  | -3. 53587800 |
| C  | -1. 04701600 | 0. 80253000  | -2. 81107700 |
| H  | -0. 78524900 | 1. 83583100  | -2. 61498400 |
| H  | -2. 10798600 | 0. 59569400  | -2. 92126200 |
| Ni | -0. 13673400 | -0. 33113300 | -1. 45239900 |
| H  | 0. 50966200  | -1. 09077200 | -2. 59621200 |
| C  | 4. 21375900  | -2. 35554000 | -1. 65185300 |
| C  | -0. 64125400 | -1. 03735900 | -4. 51685800 |
| H  | 0. 07432700  | -1. 85341700 | -4. 67181200 |
| H  | -0. 82318500 | -0. 57017100 | -5. 49321900 |
| H  | -1. 58199600 | -1. 46167100 | -4. 16433100 |
| F  | 0. 88840000  | -3. 53348700 | -0. 85904700 |
| F  | 3. 45737300  | -4. 39673100 | -0. 71829500 |
| F  | 5. 48819800  | -2. 78610100 | -1. 58724700 |
| F  | 4. 95852500  | -0. 35587900 | -2. 62535600 |
| C  | -0. 62031600 | 0. 18141800  | 0. 29715700  |
| C  | -0. 89552400 | 1. 45682300  | 2. 27849900  |
| C  | -1. 69883400 | 0. 16819300  | 2. 40259200  |
| H  | -0. 01771600 | 1. 43168400  | 2. 92830400  |
| H  | -1. 47869600 | 2. 35233800  | 2. 48725700  |
| H  | -1. 50762300 | -0. 36547800 | 3. 33098900  |
| H  | -2. 77616500 | 0. 34442600  | 2. 30462900  |
| N  | -1. 20562100 | -0. 60048900 | 1. 23721800  |
| N  | -0. 48566600 | 1. 41367800  | 0. 85535600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.58302300 | -1.96867800 | 1.08022500  |
| C | -0.70608900 | -2.97657300 | 1.53821800  |
| C | -2.85113500 | -2.28183300 | 0.56849000  |
| C | -1.14458100 | -4.29838000 | 1.49322700  |
| C | -3.25295000 | -3.62448300 | 0.56053200  |
| C | -2.41700300 | -4.64153100 | 1.01723600  |
| H | -0.48486400 | -5.09105900 | 1.82857100  |
| H | -4.23930500 | -3.88032500 | 0.18495800  |
| C | 0.08218100  | 2.53242400  | 0.17119000  |
| C | 1.44109600  | 2.84962300  | 0.33880600  |
| C | -0.74984500 | 3.31063600  | -0.66199100 |
| C | 1.97890500  | 3.89525600  | -0.41967100 |
| C | -0.17112100 | 4.34925000  | -1.39120800 |
| C | 1.19709500  | 4.63732000  | -1.30433000 |
| H | 3.03400900  | 4.12787100  | -0.32476900 |
| H | -0.78903400 | 4.94876200  | -2.05066600 |
| C | -3.78318600 | -1.19507500 | 0.06377400  |
| C | 0.68541600  | -2.60813800 | 2.04031400  |
| C | 2.26521500  | 2.15795700  | 1.42085200  |
| C | -2.24506000 | 3.02129300  | -0.71883100 |
| H | -2.35233400 | 1.94042400  | -0.84194400 |
| H | -3.30447400 | -0.23721500 | 0.27338000  |
| H | 1.10212900  | -1.91222500 | 1.30535200  |
| H | 1.76681200  | 1.21313300  | 1.64274500  |
| C | -4.03007700 | -1.20479400 | -1.44503300 |
| C | -4.63953200 | -0.07699100 | -2.01819000 |
| C | -3.69716200 | -2.27052400 | -2.28669700 |
| C | -4.92154600 | -0.01864200 | -3.38108800 |
| H | -4.89450900 | 0.77144900  | -1.38949000 |
| C | -3.99053600 | -2.22222900 | -3.65293100 |
| H | -3.19926000 | -3.14316800 | -1.88179100 |
| C | -4.60354400 | -1.09969300 | -4.20708100 |
| H | -5.38789100 | 0.86944100  | -3.79728800 |
| H | -3.72830900 | -3.06605300 | -4.28447700 |
| H | -4.82465600 | -1.06252000 | -5.26927300 |
| C | -5.12146200 | -1.21477100 | 0.83473400  |
| H | -5.67545500 | -2.13793900 | 0.64289700  |
| H | -4.94371300 | -1.14032300 | 1.91190900  |
| H | -5.75732300 | -0.37815400 | 0.53194400  |
| C | 0.65622100  | -1.88428700 | 3.37874600  |
| C | -0.22243700 | -2.27054900 | 4.39837600  |
| C | 1.56405300  | -0.84981300 | 3.63421500  |
| C | -0.21503200 | -1.61774100 | 5.63224600  |
| H | -0.92946800 | -3.07356400 | 4.21250400  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 1. 57585600  | -0. 19410500 | 4. 86614500  |
| H | 2. 27255800  | -0. 56120800 | 2. 86344200  |
| C | 0. 67859800  | -0. 57040100 | 5. 86777200  |
| H | -0. 91088500 | -1. 92370500 | 6. 40804500  |
| H | 2. 28341900  | 0. 61061300  | 5. 04192300  |
| H | 0. 68021000  | -0. 05733700 | 6. 82460500  |
| C | 1. 65401400  | -3. 80016600 | 2. 14829100  |
| H | 1. 73031000  | -4. 33983500 | 1. 20397800  |
| H | 2. 64817500  | -3. 43174700 | 2. 41623500  |
| H | 1. 34223800  | -4. 49600100 | 2. 93344000  |
| C | 3. 69702500  | 1. 81081400  | 1. 04223000  |
| C | 4. 73016100  | 2. 75953500  | 1. 07865700  |
| C | 4. 02349500  | 0. 49108200  | 0. 70439600  |
| C | 6. 04348900  | 2. 40429900  | 0. 77161100  |
| H | 4. 51723100  | 3. 78397900  | 1. 36520600  |
| C | 5. 33996900  | 0. 12764300  | 0. 41313900  |
| H | 3. 23734800  | -0. 25707100 | 0. 66210600  |
| C | 6. 35355800  | 1. 08457000  | 0. 44061200  |
| H | 6. 82539700  | 3. 15744600  | 0. 80236500  |
| H | 5. 57639700  | -0. 89862800 | 0. 15543100  |
| H | 7. 37644000  | 0. 80303100  | 0. 21017000  |
| C | 2. 22386500  | 3. 02644800  | 2. 69927900  |
| H | 1. 19426900  | 3. 21112800  | 3. 01362700  |
| H | 2. 75748700  | 2. 53370400  | 3. 51711200  |
| H | 2. 68736100  | 4. 00121600  | 2. 52583000  |
| C | -2. 93444600 | 3. 39686400  | 0. 58732500  |
| C | -2. 56750900 | 4. 53880200  | 1. 31021200  |
| C | -3. 97753400 | 2. 60368500  | 1. 07866300  |
| C | -3. 21218200 | 4. 86395500  | 2. 50476400  |
| H | -1. 75722800 | 5. 16205500  | 0. 94476900  |
| C | -4. 62364000 | 2. 92122300  | 2. 27357500  |
| H | -4. 27590300 | 1. 71902900  | 0. 52619100  |
| C | -4. 23780200 | 4. 05239400  | 2. 99537200  |
| H | -2. 90776200 | 5. 74827500  | 3. 05696600  |
| H | -5. 42065600 | 2. 28213300  | 2. 64210700  |
| H | -4. 73167100 | 4. 30008100  | 3. 92995000  |
| C | -2. 97685800 | 3. 68774800  | -1. 89626500 |
| H | -2. 98426400 | 4. 77794200  | -1. 80172100 |
| H | -2. 51889100 | 3. 42095800  | -2. 85255400 |
| H | -4. 01779300 | 3. 35336300  | -1. 91225100 |
| C | -2. 85436700 | -6. 08508800 | 0. 98292700  |
| C | 1. 80803600  | 5. 72144500  | -2. 15686100 |
| H | 2. 05342800  | 5. 33970400  | -3. 15541400 |
| H | 1. 11839900  | 6. 56014700  | -2. 29147000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.73295300  | 6.10312700  | -1.71604100 |
| H | -2.67058200 | -6.57875600 | 1.94289500  |
| H | -3.91916200 | -6.17391600 | 0.75219000  |
| H | -2.29943900 | -6.64599600 | 0.22185900  |

TS1'-D3

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.82753200  | 0.72767800  | -0.46863200 |
| C  | 3.47482600  | 1.05560400  | -0.46989500 |
| C  | 2.49759700  | 0.23955400  | -1.01199700 |
| C  | 2.90313500  | -1.01185300 | -1.55689100 |
| C  | 4.25763400  | -1.33683600 | -1.55443600 |
| C  | 1.88831900  | -2.04759300 | -2.02023100 |
| H  | 1.26556400  | -2.29346200 | -1.15478100 |
| H  | 2.42671200  | -2.96065800 | -2.28905300 |
| C  | 0.94809700  | -1.70858400 | -3.20356600 |
| H  | 1.56489500  | -1.54462000 | -4.09842700 |
| H  | 0.35610400  | -2.60729100 | -3.39206600 |
| C  | -0.00625600 | -0.51657000 | -3.05263800 |
| C  | 0.55958300  | 0.75287200  | -3.31239600 |
| H  | 1.50104800  | 0.81559900  | -3.86087500 |
| H  | -0.10464000 | 1.60184000  | -3.46832200 |
| Ni | 0.52789900  | 0.33889400  | -1.24030500 |
| H  | 1.53545400  | 1.00522700  | -2.09600400 |
| C  | -0.52678800 | -0.03435000 | 0.27388800  |
| C  | -1.80753400 | 0.81570700  | 2.07464600  |
| C  | -1.38642600 | -0.61325500 | 2.40375900  |
| H  | -1.23213600 | 1.53748900  | 2.65996000  |
| H  | -2.87150800 | 0.99542100  | 2.21613800  |
| H  | -0.89454800 | -0.69674700 | 3.37081800  |
| H  | -2.23243300 | -1.30789200 | 2.36915400  |
| N  | -0.43347600 | -0.90622000 | 1.30652500  |
| N  | -1.43330500 | 0.91094600  | 0.64574800  |
| C  | 0.32500800  | -2.11753700 | 1.31514900  |
| C  | 1.66046400  | -2.09441700 | 1.77324500  |
| C  | -0.29466400 | -3.32228000 | 0.94318700  |
| C  | 2.35711000  | -3.30120800 | 1.83229500  |
| C  | 0.43960300  | -4.51109600 | 1.04619900  |
| C  | 1.76532300  | -4.51922100 | 1.47441100  |
| H  | 3.38762000  | -3.30592300 | 2.16874500  |
| H  | -0.03511700 | -5.45011000 | 0.77739000  |
| C  | -1.93634300 | 1.92492000  | -0.23022900 |
| C  | -1.31353600 | 3.18083900  | -0.30756100 |
| C  | -3.09788900 | 1.64522900  | -0.99002200 |
| C  | -1.86243900 | 4.15183800  | -1.15474800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.59208100 | 2.63636300  | -1.83701600 |
| C | -2.98855900 | 3.89766400  | -1.93275800 |
| H | -1.37794900 | 5.12152100  | -1.21694100 |
| H | -4.47536400 | 2.43722100  | -2.43391800 |
| C | -1.74127800 | -3.35942000 | 0.48355700  |
| C | 2.31251200  | -0.77308900 | 2.15273800  |
| C | -0.09743000 | 3.53016500  | 0.54115500  |
| C | -3.82097100 | 0.31381300  | -0.82931000 |
| H | -3.05566300 | -0.46668300 | -0.79075900 |
| H | -2.12223500 | -2.33898600 | 0.54438200  |
| H | 2.11951900  | -0.09883800 | 1.31799700  |
| H | 0.38699500  | 2.58719100  | 0.81675800  |
| C | -1.96406200 | -3.78984900 | -0.96694800 |
| C | -3.24207200 | -3.59764400 | -1.51823200 |
| C | -0.97883000 | -4.35526900 | -1.78146400 |
| C | -3.52783300 | -3.95416400 | -2.83379700 |
| H | -4.02670200 | -3.15654000 | -0.91131000 |
| C | -1.26308700 | -4.72310300 | -3.10031200 |
| H | 0.02377800  | -4.49699700 | -1.39799900 |
| C | -2.53450400 | -4.52328800 | -3.63420700 |
| H | -4.52262800 | -3.78243100 | -3.23386100 |
| H | -0.47870700 | -5.15962600 | -3.71174600 |
| H | -2.74977300 | -4.80323300 | -4.66072800 |
| C | -2.58767500 | -4.22268000 | 1.44640800  |
| H | -2.26730700 | -5.26790400 | 1.42036100  |
| H | -2.48602900 | -3.86021900 | 2.47373400  |
| H | -3.64612200 | -4.19260000 | 1.17312000  |
| C | 1.70076800  | -0.12359700 | 3.38115100  |
| C | 1.36872000  | -0.86424600 | 4.52145700  |
| C | 1.51323600  | 1.26417300  | 3.39776800  |
| C | 0.83552500  | -0.23470000 | 5.64771600  |
| H | 1.51157000  | -1.94131400 | 4.51553800  |
| C | 0.98249500  | 1.89696100  | 4.52265700  |
| H | 1.79439600  | 1.84205100  | 2.52115100  |
| C | 0.63379400  | 1.14764600  | 5.64893600  |
| H | 0.57370900  | -0.82315800 | 6.52235500  |
| H | 0.83636800  | 2.97294600  | 4.51907800  |
| H | 0.21396400  | 1.63747100  | 6.52227500  |
| C | 3.83666100  | -0.86192100 | 2.33033700  |
| H | 4.30943000  | -1.32163000 | 1.45994700  |
| H | 4.24962100  | 0.14328100  | 2.44739700  |
| H | 4.10383900  | -1.43853400 | 3.22180600  |
| C | 0.93602700  | 4.33684100  | -0.24133700 |
| C | 1.30188700  | 3.91567100  | -1.52821200 |



|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 1. 57182400  | 5. 46527100  | 0. 28478000  |
| C | 2. 27541200  | 4. 58595000  | -2. 26107800 |
| H | 0. 81704000  | 3. 04467800  | -1. 94980100 |
| C | 2. 55178200  | 6. 14482800  | -0. 44704900 |
| H | 1. 31514700  | 5. 82762600  | 1. 27355800  |
| C | 2. 90942200  | 5. 70885300  | -1. 72088800 |
| H | 2. 54236400  | 4. 23147600  | -3. 25281300 |
| H | 3. 03263400  | 7. 01764700  | -0. 01480900 |
| H | 3. 67057300  | 6. 23595800  | -2. 28830500 |
| C | -0. 55769300 | 4. 22648200  | 1. 83510800  |
| H | -1. 33069000 | 3. 63878700  | 2. 33357300  |
| H | 0. 27214300  | 4. 35377400  | 2. 53573300  |
| H | -0. 97908300 | 5. 21292400  | 1. 61703500  |
| C | -4. 59815600 | 0. 25648900  | 0. 48377400  |
| C | -5. 23492200 | 1. 38800500  | 1. 00906400  |
| C | -4. 71670900 | -0. 95433500 | 1. 17561700  |
| C | -5. 94875200 | 1. 31352900  | 2. 20611100  |
| H | -5. 15032700 | 2. 33647700  | 0. 48831300  |
| C | -5. 42613900 | -1. 03467800 | 2. 37405100  |
| H | -4. 23570700 | -1. 84111700 | 0. 77895100  |
| C | -6. 04153300 | 0. 10372400  | 2. 89765700  |
| H | -6. 42689900 | 2. 20429700  | 2. 60288700  |
| H | -5. 49091200 | -1. 98301400 | 2. 89927500  |
| H | -6. 58841800 | 0. 04886900  | 3. 83388400  |
| C | -4. 77380400 | -0. 03520100 | -1. 98711600 |
| H | -5. 15947900 | -1. 04839500 | -1. 84724200 |
| H | -5. 63386300 | 0. 64024000  | -2. 01531400 |
| H | -4. 26565300 | 0. 00486400  | -2. 95362800 |
| C | 2. 55836000  | -5. 80112900 | 1. 52992700  |
| C | -3. 54146800 | 4. 94243100  | -2. 87004500 |
| H | -4. 63509300 | 4. 97109400  | -2. 83457500 |
| H | -3. 16341300 | 5. 93795700  | -2. 62343600 |
| H | -3. 25764400 | 4. 72830200  | -3. 90745000 |
| H | 3. 21111000  | -5. 82787400 | 2. 40766700  |
| H | 1. 90291500  | -6. 67561400 | 1. 56174100  |
| H | 3. 20030200  | -5. 90087400 | 0. 64639600  |
| C | 5. 22508500  | -0. 47669800 | -1. 03311200 |
| C | -1. 47306000 | -0. 77433000 | -3. 27753600 |
| H | -1. 64549300 | -1. 14697800 | -4. 29945600 |
| H | -1. 86186700 | -1. 53377000 | -2. 59734300 |
| H | -2. 05181000 | 0. 14340600  | -3. 15270100 |
| F | 4. 69653300  | -2. 52151900 | -2. 04737600 |
| F | 6. 52559400  | -0. 82444300 | -1. 04417700 |
| F | 5. 74388300  | 1. 53501500  | 0. 09903100  |

|   |            |            |            |
|---|------------|------------|------------|
| F | 3.12980300 | 2.21553100 | 0.15646800 |
|---|------------|------------|------------|

TS4(R)-D3

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.44190900 | -1.71632300 | -1.91550000 |
| C  | -2.30561500 | -0.92079000 | -1.84958000 |
| C  | -1.02281800 | -1.41438100 | -1.93658200 |
| C  | -0.85768000 | -2.79750400 | -2.19563200 |
| C  | -1.99786700 | -3.60332600 | -2.22969700 |
| H  | 2.10511000  | -0.46864200 | -1.36466500 |
| C  | 0.45772000  | -3.48700700 | -2.57020700 |
| H  | 0.42096900  | -3.67245200 | -3.65268700 |
| H  | 0.46311500  | -4.48406400 | -2.12037000 |
| C  | 1.83008100  | -2.85065600 | -2.25372100 |
| H  | 2.01876200  | -2.89190400 | -1.17521200 |
| H  | 2.58977500  | -3.50379900 | -2.70677500 |
| C  | 2.08299800  | -1.42202400 | -2.74515400 |
| C  | 1.06477200  | -0.81000800 | -3.50959300 |
| H  | 0.28389200  | -1.38523200 | -3.98226100 |
| H  | 1.28625500  | 0.14829900  | -3.97615700 |
| Ni | 0.61843000  | -0.50002300 | -1.56564900 |
| C  | 0.39164600  | 0.33113800  | 0.18118800  |
| C  | 0.88818900  | 2.00470100  | 1.77232300  |
| C  | -0.02069700 | 0.96512600  | 2.40499700  |
| H  | 1.76503800  | 2.22188400  | 2.37930600  |
| H  | 0.37079400  | 2.94092800  | 1.54430400  |
| H  | 0.51889000  | 0.29072100  | 3.07503100  |
| H  | -0.84702600 | 1.41057500  | 2.94553600  |
| N  | -0.47937700 | 0.19911200  | 1.21386600  |
| N  | 1.25921000  | 1.31952200  | 0.51699400  |
| C  | -1.61092600 | -0.68531500 | 1.27501100  |
| C  | -1.41748400 | -2.08383600 | 1.18443500  |
| C  | -2.90539400 | -0.16239700 | 1.47745200  |
| C  | -2.53466600 | -2.91520700 | 1.17092600  |
| C  | -3.99226000 | -1.04531900 | 1.47496300  |
| C  | -3.83585700 | -2.41342000 | 1.28203800  |
| H  | -2.40013300 | -3.98614100 | 1.07682000  |
| H  | -4.98898900 | -0.63747500 | 1.61100400  |
| C  | 2.31905700  | 1.80183600  | -0.31438200 |
| C  | 3.64576500  | 1.63263200  | 0.10655500  |
| C  | 2.02381200  | 2.44413500  | -1.54082600 |
| C  | 4.68037400  | 2.08787000  | -0.72121900 |
| C  | 3.08681300  | 2.87078400  | -2.33276300 |
| C  | 4.42427400  | 2.69747200  | -1.94447800 |
| H  | 5.70791400  | 1.93207300  | -0.40396100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.88307300  | 3.35770800  | -3.27986900 |
| C | -3.16335900 | 1.28819300  | 1.87100700  |
| C | -0.01228300 | -2.66566700 | 1.20957200  |
| C | 4.00641000  | 0.97192600  | 1.43237400  |
| C | 0.57531500  | 2.69109400  | -1.94861800 |
| H | 0.04031400  | 1.73660200  | -1.87150900 |
| H | -2.30398400 | 1.88305600  | 1.54700900  |
| H | 0.55617700  | -2.19276500 | 0.40408100  |
| H | 3.09072500  | 0.54168200  | 1.84673900  |
| C | -4.38672900 | 1.94302600  | 1.22548600  |
| C | -5.08869100 | 2.96258200  | 1.88814400  |
| C | -4.79423500 | 1.60930200  | -0.07275600 |
| C | -6.14989800 | 3.62899300  | 1.27224300  |
| H | -4.80999000 | 3.25523400  | 2.89355800  |
| C | -5.85658300 | 2.27030000  | -0.68923100 |
| H | -4.28337200 | 0.82476500  | -0.60642600 |
| C | -6.54029300 | 3.28711400  | -0.02232600 |
| H | -6.67164800 | 4.41522400  | 1.81035300  |
| H | -6.14806200 | 1.98295200  | -1.69540700 |
| H | -7.36692900 | 3.80293700  | -0.50162900 |
| C | -3.25050600 | 1.33816600  | 3.41802800  |
| H | -2.49032300 | 0.70158500  | 3.87511500  |
| H | -3.11799000 | 2.35265300  | 3.80397500  |
| H | -4.22460600 | 0.96752800  | 3.75010000  |
| C | 0.68317600  | -2.31230600 | 2.51887700  |
| C | -0.00135000 | -2.31611500 | 3.74104300  |
| C | 2.04128600  | -1.98454900 | 2.51668600  |
| C | 0.65600100  | -1.97690700 | 4.92500900  |
| H | -1.05828400 | -2.56392600 | 3.75935400  |
| C | 2.70466600  | -1.64092200 | 3.69531400  |
| H | 2.58415200  | -1.98840500 | 1.58025400  |
| C | 2.00964000  | -1.62947000 | 4.90632100  |
| H | 0.10817300  | -1.97619900 | 5.86296200  |
| H | 3.75805500  | -1.37798000 | 3.65855300  |
| H | 2.51631400  | -1.35524500 | 5.82673800  |
| C | 0.05314500  | -4.18415100 | 0.98130400  |
| H | -0.44173900 | -4.47119800 | 0.05062000  |
| H | 1.09976300  | -4.49684600 | 0.92671500  |
| H | -0.41177000 | -4.73284400 | 1.80605900  |
| C | 4.95553700  | -0.20281200 | 1.22111300  |
| C | 4.54783700  | -1.23932800 | 0.36777400  |
| C | 6.19691100  | -0.31748200 | 1.85372800  |
| C | 5.34515300  | -2.36085600 | 0.15975400  |
| H | 3.59077400  | -1.14831900 | -0.13604400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 7.00590200  | -1.43993000 | 1.64267300  |
| H | 6.54589700  | 0.46514400  | 2.51770200  |
| C | 6.58411300  | -2.46577400 | 0.79938400  |
| H | 5.00166200  | -3.15152200 | -0.50121400 |
| H | 7.96727300  | -1.50759300 | 2.14336500  |
| H | 7.21099500  | -3.33769000 | 0.64009000  |
| C | 4.52943300  | 2.01788700  | 2.42957500  |
| H | 4.69602800  | 1.57362400  | 3.41544800  |
| H | 5.46991100  | 2.45955700  | 2.08656600  |
| H | 3.81085400  | 2.83390400  | 2.54092200  |
| C | -0.10307400 | 3.66374800  | -0.99253500 |
| C | 0.57444000  | 4.79341900  | -0.51629600 |
| C | -1.43122300 | 3.45856400  | -0.60045400 |
| C | -0.05746300 | 5.69508700  | 0.34084200  |
| H | 1.60797200  | 4.95610700  | -0.80725900 |
| C | -2.06923000 | 4.36410800  | 0.25054500  |
| H | -1.96196800 | 2.57980900  | -0.95165200 |
| C | -1.38222200 | 5.48166200  | 0.72842100  |
| H | 0.48503700  | 6.56219100  | 0.70671600  |
| H | -3.09900600 | 4.18971100  | 0.54314400  |
| H | -1.87608500 | 6.18098000  | 1.39658400  |
| C | 0.39717000  | 3.17206800  | -3.39689100 |
| H | -0.67000400 | 3.24534200  | -3.62192700 |
| H | 0.83701400  | 4.16189400  | -3.55380000 |
| H | 0.84891500  | 2.47380500  | -4.10823700 |
| C | -5.02669400 | -3.32928000 | 1.16736100  |
| C | 5.54523700  | 3.15215700  | -2.84545600 |
| H | 6.51197800  | 3.09304500  | -2.33905300 |
| H | 5.60160200  | 2.53079900  | -3.74692000 |
| H | 5.39541200  | 4.18521100  | -3.17659700 |
| H | -5.91570600 | -2.89068800 | 1.62858400  |
| H | -5.25474400 | -3.51799000 | 0.11286200  |
| H | -4.83428800 | -4.29859800 | 1.63765800  |
| C | -3.28026200 | -3.08416700 | -2.09065300 |
| C | 3.53218000  | -1.04411100 | -3.00791600 |
| H | 3.86581400  | -1.56701600 | -3.91382000 |
| H | 3.62717500  | 0.03150400  | -3.17329800 |
| H | 4.20131800  | -1.32494700 | -2.19448500 |
| F | -2.49528800 | 0.42364300  | -1.68239200 |
| F | -4.68491200 | -1.20755900 | -1.78281800 |
| F | -4.35909800 | -3.89525200 | -2.11892800 |
| F | -1.88868400 | -4.94437000 | -2.41813300 |

TS6-D3

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 5.58887600  | 0.07705500  | -1.34696200 |
| C  | 4.66722400  | 0.97234100  | -0.81300200 |
| C  | 3.44226300  | 1.18936300  | -1.42101100 |
| C  | 3.10942500  | 0.51820800  | -2.60675500 |
| C  | 4.04581600  | -0.36368800 | -3.13934800 |
| C  | 1.76363000  | 0.69808800  | -3.26148600 |
| H  | 1.88686500  | 0.67689600  | -4.35116300 |
| H  | 1.37987600  | 1.68910500  | -3.00092300 |
| C  | 0.71065600  | -0.35264300 | -2.81532400 |
| H  | 1.17245700  | -0.39155700 | -1.24387100 |
| H  | -0.24319700 | -0.02840600 | -3.29116600 |
| C  | 1.00831400  | -1.75752900 | -3.27718900 |
| C  | 1.45579800  | -2.71328500 | -2.45105300 |
| H  | 1.58670100  | -2.52044400 | -1.39282800 |
| H  | 1.69222700  | -3.71147500 | -2.81124200 |
| Ni | -0.22234800 | -0.13781700 | -1.13864600 |
| H  | 2.73490600  | 1.86592000  | -0.95713400 |
| C  | -1.03862800 | 0.04458900  | 0.55589700  |
| C  | -2.50289800 | -0.27187400 | 2.39654200  |
| C  | -1.53902200 | 0.88770700  | 2.71520100  |
| H  | -3.54800800 | 0.05167800  | 2.38666500  |
| H  | -2.40416100 | -1.10858600 | 3.08946000  |
| H  | -2.05296900 | 1.84205600  | 2.84683600  |
| H  | -0.93864500 | 0.68730000  | 3.60594100  |
| N  | -0.68566100 | 0.93660900  | 1.50617300  |
| N  | -2.07366900 | -0.67505700 | 1.03852800  |
| C  | 0.39562000  | 1.86110200  | 1.35305700  |
| C  | 0.27055800  | 2.95274200  | 0.46675500  |
| C  | 1.58077900  | 1.66014600  | 2.07857500  |
| C  | 1.34457900  | 3.83809300  | 0.34945400  |
| C  | 2.62437100  | 2.57760400  | 1.93679300  |
| C  | 2.52702300  | 3.67309300  | 1.08058800  |
| H  | 1.26826200  | 4.67831500  | -0.33144600 |
| H  | 3.55321000  | 2.39852700  | 2.46948000  |
| C  | -2.70206800 | -1.72244000 | 0.29321300  |
| C  | -3.91818100 | -1.46939500 | -0.35434100 |
| C  | -2.07397200 | -2.98514200 | 0.18806000  |
| C  | -4.52501700 | -2.49795200 | -1.08516000 |
| C  | -2.71376500 | -3.97830300 | -0.55080600 |
| C  | -3.94503600 | -3.75918000 | -1.18664600 |
| H  | -5.45634500 | -2.29527700 | -1.60668800 |
| H  | -2.24765600 | -4.95249500 | -0.64768300 |
| C  | 1.78355400  | 0.44297400  | 2.97278300  |
| C  | -1.01228000 | 3.14974000  | -0.32342600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.54148300 | -0.08407600 | -0.35216700 |
| C | -0.72905500 | -3.22481100 | 0.85703400  |
| H | -0.09043600 | -2.38156600 | 0.57057900  |
| H | 0.89265500  | -0.18110400 | 2.88290100  |
| H | -1.27004600 | 2.17145800  | -0.74695500 |
| H | -3.94850300 | 0.54194100  | 0.32023400  |
| C | 2.94059100  | -0.40011400 | 2.44618900  |
| C | 4.14733600  | -0.56738300 | 3.13129800  |
| C | 2.78339200  | -1.03267600 | 1.20312000  |
| C | 5.17622800  | -1.34066000 | 2.58337700  |
| H | 4.29804700  | -0.09305200 | 4.09519500  |
| C | 3.80137400  | -1.81217400 | 0.66117900  |
| H | 1.86449300  | -0.88225900 | 0.64160900  |
| C | 5.00873300  | -1.96530900 | 1.34835600  |
| H | 6.11042800  | -1.45133800 | 3.12634600  |
| H | 3.66091500  | -2.27583600 | -0.31050100 |
| H | 5.81151300  | -2.55726100 | 0.92010800  |
| C | 1.91477500  | 0.85181600  | 4.44614900  |
| H | 2.77238300  | 1.51083100  | 4.61026200  |
| H | 1.02068200  | 1.39340700  | 4.76783900  |
| H | 2.03170800  | -0.02680900 | 5.08761400  |
| C | -2.17500500 | 3.56871700  | 0.56755900  |
| C | -1.99000400 | 4.27035200  | 1.76442600  |
| C | -3.48182500 | 3.27072700  | 0.16275500  |
| C | -3.08489500 | 4.64104100  | 2.54965800  |
| H | -0.98435500 | 4.51467300  | 2.09143800  |
| C | -4.57695400 | 3.63431500  | 0.94503600  |
| H | -3.63881500 | 2.74946200  | -0.77406900 |
| C | -4.38217900 | 4.31709100  | 2.14830700  |
| H | -2.92171900 | 5.18013200  | 3.47846300  |
| H | -5.58075100 | 3.38585600  | 0.61200600  |
| H | -5.23175700 | 4.59829400  | 2.76328000  |
| C | -0.88068000 | 4.10896000  | -1.51779600 |
| H | -0.05961600 | 3.80398200  | -2.17472500 |
| H | -1.80616800 | 4.09205500  | -2.09951800 |
| H | -0.70649600 | 5.14072500  | -1.19749700 |
| C | -4.39781100 | 0.57301700  | -1.72329100 |
| C | -5.39560900 | 1.38176000  | -2.27833600 |
| C | -3.18040100 | 0.45832600  | -2.41390900 |
| C | -5.17402800 | 2.07789400  | -3.47079700 |
| H | -6.35096600 | 1.48876300  | -1.77703400 |
| C | -2.95204700 | 1.15610000  | -3.59654000 |
| H | -2.40589700 | -0.19566600 | -2.01735200 |
| C | -3.95016300 | 1.97626500  | -4.13035900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.96202200 | 2.70379600  | -3.87913600 |
| H | -1.99514200 | 1.05951600  | -4.10173100 |
| H | -3.77606800 | 2.52272000  | -5.05210600 |
| C | -5.97255900 | -0.10196600 | 0.20314300  |
| H | -5.98817200 | -0.61789100 | 1.16702700  |
| H | -6.34630100 | 0.91309500  | 0.36266800  |
| H | -6.66623300 | -0.61844600 | -0.46701900 |
| C | -0.83444000 | -3.21384200 | 2.37604200  |
| C | -1.97271800 | -3.68125100 | 3.04342700  |
| C | 0.24801500  | -2.75691300 | 3.13714800  |
| C | -2.03876000 | -3.66250900 | 4.43853100  |
| H | -2.81876200 | -4.04164400 | 2.46614400  |
| C | 0.18431900  | -2.73070200 | 4.53026100  |
| H | 1.14685500  | -2.42176800 | 2.63036900  |
| C | -0.96463600 | -3.17719300 | 5.18740800  |
| H | -2.93315400 | -4.02122300 | 4.93978900  |
| H | 1.03254800  | -2.36220500 | 5.09986500  |
| H | -1.02021500 | -3.15265500 | 6.27151800  |
| C | -0.01315900 | -4.50328600 | 0.39129300  |
| H | 0.98608000  | -4.53922900 | 0.83374400  |
| H | -0.54783400 | -5.40450600 | 0.70734600  |
| H | 0.09451400  | -4.51835200 | -0.69676000 |
| C | 3.68976100  | 4.61824800  | 0.91228800  |
| C | -4.61358900 | -4.87014500 | -1.95746100 |
| H | -5.43451600 | -4.49098000 | -2.57149100 |
| H | -3.90245700 | -5.38158900 | -2.61397600 |
| H | -5.02664500 | -5.62625900 | -1.27907300 |
| H | 3.45565600  | 5.42025200  | 0.20752900  |
| H | 3.97249400  | 5.07668400  | 1.86627200  |
| H | 4.56589400  | 4.07714200  | 0.54062900  |
| C | 5.27157300  | -0.59663900 | -2.51956600 |
| C | 0.78781800  | -2.03442000 | -4.74519500 |
| H | 1.40591300  | -1.37553300 | -5.36482900 |
| H | 1.02875600  | -3.06872100 | -5.00634100 |
| H | -0.25749300 | -1.84312500 | -5.01970300 |
| F | 5.00018200  | 1.60624000  | 0.32926500  |
| F | 6.75631800  | -0.15888500 | -0.72989000 |
| F | 6.14607800  | -1.46604900 | -3.04871700 |
| F | 3.79466700  | -1.01980400 | -4.29158300 |

### TS8-D3

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.66496700 | -1.64043400 | -1.47469300 |
| C | -2.29787700 | -1.60069300 | -1.64108800 |
| C | -1.63335100 | -0.47849900 | -2.18445500 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.43839400 | 0.54055100  | -2.76948800 |
| C  | -3.82460700 | 0.49719500  | -2.56162300 |
| C  | -1.88835800 | 1.70545700  | -3.56921200 |
| H  | -1.74235000 | 2.56868100  | -2.91137500 |
| H  | -2.66874700 | 2.01335600  | -4.27277800 |
| C  | -0.60126700 | 1.44350600  | -4.36178400 |
| H  | -0.69516300 | 0.50891700  | -4.92148800 |
| H  | -0.48537800 | 2.24096500  | -5.10984700 |
| C  | 0.66558200  | 1.39905200  | -3.53751100 |
| C  | 0.80680500  | 2.09184100  | -2.37824000 |
| H  | 0.04010000  | 2.75010700  | -1.98769500 |
| H  | 1.77767600  | 2.12929200  | -1.90458600 |
| Ni | 0.08886100  | 0.12333600  | -1.49429300 |
| C  | 0.34692700  | -0.00261200 | 0.39299200  |
| C  | 1.70330700  | -0.09665300 | 2.34091000  |
| C  | 0.25035000  | 0.03944100  | 2.75799800  |
| H  | 2.07172700  | -1.11500600 | 2.50197400  |
| H  | 2.36638600  | 0.61150700  | 2.83347500  |
| H  | -0.05442300 | -0.68113900 | 3.51242700  |
| H  | 0.02137600  | 1.05145100  | 3.11166600  |
| N  | -0.44834900 | -0.20743400 | 1.47189500  |
| N  | 1.60472600  | 0.18173500  | 0.89187400  |
| C  | -1.87105200 | -0.31577600 | 1.48134500  |
| C  | -2.44488100 | -1.59422100 | 1.64310900  |
| C  | -2.65777500 | 0.84892100  | 1.46100200  |
| C  | -3.83213400 | -1.68058200 | 1.75319400  |
| C  | -4.04528000 | 0.70611200  | 1.58636000  |
| C  | -4.64825100 | -0.54589700 | 1.70380600  |
| H  | -4.30176300 | -2.65232800 | 1.84659600  |
| H  | -4.67414900 | 1.59024600  | 1.60653600  |
| C  | 2.77555400  | 0.37672500  | 0.09994600  |
| C  | 3.46672100  | -0.72594100 | -0.42239400 |
| C  | 3.24238300  | 1.69604600  | -0.10479400 |
| C  | 4.60869600  | -0.49069900 | -1.19882600 |
| C  | 4.38957800  | 1.87983100  | -0.87390700 |
| C  | 5.08080400  | 0.79743500  | -1.43856600 |
| H  | 5.13131000  | -1.33794200 | -1.63204900 |
| H  | 4.75566100  | 2.88409600  | -1.05813800 |
| C  | -2.01298800 | 2.22546500  | 1.42086100  |
| C  | -1.56010100 | -2.83724300 | 1.66151600  |
| C  | 3.03522100  | -2.15961100 | -0.12154500 |
| C  | 2.47588300  | 2.87094100  | 0.49212100  |
| H  | 1.41487200  | 2.65663100  | 0.33348600  |
| H  | -0.93292700 | 2.07391200  | 1.41726100  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.82891400 | -2.70165400 | 0.86304800  |
| H | 2.03485200  | -2.11326700 | 0.31422300  |
| C | -2.30572800 | 3.10064800  | 0.20387300  |
| C | -1.35266200 | 4.07341700  | -0.13647500 |
| C | -3.49062600 | 3.05806700  | -0.53710700 |
| C | -1.57562600 | 4.98407000  | -1.16784200 |
| H | -0.42044600 | 4.11960700  | 0.41910900  |
| C | -3.72262500 | 3.97120300  | -1.56846800 |
| H | -4.23186900 | 2.29757000  | -0.33266300 |
| C | -2.77197800 | 4.94036900  | -1.88732800 |
| H | -0.81560100 | 5.72083000  | -1.41030400 |
| H | -4.64993400 | 3.91439500  | -2.13110100 |
| H | -2.95480900 | 5.64530100  | -2.69242300 |
| C | -2.35324000 | 3.01005700  | 2.71022500  |
| H | -3.42405500 | 3.22463900  | 2.76841800  |
| H | -2.07089800 | 2.43464500  | 3.59736300  |
| H | -1.82030400 | 3.96547800  | 2.72873700  |
| C | -0.77606200 | -2.99729500 | 2.95439000  |
| C | -1.36837700 | -2.78347500 | 4.20501400  |
| C | 0.56225000  | -3.40504100 | 2.90617200  |
| C | -0.63168300 | -2.94916800 | 5.37885400  |
| H | -2.40425100 | -2.46039700 | 4.25280700  |
| C | 1.30361700  | -3.57113400 | 4.07668600  |
| H | 1.02603900  | -3.58462500 | 1.93979200  |
| C | 0.70940500  | -3.33663600 | 5.31845600  |
| H | -1.10222700 | -2.76897600 | 6.34106800  |
| H | 2.34465700  | -3.87525800 | 4.01749000  |
| H | 1.28487600  | -3.45679300 | 6.23129200  |
| C | -2.31839700 | -4.14436500 | 1.36878900  |
| H | -2.88348300 | -4.06721500 | 0.43984400  |
| H | -1.60039300 | -4.96418100 | 1.27749500  |
| H | -3.00391100 | -4.40032800 | 2.18280100  |
| C | 2.91218200  | -2.97592000 | -1.39994000 |
| C | 3.95285900  | -3.76189300 | -1.90935400 |
| C | 1.71707200  | -2.89695700 | -2.12404800 |
| C | 3.80547700  | -4.43544500 | -3.12495200 |
| H | 4.88479500  | -3.85761900 | -1.36130100 |
| C | 1.56797400  | -3.56140800 | -3.33987100 |
| H | 0.89503300  | -2.30724500 | -1.73677000 |
| C | 2.61573700  | -4.33330900 | -3.84759100 |
| H | 4.62297800  | -5.04141400 | -3.50516200 |
| H | 0.63298900  | -3.46657600 | -3.88271900 |
| H | 2.50476200  | -4.85547000 | -4.79338400 |
| C | 3.97436400  | -2.78482500 | 0.92557500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.95117200  | -2.20639300 | 1.85318800  |
| H | 3.67314900  | -3.81286900 | 1.14968100  |
| H | 5.01157500  | -2.79959200 | 0.57909000  |
| C | 2.68034500  | 2.99103700  | 1.99689900  |
| C | 3.93043500  | 2.76459400  | 2.58530000  |
| C | 1.60997500  | 3.36014600  | 2.82011500  |
| C | 4.09884300  | 2.88048200  | 3.96597800  |
| H | 4.76798100  | 2.47251200  | 1.95909700  |
| C | 1.77213100  | 3.47467900  | 4.20098400  |
| H | 0.63584600  | 3.54616100  | 2.37863500  |
| C | 3.01860600  | 3.22879600  | 4.78001500  |
| H | 5.07293300  | 2.69091800  | 4.40719300  |
| H | 0.92431500  | 3.74790600  | 4.82215800  |
| H | 3.14750100  | 3.30845100  | 5.85501800  |
| C | 2.77623600  | 4.22454500  | -0.17573200 |
| H | 2.10914100  | 4.98800700  | 0.23427000  |
| H | 3.80216600  | 4.55011500  | 0.01984400  |
| H | 2.62349900  | 4.18057300  | -1.25768300 |
| C | -6.14911200 | -0.68274000 | 1.71231500  |
| C | 6.29751600  | 1.03581300  | -2.29783200 |
| H | 6.81652100  | 0.10039000  | -2.52112400 |
| H | 6.01876900  | 1.49929400  | -3.25134300 |
| H | 7.00533900  | 1.71153300  | -1.80645800 |
| H | -6.63436400 | 0.21170000  | 2.11354800  |
| H | -6.50709800 | -0.82459700 | 0.68632900  |
| H | -6.47219800 | -1.54674600 | 2.30003900  |
| C | -4.43168000 | -0.56106500 | -1.91049200 |
| C | 1.82137500  | 0.64063500  | -4.13727500 |
| H | 2.08805500  | 1.06375100  | -5.11494100 |
| H | 2.70387900  | 0.67238000  | -3.49233900 |
| H | 1.54383700  | -0.40559000 | -4.29941100 |
| F | -1.56315300 | -2.67818800 | -1.27389100 |
| F | -4.26669800 | -2.71965700 | -0.93207500 |
| F | -5.77403800 | -0.59021400 | -1.71408000 |
| H | -4.44979900 | 1.30078400  | -2.93566600 |
| F | -0.47812000 | -1.06061700 | -3.15128100 |

TS1(R)<sub>H</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.02964400 | -4.97630500 | -1.00626400 |
| C | 0.45316700  | -3.66396500 | -0.95824200 |
| C | -0.21561800 | -2.60441600 | -1.59700200 |
| C | -1.38149800 | -2.92080200 | -2.34704900 |
| C | -1.86242500 | -4.23652000 | -2.38776100 |
| C | -2.06518500 | -1.83302200 | -3.15742500 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -2.46240900 | -1.05727300 | -2.49248400 |
| H  | -2.92410000 | -2.25516900 | -3.69273200 |
| C  | -1.12678400 | -1.15444200 | -4.19105200 |
| H  | -0.76816700 | -1.92639200 | -4.88356200 |
| H  | -1.71188500 | -0.44288600 | -4.78652300 |
| C  | 0.08880500  | -0.42754200 | -3.58225900 |
| C  | -0.10347700 | 0.81117900  | -2.87007000 |
| H  | -1.10130900 | 1.23924200  | -2.80140200 |
| H  | 0.70093400  | 1.54233400  | -2.91178400 |
| Ni | 0.09234500  | -0.60836600 | -1.49261100 |
| H  | 0.38457700  | -1.55592900 | -2.62444400 |
| C  | 0.01742300  | 0.15183500  | 0.23366300  |
| C  | 0.81061200  | 1.18905600  | 2.21725500  |
| C  | -0.69689700 | 0.98872200  | 2.33798900  |
| H  | 1.35805100  | 0.50021100  | 2.87016900  |
| H  | 1.12794000  | 2.21020300  | 2.43163400  |
| H  | -0.98693900 | 0.48250400  | 3.25858000  |
| H  | -1.24557800 | 1.93653300  | 2.26902600  |
| N  | -0.98681900 | 0.14122200  | 1.15487100  |
| N  | 1.05157000  | 0.84509700  | 0.79577600  |
| C  | -2.29230800 | -0.44521800 | 1.02020700  |
| C  | -2.51414600 | -1.75052000 | 1.52813000  |
| C  | -3.36558900 | 0.32289300  | 0.51852900  |
| C  | -3.81162400 | -2.26712200 | 1.48519700  |
| C  | -4.65246800 | -0.23685500 | 0.53482600  |
| C  | -4.89549200 | -1.52837500 | 0.99699600  |
| H  | -3.99607200 | -3.27135300 | 1.85156900  |
| H  | -5.48989800 | 0.35785300  | 0.18118100  |
| C  | 2.27185300  | 1.24474800  | 0.14876200  |
| C  | 3.41277700  | 0.41759300  | 0.18619900  |
| C  | 2.34067200  | 2.52948200  | -0.45015900 |
| C  | 4.60390500  | 0.88299800  | -0.38786200 |
| C  | 3.55020400  | 2.93643200  | -1.01978600 |
| C  | 4.69542800  | 2.13137200  | -0.99857900 |
| H  | 5.47917700  | 0.23952700  | -0.36147900 |
| H  | 3.61210200  | 3.91144100  | -1.49286000 |
| C  | -3.19125500 | 1.76649000  | 0.05738700  |
| C  | -1.37158100 | -2.57243700 | 2.12703600  |
| C  | 3.42563000  | -0.94714200 | 0.88001000  |
| C  | 1.13511800  | 3.46820900  | -0.45700900 |
| H  | 0.24355400  | 2.83623600  | -0.49404600 |
| H  | -2.13212100 | 2.01550400  | 0.16551500  |
| H  | -0.49515900 | -2.39825500 | 1.49639600  |
| H  | 2.38387900  | -1.27140700 | 0.97949300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.53819900 | 2.06342900  | -1.41074800 |
| C | -3.16384100 | 3.31551300  | -1.93077400 |
| C | -4.20587100 | 1.17920800  | -2.26752200 |
| C | -3.45286200 | 3.67547000  | -3.24601300 |
| H | -2.63296500 | 4.02122000  | -1.29670200 |
| C | -4.49867400 | 1.53541300  | -3.58887700 |
| H | -4.49674600 | 0.19743700  | -1.91417200 |
| C | -4.12797900 | 2.78413900  | -4.08455500 |
| H | -3.14805800 | 4.65018600  | -3.61675900 |
| H | -5.01811300 | 0.82708100  | -4.22839700 |
| H | -4.35622600 | 3.05989900  | -5.10996700 |
| C | -3.98475400 | 2.71536500  | 0.99389700  |
| H | -5.06194600 | 2.54552200  | 0.90608300  |
| H | -3.70182300 | 2.55464400  | 2.03889700  |
| H | -3.79380900 | 3.76313000  | 0.74460800  |
| C | -1.00246900 | -2.15107900 | 3.55195800  |
| C | -1.97664400 | -1.82439900 | 4.50681700  |
| C | 0.34158900  | -2.16142400 | 3.95320000  |
| C | -1.61685400 | -1.50788700 | 5.81898100  |
| H | -3.02409600 | -1.80936100 | 4.21913500  |
| C | 0.70559300  | -1.84737400 | 5.26454000  |
| H | 1.10965100  | -2.42315900 | 3.22918500  |
| C | -0.27405300 | -1.51600600 | 6.20329100  |
| H | -2.38783200 | -1.25383900 | 6.54137700  |
| H | 1.75364700  | -1.85971400 | 5.55105800  |
| H | 0.00567100  | -1.26738300 | 7.22296700  |
| C | -1.63277600 | -4.09422300 | 2.11665200  |
| H | -1.89765100 | -4.44545400 | 1.11654900  |
| H | -0.72538200 | -4.61885100 | 2.42960800  |
| H | -2.42612100 | -4.37514600 | 2.81675100  |
| C | 4.14449300  | -2.00224400 | 0.03073000  |
| C | 5.24962300  | -2.73012000 | 0.49012100  |
| C | 3.68145100  | -2.26014100 | -1.27101800 |
| C | 5.87362700  | -3.68336600 | -0.32281500 |
| H | 5.63871500  | -2.56263200 | 1.48840000  |
| C | 4.29883300  | -3.20957100 | -2.08278000 |
| H | 2.82155500  | -1.71059500 | -1.64522800 |
| C | 5.40302700  | -3.92666400 | -1.61191100 |
| H | 6.72996000  | -4.23304500 | 0.05838100  |
| H | 3.91585500  | -3.39206200 | -3.08316000 |
| H | 5.88699000  | -4.66635700 | -2.24326400 |
| C | 4.00845100  | -0.80638300 | 2.30093700  |
| H | 3.45602200  | -0.05541200 | 2.87016900  |
| H | 3.95387100  | -1.75259300 | 2.84885500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 5.05511300  | -0.48681900 | 2.27103400  |
| C | 1.02651600  | 4.33011000  | 0.80751900  |
| C | 2.15217700  | 4.82618700  | 1.48090000  |
| C | -0.24177100 | 4.69990200  | 1.28164100  |
| C | 2.01297500  | 5.66009900  | 2.59335900  |
| H | 3.14536000  | 4.55183500  | 1.13898600  |
| C | -0.38581200 | 5.53312900  | 2.39227800  |
| H | -1.12818700 | 4.33184500  | 0.77115200  |
| C | 0.74454100  | 6.01702700  | 3.05461400  |
| H | 2.89995800  | 6.02931100  | 3.10091700  |
| H | -1.37955300 | 5.80093900  | 2.74043600  |
| H | 0.63766800  | 6.66282400  | 3.92133300  |
| C | 1.07810600  | 4.38926800  | -1.69756900 |
| H | 0.12144400  | 4.91940000  | -1.71744400 |
| H | 1.86682500  | 5.14726000  | -1.68056800 |
| H | 1.16978200  | 3.81388700  | -2.62334200 |
| C | -6.28325700 | -2.12373300 | 0.96329000  |
| C | 5.98090600  | 2.59767100  | -1.64049900 |
| H | 6.84541300  | 2.06277900  | -1.23745700 |
| H | 5.96524200  | 2.42597800  | -2.72390100 |
| H | 6.13913300  | 3.66974300  | -1.48646700 |
| H | -6.41014100 | -2.77675300 | 0.09101600  |
| H | -6.47879300 | -2.73235500 | 1.85174000  |
| H | -7.05070000 | -1.34666300 | 0.90534200  |
| C | -1.19761200 | -5.26501100 | -1.71521700 |
| C | 1.37533500  | -0.56557600 | -4.39848900 |
| H | 1.65355700  | -1.61403200 | -4.55658300 |
| H | 1.24009200  | -0.10998300 | -5.38782800 |
| H | 2.21222000  | -0.05954000 | -3.90829800 |
| H | 0.50324200  | -5.77073200 | -0.48828200 |
| H | 1.37056000  | -3.47005500 | -0.40920600 |
| H | -1.57743800 | -6.28247900 | -1.76120600 |
| H | -2.75792900 | -4.46112300 | -2.96505800 |

TS1(S)<sub>H</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.24505900  | -4.67146700 | -2.24348300 |
| C | -0.31649700 | -3.45678700 | -1.83394000 |
| C | 0.23998000  | -2.22061500 | -2.21007400 |
| C | 1.35787700  | -2.24406200 | -3.08701600 |
| C | 1.91287800  | -3.46268700 | -3.50066800 |
| C | 1.87821900  | -0.92545800 | -3.62740000 |
| H | 2.22910700  | -0.29420500 | -2.80079600 |
| H | 2.74242700  | -1.09775000 | -4.27953200 |
| C | 0.80315700  | -0.14287000 | -4.43356900 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 0.54013800  | -0.74289700 | -5.31318300 |
| H  | 1.25140100  | 0.78500200  | -4.80882100 |
| C  | -0.49156900 | 0.19595200  | -3.66061700 |
| C  | -0.49206800 | 1.30440900  | -2.73622600 |
| H  | 0.40974100  | 1.90513900  | -2.64543700 |
| H  | -1.42099900 | 1.85847800  | -2.61255400 |
| Ni | -0.28062900 | -0.32819800 | -1.62865500 |
| H  | -0.51829400 | -1.07964400 | -2.92310200 |
| C  | 1.37070900  | -4.67694400 | -3.07043200 |
| C  | -1.77304800 | -0.05999200 | -4.45490600 |
| H  | -1.84332500 | -1.10058700 | -4.79338700 |
| H  | -1.78722300 | 0.57606100  | -5.34935500 |
| H  | -2.66200800 | 0.16849000  | -3.86330300 |
| C  | -0.14882100 | 0.18005100  | 0.19217300  |
| C  | 0.48167900  | 1.20753300  | 2.24115400  |
| C  | -0.90403500 | 0.59589100  | 2.40623900  |
| H  | 1.23543000  | 0.63943900  | 2.79613900  |
| H  | 0.53035800  | 2.25379800  | 2.54418500  |
| H  | -0.98896800 | -0.03716300 | 3.28942900  |
| H  | -1.69046700 | 1.36085200  | 2.44132400  |
| N  | -1.02675500 | -0.20460600 | 1.16490900  |
| N  | 0.70556100  | 1.06960900  | 0.78100600  |
| C  | -2.05760400 | -1.20092600 | 1.07100100  |
| C  | -1.76167000 | -2.52998600 | 1.47065600  |
| C  | -3.37564200 | -0.82958600 | 0.73056300  |
| C  | -2.79840500 | -3.46738800 | 1.47541700  |
| C  | -4.38206300 | -1.80541600 | 0.79310800  |
| C  | -4.11523600 | -3.12755700 | 1.14389000  |
| H  | -2.58637900 | -4.49198600 | 1.76274300  |
| H  | -5.40571400 | -1.52092400 | 0.56723200  |
| C  | 1.76992700  | 1.78949200  | 0.13483900  |
| C  | 3.08799600  | 1.28458500  | 0.15228500  |
| C  | 1.49617900  | 3.05529600  | -0.44413600 |
| C  | 4.09327000  | 2.00723200  | -0.50476700 |
| C  | 2.53796500  | 3.73448700  | -1.08169100 |
| C  | 3.83866200  | 3.21967600  | -1.14260700 |
| H  | 5.10290900  | 1.60687800  | -0.51359600 |
| H  | 2.33965400  | 4.69464900  | -1.54688700 |
| C  | -3.75051900 | 0.61146200  | 0.40242900  |
| C  | -0.35691700 | -2.92885300 | 1.92556500  |
| C  | 3.48123700  | 0.04938500  | 0.97289500  |
| C  | 0.10908700  | 3.68996000  | -0.33738000 |
| H  | -0.61797500 | 2.87937800  | -0.42960900 |
| H  | -2.83299800 | 1.20401600  | 0.44798500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.34889700  | -2.36860000 | 1.30563600  |
| H | 2.56611800  | -0.51723000 | 1.16731700  |
| C | -4.34473800 | 0.86388800  | -0.99215600 |
| C | -4.47340800 | 2.20024300  | -1.41256700 |
| C | -4.79088600 | -0.13677300 | -1.86507800 |
| C | -5.04510900 | 2.52702600  | -2.64115700 |
| H | -4.12143600 | 2.99980700  | -0.76510800 |
| C | -5.37094000 | 0.18650600  | -3.09707800 |
| H | -4.68428000 | -1.18080500 | -1.59588300 |
| C | -5.50645400 | 1.51692500  | -3.48993100 |
| H | -5.12998100 | 3.56944500  | -2.93549100 |
| H | -5.71197200 | -0.61195800 | -3.75030600 |
| H | -5.95713300 | 1.76566900  | -4.44627500 |
| C | -4.70701200 | 1.16437600  | 1.49213900  |
| H | -5.66656600 | 0.63865300  | 1.47852100  |
| H | -4.26985000 | 1.04421300  | 2.48836500  |
| H | -4.90802700 | 2.22748800  | 1.33238600  |
| C | -0.06559700 | -2.56130500 | 3.38538100  |
| C | -1.04792700 | -2.61558400 | 4.38454600  |
| C | 1.24513300  | -2.23012500 | 3.76276600  |
| C | -0.73218100 | -2.33533900 | 5.71675800  |
| H | -2.06950800 | -2.86991700 | 4.11810100  |
| C | 1.56483000  | -1.95102400 | 5.09278800  |
| H | 2.02491600  | -2.20049900 | 3.00524900  |
| C | 0.57434400  | -1.99982400 | 6.07662500  |
| H | -1.51076600 | -2.37922000 | 6.47347200  |
| H | 2.58633700  | -1.69375200 | 5.35901300  |
| H | 0.81865100  | -1.77939700 | 7.11174700  |
| C | -0.03360000 | -4.42643700 | 1.72512500  |
| H | -0.20825700 | -4.73567600 | 0.69196100  |
| H | 1.02037400  | -4.60208300 | 1.95908000  |
| H | -0.62195600 | -5.06419600 | 2.39194000  |
| C | 4.43283800  | -0.90240500 | 0.24573600  |
| C | 5.82708900  | -0.83978900 | 0.39306200  |
| C | 3.90354100  | -1.89742000 | -0.58948000 |
| C | 6.66394300  | -1.73611000 | -0.27732800 |
| H | 6.27542600  | -0.09563200 | 1.04340600  |
| C | 4.73556000  | -2.79758000 | -1.25658400 |
| H | 2.82762500  | -1.96978600 | -0.72286900 |
| C | 6.12176400  | -2.72045700 | -1.10394100 |
| H | 7.74022100  | -1.66621800 | -0.14469700 |
| H | 4.29281500  | -3.55820900 | -1.89227700 |
| H | 6.77090500  | -3.42243800 | -1.61971900 |
| C | 4.04971500  | 0.50969100  | 2.33589500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.31964400  | 1.11186400  | 2.88171200  |
| H | 4.32023200  | -0.35126800 | 2.95569600  |
| H | 4.94042400  | 1.13141200  | 2.20771300  |
| C | -0.13505600 | 4.36381300  | 1.01784300  |
| C | 0.87204600  | 5.06208900  | 1.69965400  |
| C | -1.42236900 | 4.34730000  | 1.57623800  |
| C | 0.60191900  | 5.71597000  | 2.90439900  |
| H | 1.87738500  | 5.08723200  | 1.28994600  |
| C | -1.69698800 | 4.99967600  | 2.77979300  |
| H | -2.21954600 | 3.81925000  | 1.05841600  |
| C | -0.68277200 | 5.68652800  | 3.45080900  |
| H | 1.39893900  | 6.24783100  | 3.41683800  |
| H | -2.70136400 | 4.96905000  | 3.19315700  |
| H | -0.89136400 | 6.19258700  | 4.38895800  |
| C | -0.20585500 | 4.70414700  | -1.45974800 |
| H | 0.39734100  | 5.61288700  | -1.37046400 |
| H | -0.03797400 | 4.26899200  | -2.44883100 |
| H | -1.25503200 | 5.00662700  | -1.39258900 |
| C | -5.20904900 | -4.16902700 | 1.15825400  |
| C | 4.92878000  | 3.96048500  | -1.88038000 |
| H | 5.92191400  | 3.64556500  | -1.54810000 |
| H | 4.86962800  | 3.77413600  | -2.95983400 |
| H | 4.84619100  | 5.04238200  | -1.73558600 |
| H | -6.19681300 | -3.71040900 | 1.25905500  |
| H | -5.21068500 | -4.75034800 | 0.22790600  |
| H | -5.07539800 | -4.87835500 | 1.98094900  |
| H | -0.19726600 | -5.61215500 | -1.92224600 |
| H | 1.80798500  | -5.61649600 | -3.39833900 |
| H | 2.76697500  | -3.46196400 | -4.17583300 |
| H | -1.20271900 | -3.47666100 | -1.20475100 |

### TS3<sub>cw</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -5.04226300 | 0.34827100  | -0.88930600 |
| C  | -3.78684300 | -0.12102000 | -0.51990900 |
| C  | -2.71466500 | -0.17828300 | -1.39544100 |
| C  | -2.97551400 | 0.22090600  | -2.72722900 |
| C  | -4.21899300 | 0.71554800  | -3.12970500 |
| C  | -1.82880800 | 0.01962800  | -3.71581500 |
| H  | -2.21136300 | -0.37624300 | -4.66331400 |
| H  | -1.36557000 | 0.98345500  | -3.94641400 |
| C  | -0.79544700 | -0.93625500 | -3.10938600 |
| C  | 0.55668900  | -0.54153200 | -2.78136000 |
| Ni | -0.64971900 | -0.38151200 | -1.14255100 |
| H  | -1.65890100 | -1.17107100 | -1.90866000 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.17402500  | 0.24705600  | 0.44209500  |
| C | 0.76127600  | 0.01652000  | 2.72214700  |
| C | 0.87873600  | 1.48699700  | 2.33843300  |
| H | -0.12268600 | -0.16577300 | 3.34027500  |
| H | 1.64324200  | -0.36671000 | 3.23091200  |
| H | 0.30614200  | 2.14446800  | 2.99019600  |
| H | 1.92051900  | 1.82166200  | 2.32112100  |
| N | 0.30961200  | 1.49043100  | 0.96675700  |
| N | 0.58115600  | -0.62553300 | 1.40073100  |
| C | 0.08396600  | 2.73445700  | 0.29472800  |
| C | -1.22109800 | 3.27197200  | 0.27282800  |
| C | 1.17760700  | 3.46895700  | -0.20482200 |
| C | -1.41596100 | 4.52664200  | -0.30507900 |
| C | 0.93631200  | 4.75436700  | -0.70917500 |
| C | -0.34848700 | 5.28760400  | -0.79406600 |
| H | -2.41499300 | 4.94599600  | -0.34531000 |
| H | 1.77443200  | 5.36354300  | -1.03080100 |
| C | 0.83378800  | -2.02096700 | 1.20573900  |
| C | -0.19959900 | -2.96213000 | 1.33269500  |
| C | 2.15994700  | -2.43344100 | 0.94384000  |
| C | 0.10943000  | -4.32137400 | 1.20721400  |
| C | 2.41770800  | -3.79819800 | 0.82364500  |
| C | 1.40747700  | -4.75832400 | 0.95382700  |
| H | -0.69315700 | -5.04782100 | 1.29629700  |
| H | 3.42604100  | -4.13133200 | 0.60518200  |
| C | 2.60105100  | 2.94097500  | -0.11488600 |
| C | -2.36135000 | 2.51677100  | 0.93780900  |
| C | -1.62259200 | -2.53507700 | 1.64720100  |
| C | 3.28035500  | -1.41000300 | 0.82149700  |
| H | 2.85277300  | -0.52758600 | 0.33538100  |
| H | 2.54241100  | 1.95163800  | 0.34042700  |
| H | -2.28001200 | 1.47995900  | 0.61643100  |
| H | -1.70672900 | -1.48122200 | 1.37519100  |
| C | 3.34300100  | 2.72379600  | -1.43507200 |
| C | 4.33054800  | 1.72709500  | -1.45685000 |
| C | 3.11698900  | 3.44505000  | -2.61288400 |
| C | 5.05857300  | 1.44536900  | -2.61070200 |
| H | 4.52064000  | 1.14726400  | -0.55975400 |
| C | 3.84384700  | 3.16789800  | -3.77287400 |
| H | 2.34020200  | 4.19691000  | -2.65228200 |
| C | 4.81568200  | 2.16741400  | -3.78057300 |
| H | 5.80164500  | 0.65377000  | -2.59826000 |
| H | 3.63804500  | 3.73235500  | -4.67760200 |
| H | 5.37242900  | 1.94899100  | -4.68661600 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 3. 44992300  | 3. 83303800  | 0. 82052000  |
| H | 3. 57225800  | 4. 83453600  | 0. 39847300  |
| H | 2. 97374800  | 3. 93250200  | 1. 80054600  |
| H | 4. 44763900  | 3. 40551300  | 0. 95780400  |
| C | -2. 21779300 | 2. 52197000  | 2. 45541400  |
| C | -1. 84785600 | 3. 68133800  | 3. 14881000  |
| C | -2. 47203700 | 1. 35487300  | 3. 18583500  |
| C | -1. 71455700 | 3. 66926700  | 4. 53801100  |
| H | -1. 63994000 | 4. 59099600  | 2. 59310100  |
| C | -2. 33726500 | 1. 33846300  | 4. 57492800  |
| H | -2. 77020500 | 0. 45729500  | 2. 65652900  |
| C | -1. 95115100 | 2. 49449900  | 5. 25622900  |
| H | -1. 41815700 | 4. 57499000  | 5. 05922200  |
| H | -2. 52683100 | 0. 41953700  | 5. 12237700  |
| H | -1. 83832600 | 2. 48189000  | 6. 33609800  |
| C | -3. 75894300 | 3. 02071800  | 0. 54584600  |
| H | -3. 88313500 | 3. 03657800  | -0. 54068000 |
| H | -4. 51777700 | 2. 35639100  | 0. 96491500  |
| H | -3. 94739100 | 4. 02576300  | 0. 93570800  |
| C | -2. 65284600 | -3. 26742200 | 0. 79320500  |
| C | -3. 89132400 | -3. 67883100 | 1. 29693100  |
| C | -2. 39895000 | -3. 47695000 | -0. 57016700 |
| C | -4. 84880200 | -4. 26540500 | 0. 46445200  |
| H | -4. 12763800 | -3. 53642700 | 2. 34515200  |
| C | -3. 34774800 | -4. 05893200 | -1. 40621900 |
| H | -1. 44295800 | -3. 17176500 | -0. 97683800 |
| C | -4. 58433500 | -4. 45559400 | -0. 89128700 |
| H | -5. 80390700 | -4. 57206000 | 0. 88107500  |
| H | -3. 12126600 | -4. 20243800 | -2. 45909700 |
| H | -5. 32883700 | -4. 91009400 | -1. 53799200 |
| C | -1. 88077600 | -2. 64398500 | 3. 16089400  |
| H | -1. 08397800 | -2. 14358100 | 3. 71615500  |
| H | -2. 82756800 | -2. 17174700 | 3. 43866500  |
| H | -1. 90785000 | -3. 68987600 | 3. 48355800  |
| C | 3. 81279300  | -0. 97067800 | 2. 18351100  |
| C | 3. 90327800  | -1. 86239300 | 3. 25991100  |
| C | 4. 26427600  | 0. 34182100  | 2. 36986500  |
| C | 4. 41293700  | -1. 44665200 | 4. 49112200  |
| H | 3. 55262500  | -2. 88204500 | 3. 13687600  |
| C | 4. 77113600  | 0. 76414000  | 3. 59890400  |
| H | 4. 20922400  | 1. 04658900  | 1. 54755100  |
| C | 4. 84371200  | -0. 13029300 | 4. 66823800  |
| H | 4. 46646700  | -2. 15154800 | 5. 31569300  |
| H | 5. 10252800  | 1. 79123100  | 3. 72030900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 5.23115200  | 0.19468600  | 5.62894300  |
| C | 4.45536600  | -1.88184900 | -0.05327000 |
| H | 5.16328300  | -1.05952600 | -0.19086800 |
| H | 5.00495200  | -2.69968800 | 0.42205800  |
| H | 4.10808100  | -2.20921900 | -1.03324000 |
| C | -0.58569400 | 6.64919500  | -1.39809200 |
| C | 1.72082700  | -6.22423700 | 0.78750200  |
| H | 0.90014200  | -6.85103900 | 1.14568900  |
| H | 1.89078500  | -6.47134700 | -0.26755200 |
| H | 2.62905000  | -6.50249600 | 1.33160000  |
| H | 0.31286600  | 7.27030800  | -1.34641400 |
| H | -0.86640600 | 6.56479500  | -2.45495700 |
| H | -1.39810000 | 7.17563400  | -0.88851300 |
| C | -5.24595100 | 0.77546400  | -2.19769200 |
| F | -3.65860900 | -0.46950400 | 0.78951200  |
| F | -6.03824900 | 0.43454400  | 0.01561600  |
| F | -6.46651700 | 1.23333000  | -2.54185900 |
| H | -0.90896800 | -1.97379900 | -3.42632500 |
| C | 1.01179100  | 0.87113500  | -3.08110600 |
| H | 0.28606600  | 1.61649000  | -2.74921300 |
| H | 1.94037200  | 1.08289900  | -2.55974400 |
| H | 1.19308300  | 1.03287200  | -4.15434400 |
| H | -4.41507700 | 1.02124100  | -4.15267500 |
| C | 1.60106900  | -1.60203200 | -2.85223500 |
| C | 1.35925400  | -2.90870600 | -2.38672900 |
| C | 2.84679300  | -1.35262200 | -3.45857300 |
| C | 2.29216600  | -3.92602700 | -2.56182800 |
| H | 0.43761500  | -3.12360800 | -1.85826000 |
| C | 3.78472500  | -2.37183900 | -3.63176200 |
| H | 3.08359100  | -0.35837700 | -3.81668100 |
| C | 3.51138700  | -3.66854800 | -3.19482000 |
| H | 2.07176600  | -4.92094100 | -2.18715900 |
| H | 4.73303300  | -2.14696700 | -4.11230200 |
| H | 4.24125400  | -4.46138300 | -3.32754700 |

TS3'<sub>cw</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.38813000 | -3.12476500 | -1.17073600 |
| C | -2.02974900 | -2.82260500 | -1.11121600 |
| C | -1.50545200 | -1.62196700 | -1.54046600 |
| C | -2.39064700 | -0.69141000 | -2.13106800 |
| C | -3.75144000 | -0.98283000 | -2.18551200 |
| C | -1.89763800 | 0.64598500  | -2.71773000 |
| H | -2.42014700 | 0.80750600  | -3.67244000 |
| H | -2.22416900 | 1.46287300  | -2.07020500 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.39628300 | 0.74390800  | -2.91275200 |
| C  | 0.29806100  | -0.20100700 | -3.69652500 |
| Ni | 0.19481000  | -0.65447600 | -1.44858900 |
| H  | 0.28356800  | -1.44764800 | -2.70682000 |
| C  | 0.43567600  | 0.22506000  | 0.26402500  |
| C  | 1.85398700  | 0.89393400  | 2.05175600  |
| C  | 0.40307800  | 1.16163400  | 2.44141500  |
| H  | 2.27969500  | 0.05426500  | 2.61228100  |
| H  | 2.49818200  | 1.76584300  | 2.17171800  |
| H  | 0.12935200  | 0.72408300  | 3.40094200  |
| H  | 0.18008600  | 2.23415600  | 2.46388900  |
| N  | -0.35107700 | 0.50842900  | 1.33614400  |
| N  | 1.71392000  | 0.53623000  | 0.62107800  |
| C  | -1.76827900 | 0.29994300  | 1.50616400  |
| C  | -2.23223200 | -0.95012200 | 1.99573600  |
| C  | -2.66329500 | 1.38083500  | 1.34353300  |
| C  | -3.59941200 | -1.09838400 | 2.24105500  |
| C  | -4.01809900 | 1.18059200  | 1.65143500  |
| C  | -4.51134600 | -0.05058700 | 2.07365100  |
| H  | -3.97341800 | -2.05343200 | 2.59266300  |
| H  | -4.70559500 | 2.01626700  | 1.56180800  |
| C  | 2.85920200  | 0.47490100  | -0.24573800 |
| C  | 3.63740300  | -0.69998000 | -0.31933000 |
| C  | 3.24296300  | 1.64109400  | -0.95707800 |
| C  | 4.75750000  | -0.70835000 | -1.16180100 |
| C  | 4.37743900  | 1.57833400  | -1.77040400 |
| C  | 5.14113100  | 0.41079600  | -1.89773100 |
| H  | 5.34596900  | -1.61791600 | -1.24048700 |
| H  | 4.68037500  | 2.45730200  | -2.33045700 |
| C  | -2.20022700 | 2.78782600  | 0.97427300  |
| C  | -1.27492700 | -2.10499000 | 2.30310400  |
| C  | 3.36239300  | -1.92102400 | 0.56444600  |
| C  | 2.45449200  | 2.94362900  | -0.82252500 |
| H  | 1.40710700  | 2.66708700  | -0.67011100 |
| H  | -1.13181600 | 2.73247200  | 0.74588200  |
| H  | -0.56136200 | -2.16321900 | 1.47608200  |
| H  | 2.37491800  | -1.78039300 | 1.00943100  |
| C  | -2.85724700 | 3.44079300  | -0.25444600 |
| C  | -2.32212700 | 4.66134600  | -0.70602400 |
| C  | -3.94384500 | 2.91004700  | -0.96295900 |
| C  | -2.85955300 | 5.33400800  | -1.80221200 |
| H  | -1.46710000 | 5.09379900  | -0.19215500 |
| C  | -4.48684600 | 3.58164800  | -2.06386000 |
| H  | -4.36337600 | 1.95096200  | -0.68570800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.95461200 | 4.79820300  | -2.48561500 |
| H | -2.42058200 | 6.27423800  | -2.12442800 |
| H | -5.32316600 | 3.13633600  | -2.59510100 |
| H | -4.37737700 | 5.31828900  | -3.34024500 |
| C | -2.36378100 | 3.71429000  | 2.21008700  |
| H | -3.42066100 | 3.84071900  | 2.46279900  |
| H | -1.85790900 | 3.29218400  | 3.08365600  |
| H | -1.94540500 | 4.70623200  | 2.01910800  |
| C | -0.47759300 | -1.89320700 | 3.59405900  |
| C | -1.05036400 | -1.30736300 | 4.73296600  |
| C | 0.83562300  | -2.37724000 | 3.68866400  |
| C | -0.32651700 | -1.19277000 | 5.92240400  |
| H | -2.06841600 | -0.93157100 | 4.68632500  |
| C | 1.56252300  | -2.26556900 | 4.87614600  |
| H | 1.28699500  | -2.85961300 | 2.82513600  |
| C | 0.98465800  | -1.66782000 | 5.99834700  |
| H | -0.78937200 | -0.73180500 | 6.79076100  |
| H | 2.57907000  | -2.64627600 | 4.92345500  |
| H | 1.54820600  | -1.57691700 | 6.92240200  |
| C | -1.96283500 | -3.48633100 | 2.39958400  |
| H | -2.56651800 | -3.70986900 | 1.51896300  |
| H | -1.19635500 | -4.26131200 | 2.48669900  |
| H | -2.59651900 | -3.55716800 | 3.28915200  |
| C | 3.29486300  | -3.23505500 | -0.21554500 |
| C | 2.05831400  | -3.65866300 | -0.72434100 |
| C | 4.41343800  | -4.05355600 | -0.43080000 |
| C | 1.94032400  | -4.85394500 | -1.43490400 |
| H | 1.17038900  | -3.05230000 | -0.56473400 |
| C | 4.30089000  | -5.24823800 | -1.14797300 |
| H | 5.38259100  | -3.77357900 | -0.02919100 |
| C | 3.06457100  | -5.65343300 | -1.65404400 |
| H | 0.96389500  | -5.15749600 | -1.80150900 |
| H | 5.18159700  | -5.86583600 | -1.30196900 |
| H | 2.97701300  | -6.58615500 | -2.20402000 |
| C | 4.38672400  | -1.96378400 | 1.72068800  |
| H | 4.32917000  | -1.05167100 | 2.32169200  |
| H | 4.19558100  | -2.82080400 | 2.37417100  |
| H | 5.41323700  | -2.04073300 | 1.35066400  |
| C | 2.87271500  | 3.77958400  | 0.39329300  |
| C | 4.20125700  | 3.85189200  | 0.83545400  |
| C | 1.91068500  | 4.55609400  | 1.05744600  |
| C | 4.55487000  | 4.67131500  | 1.91053000  |
| H | 4.96460900  | 3.25815400  | 0.34193400  |
| C | 2.25969000  | 5.37626500  | 2.13168800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.87643600  | 4.51985500  | 0.72365600  |
| C | 3.58655600  | 5.43596700  | 2.56384400  |
| H | 5.59010200  | 4.70913400  | 2.23821200  |
| H | 1.49571200  | 5.96540300  | 2.63133600  |
| H | 3.86195800  | 6.07008500  | 3.40148000  |
| C | 2.49784500  | 3.83030000  | -2.08741600 |
| H | 1.80552600  | 4.66874600  | -1.96898400 |
| H | 3.49210000  | 4.25390800  | -2.25665700 |
| H | 2.20486100  | 3.26793100  | -2.97945500 |
| C | -5.98343900 | -0.25895100 | 2.33722400  |
| C | 6.33665100  | 0.36834000  | -2.81970200 |
| H | 7.03376600  | -0.42430500 | -2.53428900 |
| H | 6.02739800  | 0.17606300  | -3.85446200 |
| H | 6.87806800  | 1.31943300  | -2.81604000 |
| H | -6.14711100 | -0.89431200 | 3.21333800  |
| H | -6.49987800 | 0.69107500  | 2.50087800  |
| H | -6.46517500 | -0.75391900 | 1.48502700  |
| C | -4.26419700 | -2.18536600 | -1.70237100 |
| F | -4.63219200 | -0.08524800 | -2.70292700 |
| F | -5.58756600 | -2.43862100 | -1.75056200 |
| F | -3.86953800 | -4.29571400 | -0.69854600 |
| F | -1.21767400 | -3.78762900 | -0.57661600 |
| C | 1.74352300  | 0.06583000  | -4.08013600 |
| C | -0.43750300 | -1.04961000 | -4.73351400 |
| H | 1.78372900  | 0.52011200  | -5.07900100 |
| H | 2.24089200  | 0.73323500  | -3.37510100 |
| H | 2.31684500  | -0.86571900 | -4.12861500 |
| H | -1.40223700 | -1.41206300 | -4.37822300 |
| H | -0.60851100 | -0.43746300 | -5.62842900 |
| H | 0.16533100  | -1.91351300 | -5.03103900 |
| H | 0.08740600  | 1.68408000  | -2.66712700 |

TS4<sub>cw</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.36114000  | -4.22532100 | -1.27554700 |
| C  | -0.21149200 | -2.99882400 | -1.57407200 |
| C  | 0.54567900  | -1.90226100 | -2.02261600 |
| C  | 1.91534700  | -2.15752700 | -2.31396900 |
| C  | 2.47589300  | -3.39218200 | -2.02369700 |
| C  | 2.61175200  | -1.11192800 | -3.15309000 |
| H  | 3.33318200  | -0.52834000 | -2.57048700 |
| H  | 3.18654700  | -1.60361500 | -3.94556200 |
| C  | 1.50485100  | -0.19237200 | -3.73132200 |
| C  | 0.10841000  | -0.79429400 | -3.46992700 |
| Ni | -0.13391200 | -0.22610200 | -1.41568700 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 1. 55998400  | 0. 79861900  | -3. 26982300 |
| C | -0. 25284400 | 0. 53157800  | 0. 32031600  |
| C | 0. 05026100  | 2. 10724400  | 2. 08544100  |
| C | -1. 07691100 | 1. 14575400  | 2. 46529200  |
| H | 0. 92588200  | 1. 97283000  | 2. 72683000  |
| H | -0. 25242000 | 3. 15560800  | 2. 11959900  |
| H | -0. 92504900 | 0. 67113700  | 3. 43573500  |
| H | -2. 05150400 | 1. 64473200  | 2. 46647200  |
| N | -1. 02256100 | 0. 14133500  | 1. 37455900  |
| N | 0. 35453200  | 1. 69740300  | 0. 69392500  |
| C | -1. 83879500 | -1. 04041100 | 1. 46645800  |
| C | -1. 26732000 | -2. 24271500 | 1. 95831000  |
| C | -3. 21390500 | -0. 97537800 | 1. 16965600  |
| C | -2. 09962600 | -3. 35021400 | 2. 12923100  |
| C | -4. 00338000 | -2. 11776100 | 1. 36400300  |
| C | -3. 47040300 | -3. 31117100 | 1. 84105800  |
| H | -1. 67695500 | -4. 27978700 | 2. 49516100  |
| H | -5. 06150900 | -2. 06658900 | 1. 12018700  |
| C | 1. 23655900  | 2. 46922800  | -0. 13819400 |
| C | 2. 63345500  | 2. 39726600  | 0. 04691500  |
| C | 0. 68775400  | 3. 34997000  | -1. 10565100 |
| C | 3. 46477600  | 3. 14223100  | -0. 80010200 |
| C | 1. 56360700  | 4. 06446600  | -1. 92728000 |
| C | 2. 95541200  | 3. 96332000  | -1. 80388700 |
| H | 4. 54114500  | 3. 06790000  | -0. 67031200 |
| H | 1. 15968000  | 4. 73036700  | -2. 68260400 |
| C | -3. 90059100 | 0. 30307900  | 0. 68809900  |
| C | 0. 22290200  | -2. 33316000 | 2. 29144800  |
| C | 3. 27110300  | 1. 61493200  | 1. 20056700  |
| C | -0. 82282700 | 3. 56386400  | -1. 20877700 |
| H | -1. 29723200 | 2. 58782600  | -1. 07002300 |
| H | -3. 11163700 | 1. 02217700  | 0. 44162100  |
| H | 0. 75454700  | -1. 80077200 | 1. 49586500  |
| H | 2. 51149500  | 0. 93171700  | 1. 58961700  |
| C | -4. 70632700 | 0. 08117500  | -0. 59994500 |
| C | -5. 97882800 | 0. 63541800  | -0. 79605500 |
| C | -4. 14977400 | -0. 67383600 | -1. 64717600 |
| C | -6. 67251600 | 0. 44617100  | -1. 99630300 |
| H | -6. 44908800 | 1. 21992600  | -0. 01310000 |
| C | -4. 84103500 | -0. 86640100 | -2. 84307500 |
| H | -3. 17350400 | -1. 12918700 | -1. 51599800 |
| C | -6. 10823400 | -0. 30505000 | -3. 02556200 |
| H | -7. 65871800 | 0. 88575200  | -2. 11863500 |
| H | -4. 39206600 | -1. 46413200 | -3. 63207400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -6.64842600 | -0.45721700 | -3.95560900 |
| C | -4.73946800 | 0.91174200  | 1.83233400  |
| H | -5.60355300 | 0.28233600  | 2.06804000  |
| H | -4.14056800 | 1.00139500  | 2.74200200  |
| H | -5.10539300 | 1.91072000  | 1.57611300  |
| C | 0.59797800  | -1.66078100 | 3.61481500  |
| C | -0.25463500 | -1.67938600 | 4.72792900  |
| C | 1.86580600  | -1.07751600 | 3.76068600  |
| C | 0.14280700  | -1.12088700 | 5.94574900  |
| H | -1.23909600 | -2.12968600 | 4.63926900  |
| C | 2.26700900  | -0.51925400 | 4.97624700  |
| H | 2.55116000  | -1.07375100 | 2.91624800  |
| C | 1.40401800  | -0.53560400 | 6.07457900  |
| H | -0.53557500 | -1.14433800 | 6.79432300  |
| H | 3.25446200  | -0.07455700 | 5.06508400  |
| H | 1.71237800  | -0.10007200 | 7.02063100  |
| C | 0.76707500  | -3.78020100 | 2.31020300  |
| H | 0.48734800  | -4.33065700 | 1.40931300  |
| H | 1.85852100  | -3.75860800 | 2.37776200  |
| H | 0.40059500  | -4.33562200 | 3.17943300  |
| C | 4.44605900  | 0.74006500  | 0.75968700  |
| C | 5.78549800  | 1.10644100  | 0.95314000  |
| C | 4.18263300  | -0.49345100 | 0.14316200  |
| C | 6.82708900  | 0.27125300  | 0.53742900  |
| H | 6.03099900  | 2.04525400  | 1.43846300  |
| C | 5.21861700  | -1.33077700 | -0.27353800 |
| H | 3.15099400  | -0.79795900 | -0.01625200 |
| C | 6.54847400  | -0.94898100 | -0.07736700 |
| H | 7.85677500  | 0.57794200  | 0.69998100  |
| H | 4.98587500  | -2.27353700 | -0.75767200 |
| H | 7.35745000  | -1.59874200 | -0.39869200 |
| C | 3.64800700  | 2.59299400  | 2.33522000  |
| H | 2.76926300  | 3.14120100  | 2.68412300  |
| H | 4.07837600  | 2.05601700  | 3.18649700  |
| H | 4.37415500  | 3.33832800  | 1.99736600  |
| C | -1.36920100 | 4.47539000  | -0.10386600 |
| C | -0.64371400 | 5.56633600  | 0.39522400  |
| C | -2.66542900 | 4.25932800  | 0.38834900  |
| C | -1.19468600 | 6.41033000  | 1.36291800  |
| H | 0.36152500  | 5.75383900  | 0.02990800  |
| C | -3.21940300 | 5.10054600  | 1.35514800  |
| H | -3.24949600 | 3.42761700  | 0.00130900  |
| C | -2.48331000 | 6.18014700  | 1.84882100  |
| H | -0.61352800 | 7.24830900  | 1.73802500  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.22401200 | 4.91129500  | 1.72323800  |
| H | -2.90947500 | 6.83448200  | 2.60376400  |
| C | -1.28976000 | 4.09611600  | -2.58128100 |
| H | -2.38274200 | 4.09254900  | -2.62249500 |
| H | -0.96270300 | 5.12633100  | -2.75146300 |
| H | -0.91414300 | 3.47489300  | -3.40016400 |
| C | -4.32929300 | -4.53975800 | 2.02615600  |
| C | 3.87018900  | 4.72261600  | -2.73561700 |
| H | 3.97560800  | 4.20111500  | -3.69498200 |
| H | 3.47962500  | 5.72171300  | -2.95374500 |
| H | 4.87191900  | 4.83212100  | -2.31097400 |
| H | -4.17664600 | -4.98908100 | 3.01347100  |
| H | -5.39172900 | -4.30430300 | 1.92062600  |
| H | -4.08289700 | -5.30763300 | 1.28318100  |
| C | 1.72596900  | -4.43005300 | -1.47786800 |
| F | -1.55163000 | -2.87381200 | -1.37561300 |
| F | -0.37870300 | -5.21792300 | -0.73767100 |
| F | 2.28630500  | -5.61767000 | -1.17908600 |
| F | 3.78284800  | -3.63147300 | -2.30686600 |
| H | 1.64574600  | -0.04434100 | -4.81081500 |
| C | -0.99414700 | 0.28312600  | -3.55858000 |
| C | -0.25716600 | -1.89273900 | -4.48087300 |
| H | -0.98405500 | 1.03808900  | -2.74711800 |
| H | -0.83168900 | 0.85847600  | -4.48056200 |
| H | -1.99465500 | -0.15107000 | -3.59820100 |
| H | 0.52943400  | -2.64675300 | -4.57065700 |
| H | -1.18431300 | -2.39841800 | -4.19542900 |
| H | -0.41057800 | -1.43785600 | -5.46893100 |

TS4'<sub>ew</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.40459900 | -3.39658300 | -1.70089100 |
| C  | -1.24005500 | -2.63046700 | -1.72140900 |
| C  | -1.28300600 | -1.30550200 | -2.17353300 |
| C  | -2.49419300 | -0.86431300 | -2.77269500 |
| C  | -3.64231900 | -1.62573400 | -2.78061300 |
| C  | -1.95926900 | 0.30143500  | -3.55554800 |
| H  | -2.22126300 | 0.28919900  | -4.61905500 |
| H  | -2.20398600 | 1.28880800  | -3.15003600 |
| C  | -0.49243600 | -0.14940800 | -3.25704200 |
| C  | 0.24198100  | -0.84141900 | -4.41262000 |
| Ni | -0.11900300 | -0.09226400 | -1.22629400 |
| H  | -0.45035800 | -1.57753300 | -4.84672300 |
| C  | 0.40147600  | 0.42755800  | 0.51832400  |
| C  | 1.75295700  | 1.49089800  | 2.16990300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.42078100  | 1.07082000  | 2.80814600  |
| H | 2.60301100  | 0.96356400  | 2.61294900  |
| H | 1.93810000  | 2.56519600  | 2.24013800  |
| H | 0.54915800  | 0.40477700  | 3.66346200  |
| H | -0.16861400 | 1.93546600  | 3.12650600  |
| N | -0.26629000 | 0.36279500  | 1.69877500  |
| N | 1.56820200  | 1.08820400  | 0.75639000  |
| C | -1.53402100 | -0.27772900 | 1.92568500  |
| C | -1.57890700 | -1.67204800 | 2.18606000  |
| C | -2.71153300 | 0.49438500  | 1.96601100  |
| C | -2.81801200 | -2.25281500 | 2.46490600  |
| C | -3.92607700 | -0.13979300 | 2.26359900  |
| C | -4.00375200 | -1.50722200 | 2.51192600  |
| H | -2.87148000 | -3.31930100 | 2.65636500  |
| H | -4.83455700 | 0.45676400  | 2.28217800  |
| C | 2.56838400  | 1.35915600  | -0.23993400 |
| C | 3.71886800  | 0.54991000  | -0.31426100 |
| C | 2.40633300  | 2.46332200  | -1.11661600 |
| C | 4.67962900  | 0.83109100  | -1.29579700 |
| C | 3.39542300  | 2.69838000  | -2.07380900 |
| C | 4.53727800  | 1.89238400  | -2.18591900 |
| H | 5.55549800  | 0.19128900  | -1.36784600 |
| H | 3.28423800  | 3.53262100  | -2.75887900 |
| C | -2.71857000 | 2.00570200  | 1.73409300  |
| C | -0.30817400 | -2.52136900 | 2.17820300  |
| C | 3.98549000  | -0.59449300 | 0.66755500  |
| C | 1.18568100  | 3.37708800  | -1.00957700 |
| H | 0.32705200  | 2.72815500  | -0.80771100 |
| H | -1.72780900 | 2.28118200  | 1.35664600  |
| H | 0.30428900  | -2.16416400 | 1.34499900  |
| H | 3.07590800  | -0.73691200 | 1.25610300  |
| C | -3.73198700 | 2.41648300  | 0.65647100  |
| C | -4.55818000 | 3.54122300  | 0.78589000  |
| C | -3.83459700 | 1.65925800  | -0.52302600 |
| C | -5.45818400 | 3.89549000  | -0.22529300 |
| H | -4.51451200 | 4.15278400  | 1.68030700  |
| C | -4.73902700 | 2.00147600  | -1.52762900 |
| H | -3.20899100 | 0.78051000  | -0.64602300 |
| C | -5.55715900 | 3.12580000  | -1.38318300 |
| H | -6.08809400 | 4.77156400  | -0.09699000 |
| H | -4.81805000 | 1.37562300  | -2.41211000 |
| H | -6.26553300 | 3.39313700  | -2.16207200 |
| C | -2.92271100 | 2.74385600  | 3.07451300  |
| H | -3.93376500 | 2.58684300  | 3.46383100  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -2. 22049100 | 2. 37529800  | 3. 82667300  |
| H | -2. 76057600 | 3. 82088200  | 2. 96895000  |
| C | 0. 52764700  | -2. 37215900 | 3. 45383200  |
| C | -0. 05205100 | -2. 13929300 | 4. 70903000  |
| C | 1. 91925500  | -2. 54485700 | 3. 38876000  |
| C | 0. 73579900  | -2. 06820000 | 5. 86136800  |
| H | -1. 12708900 | -2. 00657200 | 4. 78608900  |
| C | 2. 70924000  | -2. 47521700 | 4. 53764100  |
| H | 2. 38578700  | -2. 74833200 | 2. 42786700  |
| C | 2. 11983300  | -2. 23265900 | 5. 78082100  |
| H | 0. 26468200  | -1. 88383400 | 6. 82310200  |
| H | 3. 78456500  | -2. 61165700 | 4. 46110600  |
| H | 2. 73201300  | -2. 17497600 | 6. 67623200  |
| C | -0. 56242900 | -4. 02374900 | 1. 92207300  |
| H | -1. 15212300 | -4. 18432600 | 1. 01697100  |
| H | 0. 39618300  | -4. 53538000 | 1. 79752600  |
| H | -1. 07482300 | -4. 49831100 | 2. 76481300  |
| C | 4. 23554500  | -1. 92718000 | -0. 04238400 |
| C | 3. 14311500  | -2. 60363500 | -0. 61020500 |
| C | 5. 50167100  | -2. 51952700 | -0. 13834400 |
| C | 3. 30861500  | -3. 83229200 | -1. 24849200 |
| H | 2. 15298600  | -2. 15893500 | -0. 55754000 |
| C | 5. 67237600  | -3. 74813400 | -0. 78517300 |
| H | 6. 36752000  | -2. 03257000 | 0. 29842700  |
| C | 4. 57795300  | -4. 41053700 | -1. 34056300 |
| H | 2. 44275500  | -4. 33697900 | -1. 66729300 |
| H | 6. 66422000  | -4. 18775000 | -0. 84644600 |
| H | 4. 70999000  | -5. 36831800 | -1. 83569600 |
| C | 5. 10941500  | -0. 19778100 | 1. 64644000  |
| H | 4. 84053400  | 0. 71325600  | 2. 18866500  |
| H | 5. 28936100  | -0. 99122000 | 2. 37881200  |
| H | 6. 04948200  | 0. 00597600  | 1. 12491100  |
| C | 1. 27693500  | 4. 37329400  | 0. 14959300  |
| C | 2. 49363200  | 4. 93282400  | 0. 56441700  |
| C | 0. 10039800  | 4. 79658300  | 0. 78745600  |
| C | 2. 53392200  | 5. 88061800  | 1. 59064800  |
| H | 3. 41708100  | 4. 62073200  | 0. 08563700  |
| C | 0. 13655500  | 5. 74429300  | 1. 81179200  |
| H | -0. 85523100 | 4. 38571700  | 0. 47017200  |
| C | 1. 35655700  | 6. 28900000  | 2. 22006700  |
| H | 3. 48848000  | 6. 29923100  | 1. 89778100  |
| H | -0. 78746300 | 6. 05583600  | 2. 29116200  |
| H | 1. 38859400  | 7. 02375800  | 3. 01937100  |
| C | 0. 85760300  | 4. 13445200  | -2. 31407000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.09413400 | 4.66149800  | -2.20100300 |
| H | 1.61640900  | 4.88453900  | -2.55697500 |
| H | 0.76802300  | 3.44442300  | -3.15958100 |
| C | -5.32474300 | -2.18002100 | 2.80162600  |
| C | 5.57236800  | 2.17137000  | -3.25029400 |
| H | 5.18828800  | 1.92990800  | -4.24859800 |
| H | 5.85527600  | 3.22946500  | -3.26349400 |
| H | 6.47777900  | 1.57966400  | -3.09146200 |
| H | -5.67715300 | -2.74672300 | 1.93127600  |
| H | -5.23864500 | -2.88828200 | 3.63223500  |
| H | -6.09802200 | -1.44963300 | 3.05483200  |
| C | -3.60863600 | -2.90097000 | -2.20736800 |
| F | -4.77762800 | -1.20056900 | -3.37721800 |
| F | -4.71033800 | -3.67158100 | -2.17583400 |
| F | -2.39112400 | -4.62721700 | -1.15034100 |
| F | -0.10930500 | -3.19731500 | -1.22461000 |
| C | 1.49797000  | -1.58301400 | -3.93949300 |
| C | 0.59713800  | 0.18151100  | -5.50751300 |
| H | 2.20633400  | -0.89242900 | -3.46776400 |
| H | 1.25389000  | -2.35759000 | -3.20966100 |
| H | 2.00619500  | -2.05745500 | -4.78617200 |
| H | -0.28279600 | 0.72766100  | -5.86226800 |
| H | 1.32118200  | 0.91481300  | -5.13248900 |
| H | 1.04703900  | -0.32067700 | -6.37071900 |
| H | 0.15871900  | 0.68700200  | -2.88070500 |

4'<sub>cw</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.78935200 | 1.05688700  | 0.00022200  |
| C | -0.41816800 | 1.24540400  | -0.21927800 |
| C | 0.37106500  | 0.11569200  | -0.30652700 |
| C | -0.17676500 | -1.16521600 | -0.18642500 |
| C | -1.52603200 | -1.36553400 | 0.02023600  |
| C | 1.15584600  | -1.86150100 | -0.37611200 |
| H | 1.51465200  | -2.40968700 | 0.50050400  |
| H | 1.23407600  | -2.50799700 | -1.25489900 |
| C | 1.78624600  | -0.41404100 | -0.53781000 |
| C | 2.88871400  | -0.01716600 | 0.45496800  |
| H | 2.50772800  | -0.21566500 | 1.46741900  |
| C | -2.33370700 | -0.22459300 | 0.11529400  |
| F | -2.09286200 | -2.57876300 | 0.13452900  |
| F | -3.65307200 | -0.35310800 | 0.32408100  |
| F | -2.60400900 | 2.11889200  | 0.10024500  |
| F | 0.05193500  | 2.50280300  | -0.32939700 |
| C | 3.22089400  | 1.47870600  | 0.34943600  |

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 4.14447300 | -0.87441800 | 0.23498200  |
| H | 3.62732300 | 1.71719200  | -0.64111300 |
| H | 2.33746500 | 2.10351100  | 0.50549400  |
| H | 3.97318500 | 1.76202900  | 1.09305400  |
| H | 3.93259900 | -1.94365900 | 0.33776000  |
| H | 4.55891900 | -0.70910800 | -0.76688200 |
| H | 4.92136200 | -0.61731600 | 0.96236600  |
| H | 2.13547700 | -0.23303300 | -1.56274000 |

### TS(R)-1

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 3.86922500  | -1.34685200 | -2.60188200 |
| C  | 2.75079400  | -0.58087000 | -2.28212700 |
| C  | 1.48008100  | -1.12615400 | -2.16497100 |
| C  | 1.32080500  | -2.50461100 | -2.46856700 |
| C  | 2.43885800  | -3.27036100 | -2.78879500 |
| C  | -0.07650800 | -3.08397000 | -2.54650200 |
| H  | -0.54799300 | -3.04873400 | -1.55773500 |
| H  | -0.02738800 | -4.13599600 | -2.83996900 |
| C  | -0.97108300 | -2.32472800 | -3.56622200 |
| H  | -0.51945400 | -2.43823900 | -4.55889200 |
| H  | -1.94666100 | -2.82361100 | -3.60703600 |
| C  | -1.18699300 | -0.82124200 | -3.28843000 |
| C  | -2.06215000 | -0.41793500 | -2.22302900 |
| H  | -2.58293200 | -1.17922900 | -1.65014300 |
| H  | -2.62028200 | 0.50825000  | -2.34296700 |
| Ni | -0.23455900 | -0.24844900 | -1.48123200 |
| H  | 0.26619900  | -0.60060800 | -2.87113500 |
| C  | -0.45555700 | 0.32797500  | 0.31806200  |
| C  | -0.71548500 | 1.80401200  | 2.15476700  |
| C  | -1.13871000 | 0.40260900  | 2.59117600  |
| H  | 0.00217500  | 2.25523600  | 2.83908200  |
| H  | -1.56627400 | 2.48420000  | 2.04429600  |
| H  | -0.43080600 | -0.05463400 | 3.29008500  |
| H  | -2.13177600 | 0.38532100  | 3.04505200  |
| N  | -1.12823300 | -0.33329000 | 1.30417800  |
| N  | -0.10561700 | 1.54314800  | 0.82810400  |
| C  | -1.57019800 | -1.70117300 | 1.26675300  |
| C  | -0.63252700 | -2.75347400 | 1.42009700  |
| C  | -2.95500800 | -1.98058700 | 1.19799100  |
| C  | -1.10398200 | -4.07049100 | 1.40523800  |
| C  | -3.36997400 | -3.31927800 | 1.24241100  |
| C  | -2.46518800 | -4.37802600 | 1.31314100  |
| H  | -0.39543600 | -4.88657300 | 1.50116100  |
| H  | -4.43325800 | -3.54061800 | 1.22534800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.64302900  | 2.56334400  | 0.14005900  |
| C | 1.98656900  | 2.80239200  | 0.50708100  |
| C | 0.02283000  | 3.35972000  | -0.85430800 |
| C | 2.71263500  | 3.77347100  | -0.19288800 |
| C | 0.79926000  | 4.30960700  | -1.52525200 |
| C | 2.14958600  | 4.52063200  | -1.22512400 |
| H | 3.75310300  | 3.93819100  | 0.07345000  |
| H | 0.34204900  | 4.91535100  | -2.30055900 |
| C | -4.00920400 | -0.87616000 | 1.20858800  |
| C | 0.84613900  | -2.48007800 | 1.69425700  |
| C | 2.65425900  | 2.12286300  | 1.70953900  |
| C | -1.47228400 | 3.24669200  | -1.14482800 |
| H | -1.73859800 | 2.19071500  | -1.06208500 |
| H | -3.47835400 | 0.07978200  | 1.17856400  |
| H | 1.11201600  | -1.55936700 | 1.16870900  |
| H | 2.03977800  | 1.26040600  | 1.98344000  |
| C | -4.99752800 | -0.83946600 | 0.03114300  |
| C | -5.83460600 | 0.28592400  | -0.07692200 |
| C | -5.12929500 | -1.84014200 | -0.93987800 |
| C | -6.76877200 | 0.40552300  | -1.10475200 |
| H | -5.75210400 | 1.08302200  | 0.65754500  |
| C | -6.06666800 | -1.72639400 | -1.97236300 |
| H | -4.49077000 | -2.71480300 | -0.90699800 |
| C | -6.89233900 | -0.60682500 | -2.06008200 |
| H | -7.39803200 | 1.28946700  | -1.16022100 |
| H | -6.14422000 | -2.51982600 | -2.71063400 |
| H | -7.61877600 | -0.51976500 | -2.86272300 |
| C | -4.78905900 | -0.92961000 | 2.55004600  |
| H | -5.37855000 | -1.84838100 | 2.62343000  |
| H | -4.10194600 | -0.90362900 | 3.40157600  |
| H | -5.47571000 | -0.08351100 | 2.63969700  |
| C | 1.13638500  | -2.25279600 | 3.18634200  |
| C | 0.37653000  | -2.84284700 | 4.20631000  |
| C | 2.24331500  | -1.47100800 | 3.55535800  |
| C | 0.70796000  | -2.65230200 | 5.55074500  |
| H | -0.48544900 | -3.45106700 | 3.95150300  |
| C | 2.57648400  | -1.27840000 | 4.89691500  |
| H | 2.85811000  | -1.01516000 | 2.78394400  |
| C | 1.80743800  | -1.86836300 | 5.90292000  |
| H | 0.10174500  | -3.11808300 | 6.32300700  |
| H | 3.43703700  | -0.66703000 | 5.15434700  |
| H | 2.06260700  | -1.71844200 | 6.94803500  |
| C | 1.79213800  | -3.57761600 | 1.15692000  |
| H | 1.60744200  | -3.77536800 | 0.09772400  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 2. 82972300  | -3. 24954400 | 1. 26612300  |
| H | 1. 69090500  | -4. 51435100 | 1. 71294100  |
| C | 4. 05105500  | 1. 57564600  | 1. 40249500  |
| C | 5. 22827900  | 2. 24487000  | 1. 76722900  |
| C | 4. 17434300  | 0. 34144700  | 0. 74559000  |
| C | 6. 48455100  | 1. 70162100  | 1. 48176000  |
| H | 5. 17836300  | 3. 19522800  | 2. 28787900  |
| C | 5. 42544600  | -0. 20839300 | 0. 46555200  |
| H | 3. 27646700  | -0. 19121200 | 0. 44654700  |
| C | 6. 58886700  | 0. 47243400  | 0. 83180300  |
| H | 7. 38067600  | 2. 24135900  | 1. 77553300  |
| H | 5. 49345800  | -1. 16385200 | -0. 04443100 |
| H | 7. 56423900  | 0. 04685900  | 0. 61449000  |
| C | 2. 65903600  | 3. 09493000  | 2. 91125300  |
| H | 1. 64481500  | 3. 41363100  | 3. 16450300  |
| H | 3. 10053700  | 2. 62130000  | 3. 79378700  |
| H | 3. 22604400  | 4. 00343000  | 2. 68872000  |
| C | -2. 33369500 | 4. 00787300  | -0. 13047300 |
| C | -1. 91638800 | 5. 20630700  | 0. 46534200  |
| C | -3. 61713900 | 3. 52744700  | 0. 17369900  |
| C | -2. 75412600 | 5. 90045400  | 1. 34197400  |
| H | -0. 92715000 | 5. 59727800  | 0. 24749300  |
| C | -4. 45704800 | 4. 21921700  | 1. 04830800  |
| H | -3. 96177600 | 2. 60377300  | -0. 28521300 |
| C | -4. 02707600 | 5. 41011900  | 1. 63869200  |
| H | -2. 40877500 | 6. 82599000  | 1. 79465400  |
| H | -5. 44690100 | 3. 82869200  | 1. 26947300  |
| H | -4. 67688300 | 5. 94897300  | 2. 32224100  |
| C | -1. 86249100 | 3. 69054600  | -2. 57188000 |
| H | -2. 91014800 | 3. 43963300  | -2. 76168100 |
| H | -1. 75937900 | 4. 77149300  | -2. 70704300 |
| H | -1. 24551400 | 3. 18913700  | -3. 32373500 |
| C | -2. 93777400 | -5. 81231100 | 1. 29602900  |
| C | 2. 96807000  | 5. 52433500  | -2. 00182700 |
| H | 3. 82359700  | 5. 87903300  | -1. 42001300 |
| H | 3. 36176700  | 5. 07879500  | -2. 92374000 |
| H | 2. 36765200  | 6. 39190100  | -2. 29293000 |
| H | -3. 95935600 | -5. 90122400 | 1. 67686600  |
| H | -2. 93366100 | -6. 21528000 | 0. 27561700  |
| H | -2. 28947100 | -6. 45456000 | 1. 89961400  |
| C | 3. 71301600  | -2. 70771600 | -2. 84405600 |
| C | -1. 13265500 | 0. 05373100  | -4. 54032400 |
| H | -0. 17666700 | -0. 04134400 | -5. 06787600 |
| H | -1. 92349200 | -0. 24721900 | -5. 23930400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.28523500 | 1.10803400  | -4.29664400 |
| F | 2.95002000  | 0.74682700  | -2.08585500 |
| F | 5.09857700  | -0.80071800 | -2.67024600 |
| F | 4.78212800  | -3.46460800 | -3.14787300 |
| F | 2.32709900  | -4.59028000 | -3.07212200 |

### TS(R)-2

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.23554500 | -3.44609000 | -0.08881000 |
| C  | -1.99237900 | -2.84875500 | -0.27557200 |
| C  | -1.79506900 | -1.78522600 | -1.14389200 |
| C  | -2.91344500 | -1.32847400 | -1.89171600 |
| C  | -4.15858600 | -1.92154400 | -1.69745400 |
| C  | -2.72752900 | -0.24308200 | -2.93147100 |
| H  | -2.45999100 | 0.69581300  | -2.43439500 |
| H  | -3.67326900 | -0.06321100 | -3.44931600 |
| C  | -1.64358700 | -0.58810700 | -3.98919900 |
| H  | -1.98339400 | -1.47123700 | -4.54327400 |
| H  | -1.59813200 | 0.23485400  | -4.71265900 |
| C  | -0.22739100 | -0.86444600 | -3.44350300 |
| C  | 0.59860200  | 0.22125900  | -2.99443700 |
| H  | 0.24237900  | 1.24251300  | -3.10748100 |
| H  | 1.67603500  | 0.10952100  | -3.08422400 |
| Ni | -0.15413200 | -0.60191300 | -1.34660700 |
| H  | -0.75768100 | -1.66844500 | -2.23408400 |
| C  | 0.49426200  | 0.32047300  | 0.19354900  |
| C  | 0.70731600  | 1.72960300  | 2.08545100  |
| C  | 2.05228700  | 1.06720700  | 1.81662200  |
| H  | 0.71871700  | 2.78863800  | 1.80371000  |
| H  | 0.38201300  | 1.63970200  | 3.12083200  |
| H  | 2.87943400  | 1.77602300  | 1.77259800  |
| H  | 2.27962500  | 0.29659500  | 2.56128500  |
| N  | 1.81801000  | 0.44151800  | 0.49201500  |
| N  | -0.18936900 | 0.97183700  | 1.17621700  |
| C  | 2.93334400  | 0.00423300  | -0.30309700 |
| C  | 3.56385600  | 0.93786600  | -1.16591900 |
| C  | 3.44763100  | -1.30064100 | -0.16474100 |
| C  | 4.69209800  | 0.52682100  | -1.87994800 |
| C  | 4.58567500  | -1.65617900 | -0.90297500 |
| C  | 5.22218800  | -0.76429900 | -1.76234000 |
| H  | 5.17789800  | 1.22555400  | -2.55368200 |
| H  | 4.97511900  | -2.66567200 | -0.80251900 |
| C  | -1.62094000 | 1.02337400  | 1.32026400  |
| C  | -2.35479700 | 2.09880800  | 0.77618600  |
| C  | -2.27437200 | 0.01561000  | 2.07779900  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.75145400 | 2.08301400  | 0.89276900  |
| C | -3.66783800 | 0.05528500  | 2.16531300  |
| C | -4.42749600 | 1.06223200  | 1.55721800  |
| H | -4.32434100 | 2.89141000  | 0.44893700  |
| H | -4.18754600 | -0.71811600 | 2.72033700  |
| C | 2.85553700  | -2.33306000 | 0.80056100  |
| C | 3.02639200  | 2.35995100  | -1.32515300 |
| C | -1.66875700 | 3.33928700  | 0.18642300  |
| C | -1.48207200 | -1.06138200 | 2.82498300  |
| H | -0.72064500 | -1.44139100 | 2.13790000  |
| H | 1.83920700  | -2.00941100 | 1.04633000  |
| H | 1.94400900  | 2.30294400  | -1.18055400 |
| H | -0.64105300 | 3.05739600  | -0.05876700 |
| C | 2.72869600  | -3.71208500 | 0.14425300  |
| C | 3.46621800  | -4.82841500 | 0.55891500  |
| C | 1.83423800  | -3.87389300 | -0.92651600 |
| C | 3.31917300  | -6.06600800 | -0.07805100 |
| H | 4.16282500  | -4.74821100 | 1.38656000  |
| C | 1.68467200  | -5.10394300 | -1.56331100 |
| H | 1.24659400  | -3.02188000 | -1.25692900 |
| C | 2.43001900  | -6.20944200 | -1.14153100 |
| H | 3.90294400  | -6.91641100 | 0.26364800  |
| H | 0.98306300  | -5.20181900 | -2.38731300 |
| H | 2.31422400  | -7.17007300 | -1.63525000 |
| C | 3.67088300  | -2.35330000 | 2.10951300  |
| H | 4.71109600  | -2.64233900 | 1.92901400  |
| H | 3.68783500  | -1.36151400 | 2.56755100  |
| H | 3.24098700  | -3.05492700 | 2.83175600  |
| C | 3.56489700  | 3.34588600  | -0.28184900 |
| C | 4.86927300  | 3.26782800  | 0.22636700  |
| C | 2.75271300  | 4.41108700  | 0.13887100  |
| C | 5.34386500  | 4.22015800  | 1.13219500  |
| H | 5.51655100  | 2.45205800  | -0.08074900 |
| C | 3.22367200  | 5.36489200  | 1.04272600  |
| H | 1.74147500  | 4.49660000  | -0.25269800 |
| C | 4.52360300  | 5.27152900  | 1.54536100  |
| H | 6.35709000  | 4.13747800  | 1.51582200  |
| H | 2.57483000  | 6.17839500  | 1.35530000  |
| H | 4.89227800  | 6.00972600  | 2.25164200  |
| C | 3.25157000  | 2.94874600  | -2.73719300 |
| H | 2.87837000  | 2.27284500  | -3.51215200 |
| H | 2.71910600  | 3.90029500  | -2.82542500 |
| H | 4.30871100  | 3.15186300  | -2.93248000 |
| C | -2.29303700 | 3.85036100  | -1.11249100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.35642700 | 4.76569600  | -1.14092200 |
| C | -1.77133900 | 3.41583400  | -2.33928200 |
| C | -3.89068200 | 5.21126700  | -2.35275600 |
| H | -3.77195600 | 5.14905000  | -0.21443700 |
| C | -2.29855000 | 3.85912700  | -3.55316000 |
| H | -0.93580400 | 2.72290800  | -2.33629300 |
| C | -3.36635800 | 4.75882400  | -3.56450900 |
| H | -4.71467100 | 5.91939500  | -2.34672700 |
| H | -1.86994000 | 3.50719900  | -4.48755500 |
| H | -3.77932000 | 5.10936300  | -4.50589700 |
| C | -1.60479900 | 4.44416400  | 1.26783800  |
| H | -1.07444600 | 4.09021400  | 2.15564900  |
| H | -1.08856800 | 5.33096800  | 0.88616200  |
| H | -2.60543000 | 4.74413500  | 1.59207300  |
| C | -0.76119000 | -0.51671000 | 4.06267500  |
| C | -1.34920500 | 0.44048000  | 4.90247300  |
| C | 0.48494300  | -1.04525300 | 4.43077100  |
| C | -0.70312400 | 0.86767700  | 6.06512600  |
| H | -2.31595500 | 0.86031800  | 4.63982700  |
| C | 1.13423700  | -0.62097700 | 5.59209700  |
| H | 0.94837800  | -1.80143200 | 3.80156000  |
| C | 0.54290800  | 0.34153200  | 6.41353900  |
| H | -1.17510900 | 1.61351300  | 6.69893100  |
| H | 2.10130600  | -1.04174900 | 5.85346200  |
| H | 1.04630000  | 0.67609800  | 7.31596300  |
| C | -2.32113100 | -2.27664800 | 3.27798000  |
| H | -1.65586200 | -3.02696600 | 3.71440400  |
| H | -3.04460900 | -1.99876800 | 4.05083600  |
| H | -2.85708200 | -2.74617000 | 2.45249800  |
| C | 6.43311300  | -1.17695800 | -2.56562500 |
| C | -5.93602800 | 1.03605400  | 1.62424300  |
| H | -6.36370000 | 2.02089500  | 1.41649300  |
| H | -6.34748100 | 0.33624500  | 0.88652900  |
| H | -6.28791300 | 0.70990800  | 2.60819200  |
| H | 6.88777500  | -2.08648900 | -2.16371700 |
| H | 6.16416800  | -1.37667400 | -3.61011000 |
| H | 7.19384200  | -0.38962800 | -2.57461800 |
| C | -4.33241000 | -2.97259700 | -0.79949700 |
| C | 0.47581900  | -2.04804900 | -4.10992300 |
| H | -0.10662000 | -2.97323300 | -4.03026600 |
| H | 0.61458300  | -1.84058200 | -5.17871400 |
| H | 1.46179500  | -2.22513900 | -3.67209100 |
| F | -0.96469300 | -3.33553900 | 0.47100100  |
| F | -3.40394700 | -4.44630500 | 0.79998900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | -5.54302000 | -3.52995500 | -0.62255500 |
| F | -5.24876100 | -1.50514300 | -2.38459900 |

### TS(R)-3

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.23420800 | -3.44732200 | -0.08946000 |
| C  | -1.99130300 | -2.84942100 | -0.27614500 |
| C  | -1.79447600 | -1.78564500 | -1.14427500 |
| C  | -2.91306100 | -1.32925400 | -1.89200700 |
| C  | -4.15794200 | -1.92289600 | -1.69782200 |
| C  | -2.72762500 | -0.24364700 | -2.93162600 |
| H  | -2.46048500 | 0.69530600  | -2.43444600 |
| H  | -3.67344400 | -0.06412300 | -3.44944700 |
| C  | -1.64353800 | -0.58808800 | -3.98939700 |
| H  | -1.98297400 | -1.47128700 | -4.54359000 |
| H  | -1.59842300 | 0.23498400  | -4.71275100 |
| C  | -0.22723100 | -0.86389800 | -3.44371900 |
| C  | 0.59830900  | 0.22210900  | -2.99454400 |
| H  | 0.24163100  | 1.24322300  | -3.10745300 |
| H  | 1.67578700  | 0.11085300  | -3.08440000 |
| Ni | -0.15401500 | -0.60161500 | -1.34679300 |
| H  | -0.75717400 | -1.66823600 | -2.23444300 |
| C  | 0.49413300  | 0.32070200  | 0.19352500  |
| C  | 0.70682800  | 1.72951800  | 2.08570600  |
| C  | 2.05201200  | 1.06765200  | 1.81664800  |
| H  | 0.71785100  | 2.78861400  | 1.80419500  |
| H  | 0.38161400  | 1.63928900  | 3.12108600  |
| H  | 2.87889500  | 1.77678200  | 1.77269400  |
| H  | 2.27966900  | 0.29698000  | 2.56114900  |
| N  | 1.81786100  | 0.44213700  | 0.49193500  |
| N  | -0.18965500 | 0.97163600  | 1.17636700  |
| C  | 2.93330800  | 0.00530700  | -0.30327400 |
| C  | 3.56339700  | 0.93919400  | -1.16613600 |
| C  | 3.44813600  | -1.29935700 | -0.16493300 |
| C  | 4.69178000  | 0.52860100  | -1.88020900 |
| C  | 4.58629600  | -1.65443400 | -0.90321200 |
| C  | 5.22240500  | -0.76230100 | -1.76260900 |
| H  | 5.17728700  | 1.22751200  | -2.55397400 |
| H  | 4.97616200  | -2.66376500 | -0.80276200 |
| C  | -1.62122700 | 1.02272900  | 1.32053500  |
| C  | -2.35541700 | 2.09812700  | 0.77682800  |
| C  | -2.27432700 | 0.01460300  | 2.07786600  |
| C  | -3.75205100 | 2.08198500  | 0.89358900  |
| C  | -3.66779600 | 0.05393500  | 2.16557300  |
| C  | -4.42777000 | 1.06087200  | 1.55786500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.32517200 | 2.89038000  | 0.45005600  |
| H | -4.18724600 | -0.71973700 | 2.72045600  |
| C | 2.85651800  | -2.33202000 | 0.80039300  |
| C | 3.02531600  | 2.36104900  | -1.32535400 |
| C | -1.66977200 | 3.33893100  | 0.18729400  |
| C | -1.48169700 | -1.06243400 | 2.82463000  |
| H | -0.72033100 | -1.44213100 | 2.13731000  |
| H | 1.84008800  | -2.00875000 | 1.04625700  |
| H | 1.94292600  | 2.30351100  | -1.18103300 |
| H | -0.64199300 | 3.05740300  | -0.05800200 |
| C | 2.73012300  | -3.71107600 | 0.14405600  |
| C | 3.46784600  | -4.82723100 | 0.55883100  |
| C | 1.83585200  | -3.87310400 | -0.92683500 |
| C | 3.32116300  | -6.06486800 | -0.07813500 |
| H | 4.16432600  | -4.74685800 | 1.38656500  |
| C | 1.68664700  | -5.10319600 | -1.56363100 |
| H | 1.24807100  | -3.02122800 | -1.25734500 |
| C | 2.43218200  | -6.20852200 | -1.14172900 |
| H | 3.90508100  | -6.91513400 | 0.26365600  |
| H | 0.98517000  | -5.20124000 | -2.38772500 |
| H | 2.31666700  | -7.16918700 | -1.63544600 |
| C | 3.67199800  | -2.35200200 | 2.10926300  |
| H | 4.71228300  | -2.64071400 | 1.92865000  |
| H | 3.68868700  | -1.36021600 | 2.56730700  |
| H | 3.24240400  | -3.05376600 | 2.83155300  |
| C | 3.56310800  | 3.34710300  | -0.28180400 |
| C | 4.86751200  | 3.26976600  | 0.22645400  |
| C | 2.75023000  | 4.41170100  | 0.13909500  |
| C | 5.34144700  | 4.22219200  | 1.13252500  |
| H | 5.51533000  | 2.45448300  | -0.08082200 |
| C | 3.22053000  | 5.36559900  | 1.04319900  |
| H | 1.73896700  | 4.49667300  | -0.25252900 |
| C | 4.52048900  | 5.27294500  | 1.54588900  |
| H | 6.35470400  | 4.14007400  | 1.51618500  |
| H | 2.57115300  | 6.17861900  | 1.35591600  |
| H | 4.88865500  | 6.01121200  | 2.25236200  |
| C | 3.25054700  | 2.95013600  | -2.73725500 |
| H | 2.87788800  | 2.27415300  | -3.51240200 |
| H | 2.71761100  | 3.90142100  | -2.82548300 |
| H | 4.30762900  | 3.15383500  | -2.93224600 |
| C | -2.29426100 | 3.85003400  | -1.11150800 |
| C | -3.35771100 | 4.76529900  | -1.13977400 |
| C | -1.77269300 | 3.41556300  | -2.33837500 |
| C | -3.89213300 | 5.21088300  | -2.35153200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.77315600 | 5.14859500  | -0.21322800 |
| C | -2.30007400 | 3.85886600  | -3.55217400 |
| H | -0.93713500 | 2.72266300  | -2.33549400 |
| C | -3.36792900 | 4.75851300  | -3.56336200 |
| H | -4.71616200 | 5.91896500  | -2.34538100 |
| H | -1.87156500 | 3.50698600  | -4.48663400 |
| H | -3.78102000 | 5.10906400  | -4.50468900 |
| C | -1.60610200 | 4.44360600  | 1.26892500  |
| H | -1.07563000 | 4.08961800  | 2.15665100  |
| H | -1.09012900 | 5.33063600  | 0.88742400  |
| H | -2.60680800 | 4.74322800  | 1.59325000  |
| C | -0.76067000 | -0.51798500 | 4.06233100  |
| C | -1.34865600 | 0.43889800  | 4.90249700  |
| C | 0.48560900  | -1.04645400 | 4.43004000  |
| C | -0.70240900 | 0.86587100  | 6.06514100  |
| H | -2.31551300 | 0.85867700  | 4.64014500  |
| C | 1.13506700  | -0.62240300 | 5.59135400  |
| H | 0.94902400  | -1.80239700 | 3.80052900  |
| C | 0.54376300  | 0.33980300  | 6.41317000  |
| H | -1.17437300 | 1.61147200  | 6.69924000  |
| H | 2.10224600  | -1.04310900 | 5.85242100  |
| H | 1.04728200  | 0.67419500  | 7.31558800  |
| C | -2.32046300 | -2.27797000 | 3.27745300  |
| H | -1.65499000 | -3.02828600 | 3.71356900  |
| H | -3.04386300 | -2.00041300 | 4.05049900  |
| H | -2.85647100 | -2.74736700 | 2.45193400  |
| C | 6.43347400  | -1.17449200 | -2.56592100 |
| C | -5.93628700 | 1.03433900  | 1.62508200  |
| H | -6.36417300 | 2.01935300  | 1.41858900  |
| H | -6.34772400 | 0.33536300  | 0.88656700  |
| H | -6.28795800 | 0.70692400  | 2.60868300  |
| H | 6.16455600  | -1.37449800 | -3.61035700 |
| H | 7.19380000  | -0.38677600 | -2.57507600 |
| H | 6.88862300  | -2.08373700 | -2.16391300 |
| C | -4.33129100 | -2.97418100 | -0.80004400 |
| C | 0.47648000  | -2.04714300 | -4.11024800 |
| H | -0.10558200 | -2.97257300 | -4.03068900 |
| H | 0.61518300  | -1.83952200 | -5.17901600 |
| H | 1.46251800  | -2.22387500 | -3.67240700 |
| F | -0.96338500 | -3.33592000 | 0.47029800  |
| F | -3.40216200 | -4.44776900 | 0.79916200  |
| F | -5.54165500 | -3.53209900 | -0.62318000 |
| F | -5.24830600 | -1.50686000 | -2.38488600 |

**TS(R)-4**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.23680300 | -3.44391300 | -0.08732200 |
| C  | -1.99304000 | -2.84787100 | -0.27420800 |
| C  | -1.79462700 | -1.78484800 | -1.14289500 |
| C  | -2.91252000 | -1.32715900 | -1.89085400 |
| C  | -4.15826800 | -1.91890200 | -1.69642500 |
| C  | -2.72552800 | -0.24200100 | -2.93065300 |
| H  | -2.45730800 | 0.69667800  | -2.43354400 |
| H  | -3.67105500 | -0.06134500 | -3.44861800 |
| C  | -1.64177200 | -0.58787000 | -3.98829400 |
| H  | -1.98234600 | -1.47059400 | -4.54254100 |
| H  | -1.59552700 | 0.23516600  | -4.71162200 |
| C  | -0.22581800 | -0.86564100 | -3.44267400 |
| C  | 0.60127700  | 0.21914300  | -2.99345500 |
| H  | 0.24623300  | 1.24079800  | -3.10652900 |
| H  | 1.67860500  | 0.10614100  | -3.08304900 |
| Ni | -0.15264000 | -0.60313700 | -1.34575100 |
| H  | -0.75697200 | -1.66935400 | -2.23305400 |
| C  | 0.49553200  | 0.31973400  | 0.19425300  |
| C  | 0.70775700  | 1.73043500  | 2.08513600  |
| C  | 2.05286800  | 1.06784400  | 1.81740700  |
| H  | 0.71932900  | 2.78929200  | 1.80276500  |
| H  | 0.38197200  | 1.64118600  | 3.12042200  |
| H  | 2.87994900  | 1.77672200  | 1.77286600  |
| H  | 2.28018200  | 0.29804700  | 2.56293300  |
| N  | 1.81912000  | 0.44069000  | 0.49340000  |
| N  | -0.18852500 | 0.97214000  | 1.17594800  |
| C  | 2.93536500  | 0.00196300  | -0.29959800 |
| C  | 3.56728000  | 0.93451000  | -1.16309700 |
| C  | 3.44619200  | -1.30408500 | -0.16250200 |
| C  | 4.69499200  | 0.52181600  | -1.87639700 |
| C  | 4.58393800  | -1.66159800 | -0.90083300 |
| C  | 5.22513900  | -0.76932800 | -1.75584500 |
| H  | 5.17900900  | 1.21804900  | -2.55400500 |
| H  | 4.96826500  | -2.67338500 | -0.80461800 |
| C  | -1.62017700 | 1.02374600  | 1.31923600  |
| C  | -2.35384700 | 2.09862600  | 0.77378300  |
| C  | -2.27394200 | 0.01659100  | 2.07728600  |
| C  | -3.75057500 | 2.08266200  | 0.88939900  |
| C  | -3.66748100 | 0.05607900  | 2.16380400  |
| C  | -4.42689700 | 1.06229700  | 1.55422800  |
| H  | -4.32332800 | 2.89055300  | 0.44449200  |
| H  | -4.18742500 | -0.71691800 | 2.71917000  |
| C  | 2.84917300  | -2.33736300 | 0.79893600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.02832800  | 2.35556800  | -1.32687900 |
| C | -1.66749100 | 3.33877000  | 0.18367400  |
| C | -1.48196100 | -1.05942600 | 2.82621400  |
| H | -0.71977700 | -1.43985100 | 2.14019700  |
| H | 1.83253700  | -2.01276300 | 1.04198200  |
| H | 1.94571200  | 2.29769100  | -1.18454600 |
| H | -0.63967300 | 3.05667600  | -0.06080000 |
| C | 2.72257700  | -3.71527300 | 0.14035200  |
| C | 3.46015100  | -4.83221300 | 0.55334700  |
| C | 1.82843600  | -3.87540900 | -0.93090100 |
| C | 3.31340800  | -6.06877000 | -0.08567900 |
| H | 4.15651900  | -4.75329600 | 1.38132300  |
| C | 1.67919400  | -5.10442800 | -1.56978200 |
| H | 1.24066300  | -3.02293600 | -1.25991100 |
| C | 2.42453700  | -6.21053800 | -1.14962900 |
| H | 3.89715700  | -6.91968100 | 0.25479200  |
| H | 0.97781600  | -5.20103000 | -2.39412800 |
| H | 2.30895200  | -7.17037100 | -1.64494800 |
| C | 3.66021200  | -2.36076800 | 2.11054700  |
| H | 4.70087400  | -2.65002100 | 1.93299000  |
| H | 3.67618500  | -1.36993400 | 2.57068900  |
| H | 3.22744500  | -3.06365300 | 2.82985300  |
| C | 3.56357500  | 3.34427300  | -0.28457100 |
| C | 4.86792600  | 3.27024700  | 0.22430700  |
| C | 2.74861600  | 4.40813500  | 0.13411700  |
| C | 5.33978900  | 4.22509800  | 1.12888400  |
| H | 5.51734700  | 2.45561700  | -0.08136200 |
| C | 3.21682700  | 5.36448000  | 1.03673400  |
| H | 1.73740500  | 4.49066600  | -0.25815500 |
| C | 4.51674300  | 5.27507300  | 1.54010300  |
| H | 6.35306100  | 4.14553700  | 1.51304700  |
| H | 2.56586200  | 6.17689600  | 1.34771300  |
| H | 4.88329400  | 6.01524700  | 2.24541800  |
| C | 3.25618100  | 2.94173800  | -2.73957400 |
| H | 2.88573300  | 2.26382300  | -3.51408800 |
| H | 2.72271600  | 3.89242800  | -2.83096700 |
| H | 4.31355100  | 3.14581700  | -2.93266000 |
| C | -2.29096400 | 3.84940500  | -1.11579900 |
| C | -3.35514300 | 4.76381400  | -1.14515200 |
| C | -1.76764000 | 3.41560400  | -2.34215500 |
| C | -3.88860600 | 5.20909500  | -2.35743300 |
| H | -3.77192300 | 5.14668200  | -0.21902700 |
| C | -2.29405200 | 3.85862400  | -3.55648800 |
| H | -0.93145200 | 2.72347100  | -2.33850000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.36267800 | 4.75732400  | -3.56874700 |
| H | -4.71324100 | 5.91647600  | -2.35209900 |
| H | -1.86417900 | 3.50725500  | -4.49051200 |
| H | -3.77503800 | 5.10763400  | -4.51048400 |
| C | -1.60407300 | 4.44420700  | 1.26457500  |
| H | -1.07434400 | 4.09066300  | 2.15292300  |
| H | -1.08749600 | 5.33075000  | 0.88276100  |
| H | -2.60488000 | 4.74447700  | 1.58798500  |
| C | -0.76243100 | -0.51317900 | 4.06400400  |
| C | -1.35162700 | 0.44464700  | 4.90224900  |
| C | 0.48361900  | -1.04074100 | 4.43378000  |
| C | -0.70677900 | 0.87340700  | 6.06500600  |
| H | -2.31833200 | 0.86377300  | 4.63831100  |
| C | 1.13168600  | -0.61490200 | 5.59522000  |
| H | 0.94800100  | -1.79733500 | 3.80577700  |
| C | 0.53919000  | 0.34822400  | 6.41509700  |
| H | -1.17967100 | 1.61971700  | 6.69757600  |
| H | 2.09872500  | -1.03493400 | 5.85788800  |
| H | 1.04163400  | 0.68400600  | 7.31759700  |
| C | -2.32097000 | -2.27454900 | 3.27968900  |
| H | -1.65579800 | -3.02412400 | 3.71754400  |
| H | -3.04527500 | -1.99615900 | 4.05158400  |
| H | -2.85593900 | -2.74517600 | 2.45420400  |
| C | 6.46179100  | -1.16878600 | -2.52618900 |
| C | -5.93547500 | 1.03581300  | 1.62002500  |
| H | -6.36316600 | 2.02069400  | 1.41249300  |
| H | -6.34618300 | 0.33637800  | 0.88153500  |
| H | -6.28810200 | 0.70901400  | 2.60348600  |
| H | 7.35493400  | -0.67520500 | -2.12411200 |
| H | 6.63018000  | -2.24790300 | -2.47933900 |
| H | 6.38500600  | -0.88193800 | -3.58032300 |
| C | -4.33317500 | -2.96951600 | -0.79816300 |
| C | 0.47615400  | -2.04975400 | -4.10947400 |
| H | -0.10704600 | -2.97445600 | -4.02977700 |
| H | 0.61463100  | -1.84219000 | -5.17828300 |
| H | 1.46218100  | -2.22772900 | -3.67214500 |
| F | -0.96590500 | -3.33534800 | 0.47268200  |
| F | -3.40623700 | -4.44366300 | 0.80181600  |
| F | -5.54436800 | -3.52556200 | -0.62104700 |
| F | -5.24804700 | -1.50150300 | -2.38360100 |

**TS(R)-5**

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 3.72048100 | -1.76661400 | -2.60586200 |
| C | 2.66093100 | -0.89682000 | -2.36695600 |



|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | 1. 35494100  | -1. 32835300 | -2. 20610000 |
| C  | 1. 08766800  | -2. 70723200 | -2. 41251000 |
| C  | 2. 14483700  | -3. 57994600 | -2. 65757700 |
| C  | -0. 35079200 | -3. 17935800 | -2. 46922600 |
| H  | -0. 82205000 | -3. 06344800 | -1. 48691400 |
| H  | -0. 38271900 | -4. 24477400 | -2. 71262800 |
| C  | -1. 18116200 | -2. 40169800 | -3. 52785300 |
| H  | -0. 74000600 | -2. 59704900 | -4. 51245100 |
| H  | -2. 19376300 | -2. 82149000 | -3. 54906300 |
| C  | -1. 27298800 | -0. 87401300 | -3. 32083500 |
| C  | -2. 11430700 | -0. 34890000 | -2. 27885200 |
| H  | -2. 70762400 | -1. 03355800 | -1. 67759600 |
| H  | -2. 58356600 | 0. 61584100  | -2. 45953600 |
| Ni | -0. 28009000 | -0. 28478400 | -1. 53850600 |
| H  | 0. 16784700  | -0. 74939100 | -2. 92110800 |
| C  | -0. 41186900 | 0. 38265700  | 0. 24733000  |
| C  | -1. 05610900 | 0. 61101500  | 2. 51848300  |
| C  | -0. 51031700 | 1. 94344600  | 2. 02308800  |
| H  | -2. 02586700 | 0. 71475500  | 3. 00259400  |
| H  | -0. 37241800 | 0. 10453500  | 3. 20739700  |
| H  | -1. 30104900 | 2. 68253100  | 1. 85380700  |
| H  | 0. 22720600  | 2. 37235100  | 2. 69895000  |
| N  | 0. 09493800  | 1. 55770700  | 0. 72571600  |
| N  | -1. 16354100 | -0. 15699800 | 1. 25390800  |
| C  | 0. 97927400  | 2. 46029500  | 0. 03445300  |
| C  | 0. 50239600  | 3. 25347800  | -1. 03831200 |
| C  | 2. 31117000  | 2. 60592600  | 0. 48927300  |
| C  | 1. 41077500  | 4. 07827600  | -1. 70959400 |
| C  | 3. 16837200  | 3. 46795200  | -0. 20577600 |
| C  | 2. 75161400  | 4. 18700200  | -1. 32438600 |
| H  | 1. 06597700  | 4. 67271700  | -2. 54913000 |
| H  | 4. 19508500  | 3. 56548700  | 0. 13701000  |
| C  | -1. 77946000 | -1. 45871000 | 1. 24436600  |
| C  | -3. 19073300 | -1. 56619300 | 1. 24033000  |
| C  | -0. 97494200 | -2. 62648900 | 1. 31903800  |
| C  | -3. 76504100 | -2. 84371900 | 1. 20727400  |
| C  | -1. 60797300 | -3. 87305000 | 1. 28353200  |
| C  | -2. 99815900 | -4. 00654700 | 1. 20684100  |
| H  | -4. 84651900 | -2. 93032000 | 1. 17595000  |
| H  | -1. 00546800 | -4. 77394000 | 1. 32514200  |
| C  | 2. 82061900  | 1. 97188600  | 1. 78644600  |
| C  | -0. 98341000 | 3. 29448300  | -1. 39450800 |
| C  | -4. 12178600 | -0. 35096400 | 1. 38539500  |
| C  | 0. 54197700  | -2. 55093200 | 1. 50573700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.91107800  | -1.73788200 | 0.87467300  |
| H | 2.10743300  | 1.19160300  | 2.07394600  |
| H | -1.37549200 | 2.28113400  | -1.28045200 |
| H | -3.53374800 | 0.54097400  | 1.15081900  |
| C | 4.18414800  | 1.27691000  | 1.66432600  |
| C | 5.11282800  | 1.27759700  | 2.71756500  |
| C | 4.51472800  | 0.55829400  | 0.50484100  |
| C | 6.32133300  | 0.58162400  | 2.61636000  |
| H | 4.90707900  | 1.82506700  | 3.63049900  |
| C | 5.72061000  | -0.13679400 | 0.39933800  |
| H | 3.83451600  | 0.56721300  | -0.33671800 |
| C | 6.63102700  | -0.13086700 | 1.45805800  |
| H | 7.02121500  | 0.60354900  | 3.44737000  |
| H | 5.94201400  | -0.67568500 | -0.51674900 |
| H | 7.57097300  | -0.66959000 | 1.37879200  |
| C | 2.81109400  | 3.04828500  | 2.90016800  |
| H | 3.62892500  | 3.76204900  | 2.75907400  |
| H | 1.87894200  | 3.61820700  | 2.88705100  |
| H | 2.91343900  | 2.60135600  | 3.89330700  |
| C | -1.78152000 | 4.19879100  | -0.44598300 |
| C | -1.26018600 | 5.39754500  | 0.06197600  |
| C | -3.10181500 | 3.85960300  | -0.11314200 |
| C | -2.03258700 | 6.22719300  | 0.87818100  |
| H | -0.23963500 | 5.68158000  | -0.17620900 |
| C | -3.87698100 | 4.68495300  | 0.70404700  |
| H | -3.53139200 | 2.94011700  | -0.50171000 |
| C | -3.34356900 | 5.87449100  | 1.20480500  |
| H | -1.60621000 | 7.15032900  | 1.26138100  |
| H | -4.89546100 | 4.39654300  | 0.94922200  |
| H | -3.94219800 | 6.51829500  | 1.84275800  |
| C | -1.26454700 | 3.71573800  | -2.85315400 |
| H | -0.68425500 | 3.11246400  | -3.55820900 |
| H | -2.32706200 | 3.58067400  | -3.07630200 |
| H | -1.03014400 | 4.77011300  | -3.02803200 |
| C | -5.31188700 | -0.35064900 | 0.42069600  |
| C | -6.53016600 | -0.98526500 | 0.71216000  |
| C | -5.21166200 | 0.33406200  | -0.79886400 |
| C | -7.59478700 | -0.95506600 | -0.19201300 |
| H | -6.66689300 | -1.50160500 | 1.65684800  |
| C | -6.27226200 | 0.37117900  | -1.70532600 |
| H | -4.28607300 | 0.84464400  | -1.04067400 |
| C | -7.47075500 | -0.27943800 | -1.40682600 |
| H | -8.52524500 | -1.45621900 | 0.06008800  |
| H | -6.16236800 | 0.91356300  | -2.64029500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -8.30030800 | -0.25242800 | -2.10734600 |
| C | -4.59437500 | -0.23695200 | 2.85505100  |
| H | -3.74752300 | -0.16649600 | 3.54208800  |
| H | -5.22399700 | 0.64793800  | 2.99081700  |
| H | -5.16971700 | -1.11597800 | 3.15799300  |
| C | 0.94635200  | -2.22896200 | 2.94903500  |
| C | 0.20317900  | -2.66456100 | 4.05516400  |
| C | 2.14358700  | -1.53583900 | 3.18517300  |
| C | 0.63847900  | -2.40513400 | 5.35765100  |
| H | -0.72585900 | -3.20470500 | 3.89905200  |
| C | 2.58174200  | -1.27547200 | 4.48495700  |
| H | 2.74385500  | -1.20250300 | 2.34229000  |
| C | 1.82767300  | -1.70785400 | 5.57874800  |
| H | 0.04485400  | -2.74947700 | 6.20024800  |
| H | 3.51189100  | -0.73513600 | 4.63696800  |
| H | 2.16403000  | -1.50500100 | 6.59151200  |
| C | 1.29427300  | -3.82717100 | 1.06504700  |
| H | 2.37121200  | -3.63965300 | 1.09489200  |
| H | 1.09517900  | -4.66845100 | 1.73599500  |
| H | 1.03058000  | -4.12218300 | 0.04641100  |
| C | 3.71259500  | 5.05921000  | -2.09642900 |
| C | -3.64208600 | -5.37035300 | 1.12783700  |
| H | -4.68262900 | -5.34169200 | 1.46324600  |
| H | -3.64003300 | -5.74760200 | 0.09768500  |
| H | -3.10483600 | -6.10177300 | 1.73961200  |
| H | 4.52028100  | 5.42785000  | -1.45739900 |
| H | 4.17676500  | 4.49866500  | -2.91733900 |
| H | 3.20455700  | 5.92132700  | -2.53919200 |
| C | 3.46094300  | -3.12687900 | -2.73702700 |
| C | -1.15744200 | -0.06632700 | -4.61401600 |
| H | -0.21499800 | -0.26172800 | -5.13848900 |
| H | -1.97360800 | -0.33665300 | -5.29594300 |
| H | -1.22407700 | 1.00715400  | -4.41978300 |
| F | 2.95832100  | 0.43021300  | -2.29596700 |
| F | 4.98919200  | -1.31807100 | -2.70343300 |
| F | 4.46799400  | -3.98716100 | -2.96418100 |
| F | 1.93102300  | -4.90585200 | -2.83145000 |

### TS(S)-1

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 2.98856600 | -3.53244600 | -1.12282300 |
| C | 1.74122900 | -2.91587800 | -1.13951300 |
| C | 1.52940800 | -1.66492700 | -1.69649300 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | 2. 61257200  | -1. 04966400 | -2. 37725900 |
| C  | 3. 85560600  | -1. 67508100 | -2. 38251100 |
| C  | 2. 36890300  | 0. 23252000  | -3. 14576100 |
| H  | 2. 12608500  | 1. 04175400  | -2. 44668400 |
| H  | 3. 27995900  | 0. 52973500  | -3. 67180400 |
| C  | 1. 21886600  | 0. 08701400  | -4. 18129000 |
| H  | 1. 51627000  | -0. 67842000 | -4. 90757100 |
| H  | 1. 13302500  | 1. 02886300  | -4. 73591700 |
| C  | -0. 16514900 | -0. 28741300 | -3. 60634900 |
| C  | -0. 91770100 | 0. 70168200  | -2. 88528600 |
| H  | -0. 50090900 | 1. 70040500  | -2. 78950700 |
| H  | -2. 00410500 | 0. 65711100  | -2. 92943000 |
| Ni | -0. 07595800 | -0. 43001000 | -1. 49014300 |
| H  | 0. 41580800  | -1. 30009000 | -2. 63766300 |
| C  | 4. 05859800  | -2. 89651700 | -1. 74230300 |
| C  | -0. 93553400 | -1. 30203500 | -4. 44975800 |
| H  | -0. 37014100 | -2. 23072100 | -4. 59150900 |
| H  | -1. 12987200 | -0. 88437500 | -5. 44605300 |
| H  | -1. 89686000 | -1. 55057900 | -3. 99500700 |
| F  | 0. 71207900  | -3. 59942900 | -0. 56955000 |
| F  | 3. 17622200  | -4. 71707300 | -0. 50887700 |
| F  | 5. 28672200  | -3. 44845100 | -1. 70458900 |
| F  | 4. 92510300  | -1. 11131000 | -2. 99194000 |
| C  | -0. 53505500 | 0. 26531800  | 0. 22564200  |
| C  | -0. 77317100 | 1. 68881700  | 2. 11178800  |
| C  | -1. 75988600 | 0. 53478800  | 2. 23887000  |
| H  | 0. 04037900  | 1. 59387000  | 2. 83691900  |
| H  | -1. 23804800 | 2. 66872000  | 2. 22241300  |
| H  | -1. 70809500 | 0. 03347900  | 3. 20516600  |
| H  | -2. 79443300 | 0. 85301900  | 2. 05985800  |
| N  | -1. 31199600 | -0. 36692300 | 1. 14951100  |
| N  | -0. 25698700 | 1. 50150500  | 0. 73225100  |
| C  | -1. 80324900 | -1. 71825600 | 1. 11793600  |
| C  | -1. 06515900 | -2. 73045700 | 1. 78418600  |
| C  | -3. 07042700 | -1. 99894200 | 0. 56306000  |
| C  | -1. 60951300 | -4. 01542200 | 1. 84568600  |
| C  | -3. 58025200 | -3. 30045100 | 0. 68768800  |
| C  | -2. 86485300 | -4. 32283000 | 1. 30864100  |
| H  | -1. 05080800 | -4. 80522100 | 2. 33673800  |
| H  | -4. 56996800 | -3. 51845000 | 0. 29683500  |
| C  | 0. 49629100  | 2. 53622500  | 0. 07354700  |
| C  | 1. 87956200  | 2. 68915600  | 0. 32505300  |
| C  | -0. 18332100 | 3. 45123300  | -0. 77101900 |
| C  | 2. 58006500  | 3. 67946600  | -0. 37660900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.56710500  | 4.42289900  | -1.44008600 |
| C | 1.95207700  | 4.53837700  | -1.27801200 |
| H | 3.64724700  | 3.78498500  | -0.20898700 |
| H | 0.06532700  | 5.11738300  | -2.10541100 |
| C | -3.93860700 | -0.91484900 | -0.06646800 |
| C | 0.27797000  | -2.42964000 | 2.45246600  |
| C | 2.59560800  | 1.91462500  | 1.44199700  |
| C | -1.70686500 | 3.42344500  | -0.90953700 |
| H | -2.00889900 | 2.37322500  | -0.91486500 |
| H | -3.37229000 | 0.01938600  | -0.02788300 |
| H | 0.79020600  | -1.69607800 | 1.82266500  |
| H | 2.00877800  | 1.01375200  | 1.64223000  |
| C | -4.31802000 | -1.11250300 | -1.54271600 |
| C | -4.90808500 | -0.02554600 | -2.21381500 |
| C | -4.14126200 | -2.30118900 | -2.26306600 |
| C | -5.32652100 | -0.12624200 | -3.53998600 |
| H | -5.04443100 | 0.91623000  | -1.68784100 |
| C | -4.56503100 | -2.40905100 | -3.59305900 |
| H | -3.66669300 | -3.15578000 | -1.79577300 |
| C | -5.16318600 | -1.32692900 | -4.23709700 |
| H | -5.77983900 | 0.73204900  | -4.02811400 |
| H | -4.42086300 | -3.34659300 | -4.12303000 |
| H | -5.49246700 | -1.41316100 | -5.26845300 |
| C | -5.21888500 | -0.70744600 | 0.78544000  |
| H | -5.85406700 | -1.59813600 | 0.76657700  |
| H | -4.95983900 | -0.49891000 | 1.82811100  |
| H | -5.80844600 | 0.13164900  | 0.40566300  |
| C | 0.13295300  | -1.80311800 | 3.84390600  |
| C | -0.87422200 | -2.19364600 | 4.73859900  |
| C | 1.08034000  | -0.86478900 | 4.28134300  |
| C | -0.93829200 | -1.65417200 | 6.02609300  |
| H | -1.61870200 | -2.91904200 | 4.42408600  |
| C | 1.02024100  | -0.32366500 | 5.56735700  |
| H | 1.88039000  | -0.56389700 | 3.60902700  |
| C | 0.00672200  | -0.71531500 | 6.44543200  |
| H | -1.72968800 | -1.96841000 | 6.70107900  |
| H | 1.76385600  | 0.40350500  | 5.88155200  |
| H | -0.04529200 | -0.29412000 | 7.44522000  |
| C | 1.21455600  | -3.65464400 | 2.56709500  |
| H | 1.36002900  | -4.13640900 | 1.59879500  |
| H | 2.18919200  | -3.32780200 | 2.94172600  |
| H | 0.83073900  | -4.39433200 | 3.27651900  |
| C | 4.01232800  | 1.44509500  | 1.10170800  |
| C | 5.13905800  | 2.26485200  | 1.28140400  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 4. 22183300  | 0. 13909600  | 0. 63417900  |
| C | 6. 42382400  | 1. 80346300  | 0. 98690300  |
| H | 5. 02509000  | 3. 27253300  | 1. 66737600  |
| C | 5. 50614800  | -0. 32925900 | 0. 34372300  |
| H | 3. 36926900  | -0. 52073100 | 0. 49904500  |
| C | 6. 61313900  | 0. 50350100  | 0. 51593100  |
| H | 7. 27645600  | 2. 46040200  | 1. 13482200  |
| H | 5. 64429300  | -1. 34314500 | -0. 01872300 |
| H | 7. 61210800  | 0. 14059600  | 0. 29226200  |
| C | 2. 58847500  | 2. 77782100  | 2. 72881100  |
| H | 1. 57048700  | 3. 04946600  | 3. 01645700  |
| H | 3. 05035100  | 2. 23591700  | 3. 56017300  |
| H | 3. 13717200  | 3. 71221900  | 2. 58264200  |
| C | -2. 42104300 | 4. 09074200  | 0. 27216000  |
| C | -1. 91453900 | 5. 23682000  | 0. 90212900  |
| C | -3. 65920900 | 3. 59048500  | 0. 70358000  |
| C | -2. 61978100 | 5. 85730800  | 1. 93651600  |
| H | -0. 95824600 | 5. 64395000  | 0. 58752200  |
| C | -4. 36745900 | 4. 20760500  | 1. 73681300  |
| H | -4. 07478100 | 2. 70944300  | 0. 22061500  |
| C | -3. 84808000 | 5. 34496400  | 2. 35976100  |
| H | -2. 20605500 | 6. 74185900  | 2. 41297400  |
| H | -5. 32205200 | 3. 79826800  | 2. 05558600  |
| H | -4. 39401300 | 5. 82560500  | 3. 16637000  |
| C | -2. 23333500 | 4. 05119000  | -2. 22003700 |
| H | -2. 08254000 | 5. 13469100  | -2. 24178300 |
| H | -1. 74941400 | 3. 61593600  | -3. 09907700 |
| H | -3. 30962100 | 3. 87315200  | -2. 30026200 |
| C | -3. 41831200 | -5. 72570800 | 1. 39249100  |
| C | 2. 74018200  | 5. 56735100  | -2. 05335400 |
| H | 3. 64818200  | 5. 86130700  | -1. 51911400 |
| H | 3. 04927100  | 5. 17206000  | -3. 02898500 |
| H | 2. 14624700  | 6. 46660600  | -2. 24244100 |
| H | -4. 50567700 | -5. 73415100 | 1. 27611400  |
| H | -2. 99833900 | -6. 36130300 | 0. 60315700  |
| H | -3. 17149000 | -6. 19569000 | 2. 34949800  |

### TS(S)-2

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 3. 21528300 | -3. 36077200 | -0. 85933500 |
| C | 1. 96718500 | -2. 75533300 | -0. 96835600 |
| C | 1. 78431900 | -1. 50971500 | -1. 54752700 |
| C | 2. 91446400 | -0. 88371100 | -2. 13569500 |
| C | 4. 15928600 | -1. 50148200 | -2. 05359200 |
| C | 2. 72068400 | 0. 39758300  | -2. 91901000 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 2.39433200  | 1.19414400  | -2.24086700 |
| H  | 3.67271500  | 0.71766000  | -3.35002000 |
| C  | 1.68138800  | 0.24222100  | -4.06108600 |
| H  | 2.06098200  | -0.51095500 | -4.76185900 |
| H  | 1.63041900  | 1.18735500  | -4.61521500 |
| C  | 0.25592100  | -0.16223700 | -3.62780500 |
| C  | -0.59130400 | 0.80280900  | -2.98206100 |
| H  | -0.21552800 | 1.81263000  | -2.83821100 |
| H  | -1.66458100 | 0.73367800  | -3.14885100 |
| Ni | 0.12845200  | -0.32117300 | -1.51560800 |
| H  | 0.76383500  | -1.17409200 | -2.60145200 |
| C  | 4.32538700  | -2.72216900 | -1.40121600 |
| C  | -0.40141600 | -1.17544000 | -4.56303900 |
| H  | 0.17366300  | -2.10634100 | -4.63240700 |
| H  | -0.46384400 | -0.75517100 | -5.57520200 |
| H  | -1.41470200 | -1.41830800 | -4.23852300 |
| F  | 0.90730300  | -3.44850600 | -0.47167100 |
| F  | 3.36242900  | -4.54514100 | -0.23262200 |
| F  | 5.54106700  | -3.28999900 | -1.31314000 |
| F  | 5.25879100  | -0.94235200 | -2.61197900 |
| C  | -0.50588900 | 0.34884500  | 0.15143100  |
| C  | -1.83360100 | 0.58158300  | 2.10502300  |
| C  | -0.90773100 | 1.78601700  | 2.00418000  |
| H  | -2.87041700 | 0.85072800  | 1.87536300  |
| H  | -1.80032700 | 0.09131900  | 3.07777400  |
| H  | -1.43405200 | 2.73833200  | 2.07457400  |
| H  | -0.11791800 | 1.76135200  | 2.76432300  |
| N  | -0.32525200 | 1.60665000  | 0.65129700  |
| N  | -1.29742300 | -0.30948900 | 1.04631100  |
| C  | 0.38840800  | 2.70493200  | 0.05789600  |
| C  | -0.31654000 | 3.61213100  | -0.77412700 |
| C  | 1.72623300  | 2.96490700  | 0.43176900  |
| C  | 0.36555300  | 4.72532100  | -1.27307100 |
| C  | 2.34078500  | 4.12723000  | -0.05971200 |
| C  | 1.69314400  | 5.00315300  | -0.92941400 |
| H  | -0.15464200 | 5.41518100  | -1.92921900 |
| H  | 3.35153500  | 4.36289800  | 0.25934100  |
| C  | -1.70651300 | -1.68995400 | 1.02808900  |
| C  | -2.89996700 | -2.07401900 | 0.38205600  |
| C  | -0.96317200 | -2.63412400 | 1.78246500  |
| C  | -3.32037200 | -3.40762200 | 0.48042900  |
| C  | -1.42378400 | -3.95152200 | 1.83569500  |
| C  | -2.59713800 | -4.36165100 | 1.19232100  |
| H  | -4.23806300 | -3.70303700 | -0.02108700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.85541900 | -4.68924200 | 2.39253700  |
| C | 2.46437600  | 2.10284500  | 1.45218400  |
| C | -1.80200100 | 3.41826700  | -1.08228400 |
| C | -3.80806800 | -1.07521800 | -0.33634700 |
| C | 0.29682300  | -2.23024400 | 2.54972800  |
| H | 0.79186900  | -1.45075900 | 1.96299500  |
| H | 1.80196800  | 1.27341800  | 1.71256900  |
| H | -1.97373800 | 2.34163400  | -1.15411000 |
| H | -3.21823300 | -0.16918600 | -0.51703800 |
| C | 3.78707900  | 1.45660300  | 1.01066100  |
| C | 4.30337800  | 0.43086600  | 1.82234500  |
| C | 4.53574200  | 1.83397500  | -0.11129900 |
| C | 5.52380100  | -0.18005000 | 1.53942500  |
| H | 3.74057700  | 0.10417000  | 2.69347600  |
| C | 5.76217200  | 1.22593900  | -0.39839100 |
| H | 4.16301900  | 2.59757600  | -0.78291600 |
| C | 6.26550000  | 0.22105500  | 0.42548500  |
| H | 5.89278100  | -0.97122300 | 2.18614600  |
| H | 6.31719200  | 1.53593600  | -1.27880500 |
| H | 7.21552500  | -0.25300800 | 0.19769600  |
| C | 2.69819200  | 2.92724500  | 2.74717300  |
| H | 3.38532700  | 3.75866800  | 2.56347300  |
| H | 1.75732800  | 3.34317000  | 3.12104300  |
| H | 3.13460200  | 2.30312000  | 3.53215800  |
| C | -2.72034200 | 3.94492800  | 0.02651700  |
| C | -2.43449100 | 5.11219800  | 0.74922800  |
| C | -3.92915800 | 3.28259800  | 0.29029000  |
| C | -3.32550000 | 5.59676100  | 1.71028500  |
| H | -1.50438800 | 5.64210300  | 0.56684700  |
| C | -4.82275500 | 3.76422000  | 1.24885600  |
| H | -4.17509900 | 2.38240500  | -0.26808900 |
| C | -4.52245100 | 4.92473500  | 1.96560200  |
| H | -3.08121100 | 6.50103000  | 2.26098700  |
| H | -5.75109800 | 3.23174600  | 1.43646800  |
| H | -5.21324600 | 5.30050900  | 2.71477800  |
| C | -2.24532100 | 4.03471200  | -2.42890600 |
| H | -1.61256100 | 3.69329700  | -3.25323800 |
| H | -3.27585400 | 3.73699800  | -2.64306800 |
| H | -2.22426300 | 5.12849800  | -2.40406600 |
| C | -4.28792300 | -1.57594200 | -1.70643200 |
| C | -5.57349200 | -1.29164000 | -2.19055500 |
| C | -3.42817700 | -2.31428400 | -2.53714000 |
| C | -5.98698600 | -1.72904800 | -3.45254500 |
| H | -6.27366000 | -0.72686000 | -1.58539100 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.84018500 | -2.75994000 | -3.79370100 |
| H | -2.42888600 | -2.55589600 | -2.18874900 |
| C | -5.12443300 | -2.46901100 | -4.25980300 |
| H | -6.99020100 | -1.49367400 | -3.79724300 |
| H | -3.15615700 | -3.33960700 | -4.40728900 |
| H | -5.44706900 | -2.81754800 | -5.23659200 |
| C | -4.97881900 | -0.69353600 | 0.59970500  |
| H | -4.60779600 | -0.43501100 | 1.59393100  |
| H | -5.53773000 | 0.16742800  | 0.22125300  |
| H | -5.67605400 | -1.52968400 | 0.71416400  |
| C | -0.00492600 | -1.63440700 | 3.93063600  |
| C | -1.03859800 | -2.11795800 | 4.74597600  |
| C | 0.81913800  | -0.62072400 | 4.44254100  |
| C | -1.24510400 | -1.59909400 | 6.02669000  |
| H | -1.69225500 | -2.90072800 | 4.37329800  |
| C | 0.61750000  | -0.09940900 | 5.72194600  |
| H | 1.63262500  | -0.23909400 | 3.83070400  |
| C | -0.41945700 | -0.58685700 | 6.52029200  |
| H | -2.05464500 | -1.98747400 | 6.63865700  |
| H | 1.26887300  | 0.68716200  | 6.09282200  |
| H | -0.58217100 | -0.18244100 | 7.51510600  |
| C | 1.32093400  | -3.37619800 | 2.72244100  |
| H | 0.95479600  | -4.14830100 | 3.40620600  |
| H | 1.56232900  | -3.83999700 | 1.76455400  |
| H | 2.24153300  | -2.97507300 | 3.15684900  |
| C | 2.39934400  | 6.21674400  | -1.48563400 |
| C | -3.04943700 | -5.80140000 | 1.25546500  |
| H | -4.11531600 | -5.89612700 | 1.02971300  |
| H | -2.50383000 | -6.41656300 | 0.52934100  |
| H | -2.86870700 | -6.23446200 | 2.24434500  |
| H | 3.21483000  | 6.53980300  | -0.83213000 |
| H | 2.83483400  | 6.00153500  | -2.46932000 |
| H | 1.71010400  | 7.05681000  | -1.61448400 |

### TS(S)-3

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 1.56808500 | -4.49892800 | -0.63202600 |
| C | 0.65718000 | -3.45438300 | -0.75904200 |
| C | 0.95283300 | -2.27187800 | -1.41955800 |
| C | 2.20996600 | -2.18170300 | -2.07455300 |
| C | 3.11338000 | -3.23564500 | -1.96602100 |
| C | 2.49473300 | -0.98142100 | -2.95332700 |
| H | 2.53562700 | -0.07483900 | -2.33797100 |
| H | 3.47509900 | -1.08799600 | -3.42498500 |
| C | 1.42364100 | -0.79855900 | -4.06356700 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 1.46343900  | -1.67848600 | -4.71629900 |
| H  | 1.71145400  | 0.06133500  | -4.68011700 |
| C  | -0.03219200 | -0.60670300 | -3.58308000 |
| C  | -0.43242300 | 0.65357900  | -3.02295100 |
| H  | 0.29260700  | 1.46159500  | -2.98201700 |
| H  | -1.46381300 | 0.97094900  | -3.16476000 |
| Ni | -0.11109800 | -0.52006700 | -1.45675300 |
| H  | 0.09802700  | -1.63983900 | -2.46981300 |
| C  | 2.81684400  | -4.38300400 | -1.23211000 |
| C  | -1.05699600 | -1.37809100 | -4.41236700 |
| H  | -0.86909300 | -2.45827600 | -4.40063100 |
| H  | -1.00486100 | -1.05003900 | -5.45855300 |
| H  | -2.07309700 | -1.20069700 | -4.05561100 |
| F  | -0.56386400 | -3.64332100 | -0.19533900 |
| F  | 1.26326600  | -5.60516500 | 0.07346900  |
| F  | 3.71636500  | -5.37510200 | -1.12164600 |
| F  | 4.33194000  | -3.18177200 | -2.56109300 |
| C  | -0.37441300 | 0.49265000  | 0.14479300  |
| C  | -0.19382400 | 2.14486000  | 1.84489900  |
| C  | -1.45006400 | 1.32372000  | 2.09126600  |
| H  | 0.57918600  | 1.92151600  | 2.58636700  |
| H  | -0.37768300 | 3.21972200  | 1.83092900  |
| H  | -1.51968500 | 0.94168100  | 3.10979100  |
| H  | -2.35822000 | 1.89030000  | 1.85850000  |
| N  | -1.28376600 | 0.21213300  | 1.12210900  |
| N  | 0.22695600  | 1.66706100  | 0.50389900  |
| C  | -2.09842100 | -0.96287100 | 1.29276000  |
| C  | -1.62029200 | -2.01496500 | 2.11662100  |
| C  | -3.40785600 | -1.00484500 | 0.77355200  |
| C  | -2.47609000 | -3.08282300 | 2.39323600  |
| C  | -4.22473000 | -2.09995200 | 1.08905200  |
| C  | -3.78336100 | -3.14492100 | 1.89582400  |
| H  | -2.11887500 | -3.90086000 | 3.01015900  |
| H  | -5.23187700 | -2.13186000 | 0.68189600  |
| C  | 1.17745600  | 2.42919000  | -0.26274600 |
| C  | 2.55989200  | 2.33804400  | 0.01221600  |
| C  | 0.70229900  | 3.35826700  | -1.22554400 |
| C  | 3.45113000  | 3.08946700  | -0.76658800 |
| C  | 1.63680800  | 4.08226600  | -1.97092300 |
| C  | 3.01634000  | 3.94702000  | -1.77463600 |
| H  | 4.51576900  | 2.99896000  | -0.57111000 |
| H  | 1.28849800  | 4.77973400  | -2.72551300 |
| C  | -4.00557600 | 0.12194400  | -0.07066300 |
| C  | -0.20448800 | -1.99685600 | 2.69470100  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 3. 11794200  | 1. 56316200  | 1. 21446200  |
| C | -0. 79457800 | 3. 61248800  | -1. 41200900 |
| H | -1. 29832800 | 2. 64822800  | -1. 30945100 |
| H | -3. 17572200 | 0. 75526700  | -0. 40513600 |
| H | 0. 43590100  | -1. 51497800 | 1. 94977700  |
| H | 2. 36644400  | 0. 82338800  | 1. 50785400  |
| C | -4. 69692300 | -0. 41224800 | -1. 33314500 |
| C | -5. 93465000 | 0. 07372700  | -1. 77687500 |
| C | -4. 07480300 | -1. 41326900 | -2. 09896900 |
| C | -6. 53171000 | -0. 42140200 | -2. 94120000 |
| H | -6. 45393700 | 0. 84325800  | -1. 21674200 |
| C | -4. 67030200 | -1. 91412400 | -3. 25630200 |
| H | -3. 11931000 | -1. 81413400 | -1. 77326900 |
| C | -5. 90513100 | -1. 41931300 | -3. 68516800 |
| H | -7. 49287000 | -0. 02604200 | -3. 25824300 |
| H | -4. 17084300 | -2. 69613200 | -3. 82138200 |
| H | -6. 37125300 | -1. 81028900 | -4. 58494500 |
| C | -4. 93655900 | 0. 99057800  | 0. 80267600  |
| H | -5. 83137000 | 0. 43356600  | 1. 09856400  |
| H | -4. 42680400 | 1. 30234100  | 1. 71691600  |
| H | -5. 25668700 | 1. 89441700  | 0. 27520400  |
| C | -0. 07772700 | -1. 18528600 | 3. 98849100  |
| C | -1. 10049300 | -1. 13586700 | 4. 94655000  |
| C | 1. 12917700  | -0. 52832300 | 4. 27449300  |
| C | -0. 92588700 | -0. 44318300 | 6. 14763900  |
| H | -2. 04309200 | -1. 63736600 | 4. 74857800  |
| C | 1. 30815600  | 0. 16357800  | 5. 47402000  |
| H | 1. 94153300  | -0. 57032400 | 3. 55246600  |
| C | 0. 27785300  | 0. 21120000  | 6. 41603100  |
| H | -1. 73379400 | -0. 41585300 | 6. 87377400  |
| H | 2. 25162300  | 0. 66500600  | 5. 67158800  |
| H | 0. 41252800  | 0. 75113400  | 7. 34879800  |
| C | 0. 37994600  | -3. 40775700 | 2. 94084900  |
| H | 0. 28461200  | -4. 03756600 | 2. 05448900  |
| H | 1. 44022100  | -3. 32253900 | 3. 19656100  |
| H | -0. 11235800 | -3. 90928400 | 3. 77982200  |
| C | 4. 39940700  | 0. 78899100  | 0. 89545300  |
| C | 5. 67651100  | 1. 26543000  | 1. 22635500  |
| C | 4. 30902600  | -0. 44997700 | 0. 24363900  |
| C | 6. 82413600  | 0. 53451600  | 0. 90536700  |
| H | 5. 79042600  | 2. 21134300  | 1. 74491000  |
| C | 5. 45164000  | -1. 18072500 | -0. 08475700 |
| H | 3. 32982200  | -0. 84562800 | -0. 01070300 |
| C | 6. 71710600  | -0. 68896600 | 0. 24528100  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 7. 80124500  | 0. 92618500  | 1. 17475600  |
| H | 5. 35570900  | -2. 12491600 | -0. 61020200 |
| H | 7. 60818000  | -1. 25645100 | -0. 00728600 |
| C | 3. 30701900  | 2. 54272700  | 2. 39582500  |
| H | 2. 36541100  | 3. 02967900  | 2. 65679400  |
| H | 3. 68141400  | 2. 01904800  | 3. 28124200  |
| H | 4. 01415600  | 3. 33786600  | 2. 14279700  |
| C | -1. 37764900 | 4. 54077000  | -0. 33980700 |
| C | -0. 66031500 | 5. 62576900  | 0. 18403900  |
| C | -2. 70108400 | 4. 35328700  | 0. 08757900  |
| C | -1. 24557700 | 6. 49079200  | 1. 11224100  |
| H | 0. 36555900  | 5. 79206500  | -0. 13070100 |
| C | -3. 28986700 | 5. 21581000  | 1. 01430600  |
| H | -3. 27775400 | 3. 52480000  | -0. 31699800 |
| C | -2. 56172100 | 6. 28907700  | 1. 53270700  |
| H | -0. 66975600 | 7. 32312700  | 1. 50756900  |
| H | -4. 31521500 | 5. 04772900  | 1. 33201300  |
| H | -3. 01504400 | 6. 96027300  | 2. 25637100  |
| C | -1. 17105100 | 4. 16837700  | -2. 80386500 |
| H | -0. 81223300 | 5. 19252400  | -2. 94516300 |
| H | -0. 76898400 | 3. 54451000  | -3. 60699800 |
| H | -2. 26020000 | 4. 19272300  | -2. 90276200 |
| C | -4. 67119800 | -4. 32674100 | 2. 20658400  |
| C | 3. 99813700  | 4. 71242900  | -2. 62965700 |
| H | 4. 97102600  | 4. 80200800  | -2. 13843900 |
| H | 4. 16081300  | 4. 20680500  | -3. 58952500 |
| H | 3. 63324400  | 5. 71970100  | -2. 85417200 |
| H | -5. 71976200 | -4. 10774200 | 1. 98706900  |
| H | -4. 38444200 | -5. 20170000 | 1. 61055500  |
| H | -4. 59572300 | -4. 61708800 | 3. 25959300  |

#### TS(S)-4

|   |              |              |             |
|---|--------------|--------------|-------------|
| C | -4. 22681900 | -1. 25567000 | 2. 09182600 |
| C | -2. 88387200 | -1. 35989900 | 1. 74433300 |
| C | -1. 93416900 | -0. 40648500 | 2. 08504200 |
| C | -2. 37749800 | 0. 69991900  | 2. 86182400 |
| C | -3. 72719900 | 0. 82369400  | 3. 18405100 |
| C | -1. 35970300 | 1. 67071700  | 3. 42254000 |
| H | -0. 86447000 | 2. 19656300  | 2. 59864900 |
| H | -1. 86367500 | 2. 42927000  | 4. 02696400 |
| C | -0. 28937500 | 0. 96277800  | 4. 29994900 |
| H | -0. 80465200 | 0. 49614200  | 5. 14791800 |
| H | 0. 37446200  | 1. 72773500  | 4. 72030100 |
| C | 0. 55616100  | -0. 10693100 | 3. 57976700 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.57927000  | 0.30065700  | 2.65878400  |
| H  | 1.77254800  | 1.36402700  | 2.52451200  |
| H  | 2.45391900  | -0.33627500 | 2.55434800  |
| Ni | 0.04208500  | -0.24979800 | 1.53361100  |
| H  | -0.65209300 | -0.66444600 | 2.81341100  |
| C  | -4.65630700 | -0.14175900 | 2.80210500  |
| C  | 0.80660800  | -1.37770000 | 4.39214100  |
| H  | -0.12750600 | -1.84980900 | 4.71753600  |
| H  | 1.38446900  | -1.13857700 | 5.29401800  |
| H  | 1.37601100  | -2.10975200 | 3.81215800  |
| F  | -2.54057600 | -2.46437100 | 1.02703000  |
| F  | -5.11975800 | -2.19021300 | 1.72089900  |
| F  | -5.96126100 | 0.00127500  | 3.09987000  |
| F  | -4.18259900 | 1.87457500  | 3.90588900  |
| C  | 0.51557900  | -0.08615900 | -0.30641000 |
| C  | 1.42959700  | -0.67286200 | -2.40999100 |
| C  | 0.71929800  | 0.66918700  | -2.54374200 |
| H  | 2.43977200  | -0.65248200 | -2.81495700 |
| H  | 0.87806500  | -1.48919500 | -2.88667800 |
| H  | 1.41484400  | 1.50788200  | -2.65457600 |
| H  | 0.01772700  | 0.68778500  | -3.37713300 |
| N  | 0.01321400  | 0.76877300  | -1.24289400 |
| N  | 1.43865800  | -0.86808400 | -0.93965100 |
| C  | -0.87897600 | 1.87181500  | -0.99707500 |
| C  | -0.40592500 | 3.03576200  | -0.33888300 |
| C  | -2.19372600 | 1.83084200  | -1.51486000 |
| C  | -1.30522100 | 4.08269400  | -0.11212800 |
| C  | -3.03630900 | 2.92853700  | -1.29260200 |
| C  | -2.62788300 | 4.04594300  | -0.56661800 |
| H  | -0.96251200 | 4.97065800  | 0.40900500  |
| H  | -4.04501900 | 2.89955800  | -1.69462500 |
| C  | 2.26172900  | -1.89263400 | -0.34795700 |
| C  | 3.65611500  | -1.68425100 | -0.23984800 |
| C  | 1.69514300  | -3.13108800 | 0.05215200  |
| C  | 4.44803500  | -2.69398500 | 0.32402500  |
| C  | 2.53532700  | -4.09773600 | 0.61150400  |
| C  | 3.91189800  | -3.89938700 | 0.76715500  |
| H  | 5.51596300  | -2.52136400 | 0.42499800  |
| H  | 2.11266100  | -5.04369100 | 0.93180600  |
| C  | -2.67607200 | 0.71192200  | -2.43793100 |
| C  | 1.07040100  | 3.21432500  | 0.01548000  |
| C  | 4.37418200  | -0.43709100 | -0.77684600 |
| C  | 0.20887300  | -3.42510000 | -0.14409800 |
| H  | -0.33904800 | -2.53830300 | 0.18126900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.96301700 | -0.11593100 | -2.35677500 |
| H | 1.46896300  | 2.22949300  | 0.27011900  |
| H | 3.61351700  | 0.32136400  | -0.98382300 |
| C | -4.06203700 | 0.13062400  | -2.11316100 |
| C | -4.74226700 | -0.63512200 | -3.07716600 |
| C | -4.68033700 | 0.29494000  | -0.86544700 |
| C | -5.99256700 | -1.19536600 | -2.81187700 |
| H | -4.29876100 | -0.80009300 | -4.05342800 |
| C | -5.93581400 | -0.25850000 | -0.59752500 |
| H | -4.18119200 | 0.86512000  | -0.09068600 |
| C | -6.60100700 | -1.00311300 | -1.57046800 |
| H | -6.49145100 | -1.77936200 | -3.58045900 |
| H | -6.38617100 | -0.11176100 | 0.37932100  |
| H | -7.57712300 | -1.43183800 | -1.36321000 |
| C | -2.62332200 | 1.24176800  | -3.89759000 |
| H | -3.43896900 | 1.94825900  | -4.08001500 |
| H | -1.68428000 | 1.76729300  | -4.08928100 |
| H | -2.70375500 | 0.43319100  | -4.62835100 |
| C | 1.89815200  | 3.74495600  | -1.16631600 |
| C | 1.35288500  | 4.54974000  | -2.17650400 |
| C | 3.27340200  | 3.46397900  | -1.21602100 |
| C | 2.15495300  | 5.05278300  | -3.20476700 |
| H | 0.29281900  | 4.78156000  | -2.16601900 |
| C | 4.07695700  | 3.96458800  | -2.24146700 |
| H | 3.72363900  | 2.85273800  | -0.43842200 |
| C | 3.51923200  | 4.76211700  | -3.24367100 |
| H | 1.70830100  | 5.67222500  | -3.97780500 |
| H | 5.13763600  | 3.72939500  | -2.25665700 |
| H | 4.14078000  | 5.15123100  | -4.04497400 |
| C | 1.31362600  | 4.11891400  | 1.24515200  |
| H | 0.73013100  | 3.78517600  | 2.10851900  |
| H | 2.37271500  | 4.09173300  | 1.51710500  |
| H | 1.06097800  | 5.16361800  | 1.04166000  |
| C | 5.33104400  | 0.17862600  | 0.25040100  |
| C | 6.72050700  | -0.00564200 | 0.20904800  |
| C | 4.80712900  | 0.97155400  | 1.28352400  |
| C | 7.55360400  | 0.57242300  | 1.17214800  |
| H | 7.17097400  | -0.59758600 | -0.58045300 |
| C | 5.63357400  | 1.55301100  | 2.24504700  |
| H | 3.73550900  | 1.12942400  | 1.33424400  |
| C | 7.01539100  | 1.35316100  | 2.19472000  |
| H | 8.62685400  | 0.41269300  | 1.11596700  |
| H | 5.19803400  | 2.16394100  | 3.03094100  |
| H | 7.66330400  | 1.80474400  | 2.94030200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 5.08358800  | -0.77032400 | -2.10808400 |
| H | 4.37544500  | -1.14538400 | -2.85078100 |
| H | 5.57430700  | 0.11688700  | -2.52050400 |
| H | 5.83887300  | -1.55027900 | -1.97579900 |
| C | -0.16709000 | -3.66989600 | -1.60767800 |
| C | 0.66545500  | -4.38158400 | -2.48278600 |
| C | -1.41122100 | -3.22681200 | -2.08326800 |
| C | 0.27110800  | -4.63576700 | -3.79894300 |
| H | 1.63219300  | -4.73426600 | -2.13438800 |
| C | -1.80771900 | -3.47958500 | -3.39822400 |
| H | -2.07550200 | -2.69122000 | -1.41103500 |
| C | -0.96603300 | -4.18356800 | -4.26322500 |
| H | 0.93259900  | -5.18735700 | -4.46167000 |
| H | -2.77588700 | -3.12600200 | -3.74203300 |
| H | -1.27177000 | -4.37957000 | -5.28706100 |
| C | -0.31683500 | -4.59434400 | 0.71549800  |
| H | 0.09617000  | -5.55677600 | 0.39713000  |
| H | -0.07928900 | -4.44689600 | 1.77418600  |
| H | -1.40269700 | -4.65302100 | 0.61854300  |
| C | -3.57771200 | 5.18548600  | -0.28445200 |
| C | 4.77894400  | -4.95949500 | 1.40387400  |
| H | 5.83569700  | -4.80702300 | 1.16755200  |
| H | 4.68052800  | -4.94551300 | 2.49631700  |
| H | 4.49470200  | -5.96214700 | 1.06860600  |
| H | -4.36252400 | 5.24943900  | -1.04366500 |
| H | -4.07256600 | 5.05189200  | 0.68551000  |
| H | -3.05342800 | 6.14538400  | -0.25093700 |

### TS(S)-5

|   |             |             |            |
|---|-------------|-------------|------------|
| C | 4.04650600  | 1.05893100  | 2.66627400 |
| C | 2.75118700  | 1.16170100  | 2.16871900 |
| C | 1.80507400  | 0.15479300  | 2.29595400 |
| C | 2.19834800  | -1.01309300 | 3.00666500 |
| C | 3.50072000  | -1.12784500 | 3.48650800 |
| C | 1.16467300  | -2.07103300 | 3.32816800 |
| H | 0.78856900  | -2.50621000 | 2.39574400 |
| H | 1.62678000  | -2.88221800 | 3.89636600 |
| C | -0.02656100 | -1.50018100 | 4.14534000 |
| H | 0.36870200  | -1.11394800 | 5.09239800 |
| H | -0.70066100 | -2.32654900 | 4.40092000 |
| C | -0.83026700 | -0.38591600 | 3.44751900 |
| C | -1.71320300 | -0.71739100 | 2.36778400 |
| H | -1.82859700 | -1.76114000 | 2.08205400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -2.60461400 | -0.11449200 | 2.22902900  |
| Ni | -0.09786900 | 0.03528600  | 1.49783900  |
| H  | 0.44030600  | 0.28852500  | 2.88837000  |
| C  | 4.43164500  | -0.10425800 | 3.32168700  |
| C  | -1.23014400 | 0.77553500  | 4.35703000  |
| H  | -0.36124600 | 1.24208700  | 4.83529000  |
| H  | -1.88956700 | 0.41526700  | 5.15708800  |
| H  | -1.76834000 | 1.54722900  | 3.79931300  |
| F  | 2.45320800  | 2.31624200  | 1.50879200  |
| F  | 4.93640600  | 2.06081200  | 2.51198400  |
| F  | 5.67999900  | -0.22768300 | 3.80292500  |
| F  | 3.90418000  | -2.23105600 | 4.16019300  |
| C  | -0.49762900 | 0.08210000  | -0.36688900 |
| C  | -0.79284700 | -0.52690500 | -2.64061100 |
| C  | -1.49202900 | 0.80846200  | -2.39675900 |
| H  | -0.11680700 | -0.49176400 | -3.49417000 |
| H  | -1.49677700 | -1.35208900 | -2.78913900 |
| H  | -0.97458500 | 1.64719000  | -2.87191800 |
| H  | -2.53005400 | 0.80697600  | -2.73345900 |
| N  | -1.40884600 | 0.93368400  | -0.92120500 |
| N  | -0.04871600 | -0.72186000 | -1.37252900 |
| C  | -2.12887400 | 1.98879800  | -0.25614000 |
| C  | -1.47816500 | 3.20745600  | 0.06576800  |
| C  | -3.51883800 | 1.84401900  | -0.03731000 |
| C  | -2.22677000 | 4.22043600  | 0.67339900  |
| C  | -4.22451600 | 2.91564700  | 0.52891000  |
| C  | -3.59856100 | 4.09810300  | 0.91692800  |
| H  | -1.73736400 | 5.15005200  | 0.94286000  |
| H  | -5.29692300 | 2.81890900  | 0.67234300  |
| C  | 0.88880000  | -1.80476500 | -1.22728200 |
| C  | 2.20642500  | -1.65356400 | -1.71501400 |
| C  | 0.47512200  | -3.03646800 | -0.65985700 |
| C  | 3.12099400  | -2.69460000 | -1.51276300 |
| C  | 1.43309700  | -4.03919400 | -0.47789700 |
| C  | 2.76627100  | -3.88095400 | -0.87251700 |
| H  | 4.14152300  | -2.56628400 | -1.86255700 |
| H  | 1.13659300  | -4.98096700 | -0.02755600 |
| C  | -4.30506800 | 0.61980300  | -0.50009700 |
| C  | -0.01683900 | 3.46048700  | -0.30465900 |
| C  | 2.64162100  | -0.45199400 | -2.56427200 |
| C  | -0.99378000 | -3.31324600 | -0.34332500 |
| H  | -1.43695900 | -2.37436700 | -0.00368900 |
| H  | -3.58484100 | -0.10730200 | -0.88720400 |
| H  | 0.52990200  | 2.52971000  | -0.13640100 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.91140500  | 0.34704600  | -2.40494100 |
| C | -5.11583300 | -0.12336000 | 0.57610000  |
| C | -5.79129200 | -1.29845700 | 0.19794100  |
| C | -5.22178900 | 0.27873800  | 1.91427400  |
| C | -6.54355800 | -2.03583200 | 1.11140400  |
| H | -5.72907500 | -1.64445900 | -0.83012400 |
| C | -5.97753800 | -0.45602700 | 2.83446700  |
| H | -4.70958800 | 1.17084900  | 2.25434000  |
| C | -6.64405400 | -1.61447700 | 2.43974000  |
| H | -7.05055300 | -2.93947900 | 0.78465100  |
| H | -6.03918000 | -0.11544300 | 3.86438000  |
| H | -7.23059800 | -2.18386300 | 3.15476300  |
| C | -5.23038300 | 1.03074000  | -1.67768200 |
| H | -6.01240300 | 1.71576600  | -1.33711800 |
| H | -4.66063500 | 1.53889300  | -2.46157400 |
| H | -5.71818400 | 0.16076100  | -2.12460200 |
| C | 0.15943400  | 3.83638900  | -1.78119500 |
| C | -0.79672000 | 4.58061600  | -2.48722200 |
| C | 1.34473600  | 3.48287000  | -2.44510300 |
| C | -0.57988500 | 4.94989200  | -3.81735300 |
| H | -1.72249700 | 4.86728000  | -1.99745200 |
| C | 1.56425500  | 3.84929300  | -3.77429800 |
| H | 2.10835800  | 2.92078100  | -1.91423300 |
| C | 0.59964500  | 4.58362500  | -4.46819800 |
| H | -1.33698500 | 5.52366800  | -4.34510100 |
| H | 2.48897800  | 3.55949900  | -4.26573900 |
| H | 0.76595100  | 4.86756700  | -5.50338800 |
| C | 0.66826500  | 4.53337000  | 0.56976800  |
| H | 0.55499500  | 4.30925900  | 1.63427000  |
| H | 1.73654900  | 4.55783100  | 0.34283400  |
| H | 0.26940500  | 5.53359700  | 0.37527900  |
| C | 4.00359000  | 0.11865300  | -2.16308800 |
| C | 5.18986600  | -0.18743600 | -2.84595200 |
| C | 4.08073800  | 1.00215400  | -1.07609200 |
| C | 6.41147700  | 0.36634300  | -2.45142800 |
| H | 5.17298000  | -0.85536900 | -3.70062000 |
| C | 5.29662000  | 1.56135500  | -0.68119300 |
| H | 3.17768800  | 1.25684400  | -0.53085200 |
| C | 6.47032400  | 1.24329800  | -1.36876000 |
| H | 7.31562200  | 0.11281600  | -2.99825100 |
| H | 5.32355000  | 2.23545500  | 0.16794200  |
| H | 7.41861300  | 1.67680100  | -1.06429900 |
| C | 2.59146200  | -0.84303000 | -4.05932600 |
| H | 1.59232600  | -1.18005100 | -4.34571100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.86230900  | 0.00722200  | -4.69315300 |
| H | 3.27485500  | -1.66800500 | -4.27996300 |
| C | -1.78981000 | -3.76212000 | -1.57669600 |
| C | -1.21743300 | -4.49528700 | -2.62520500 |
| C | -3.16526400 | -3.48700500 | -1.63394900 |
| C | -1.99496400 | -4.93464400 | -3.70017800 |
| H | -0.15572400 | -4.72050000 | -2.60632600 |
| C | -3.94478000 | -3.92514000 | -2.70551200 |
| H | -3.63025200 | -2.92961200 | -0.82440500 |
| C | -3.36083400 | -4.65123800 | -3.74652000 |
| H | -1.52898200 | -5.49884800 | -4.50346400 |
| H | -5.00768700 | -3.69959000 | -2.72829900 |
| H | -3.96369800 | -4.99124800 | -4.58361500 |
| C | -1.21142500 | -4.34366900 | 0.78754200  |
| H | -0.91472700 | -5.35188800 | 0.48376500  |
| H | -0.65066600 | -4.07686900 | 1.68800500  |
| H | -2.27347700 | -4.38483400 | 1.04604500  |
| C | -4.37167400 | 5.21405900  | 1.57854700  |
| C | 3.78527500  | -4.96536500 | -0.61525900 |
| H | 4.60915500  | -4.91820300 | -1.33303800 |
| H | 4.21931300  | -4.86459100 | 0.38718300  |
| H | 3.33471900  | -5.96089400 | -0.67432000 |
| H | -5.43688300 | 5.16122600  | 1.33599400  |
| H | -4.28152100 | 5.16152600  | 2.67065900  |
| H | -3.99840800 | 6.19582700  | 1.27138800  |