

Supplementary Information

Carboxylate Breaks Arene C–H Bond via a Hydrogen-Atom-Transfer Mechanism in Electrochemical Cobalt Catalysis

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I. Computational Studies

Computation details

All density functional theory (DFT) calculations were carried out by Gaussian 09 program.^[1] The geometry optimizations were conducted using the B3LYP level of theory^[2] adding Grimme's dispersion corrections^[3] with Becke-Johnson damping employing LANL2DZ basis set^[4] for cobalt and 6-31G(d) basis set for other atoms. To confirm whether each optimized stationary point is an energy minimum or a transition state as well as evaluate the zero-point vibrational energy and thermal corrections at 298 K, the vibrational frequencies were computed at the same level of theory as for the geometry optimizations. On the basis of the gas-phase optimized structures, the single-point energies and solvent effects were evaluated with the B3LYP functional Def2-TZVP basis set^[5] for cobalt and other atoms. The solvation energies were calculated using the self-consistent reaction field with the SMD implicit solvent model.^[6] Natural bond orbital (NBO) calculations were performed with the B3LYP functional Def2-TZVP basis set. The 3D diagrams of computed species were generated using CYLView.^[7] Minimum-energy crossing points (MECPs) in the most favorable pathways were calculated with the sobMECP program^[8] using the same level of theory as for the geometry optimizations.

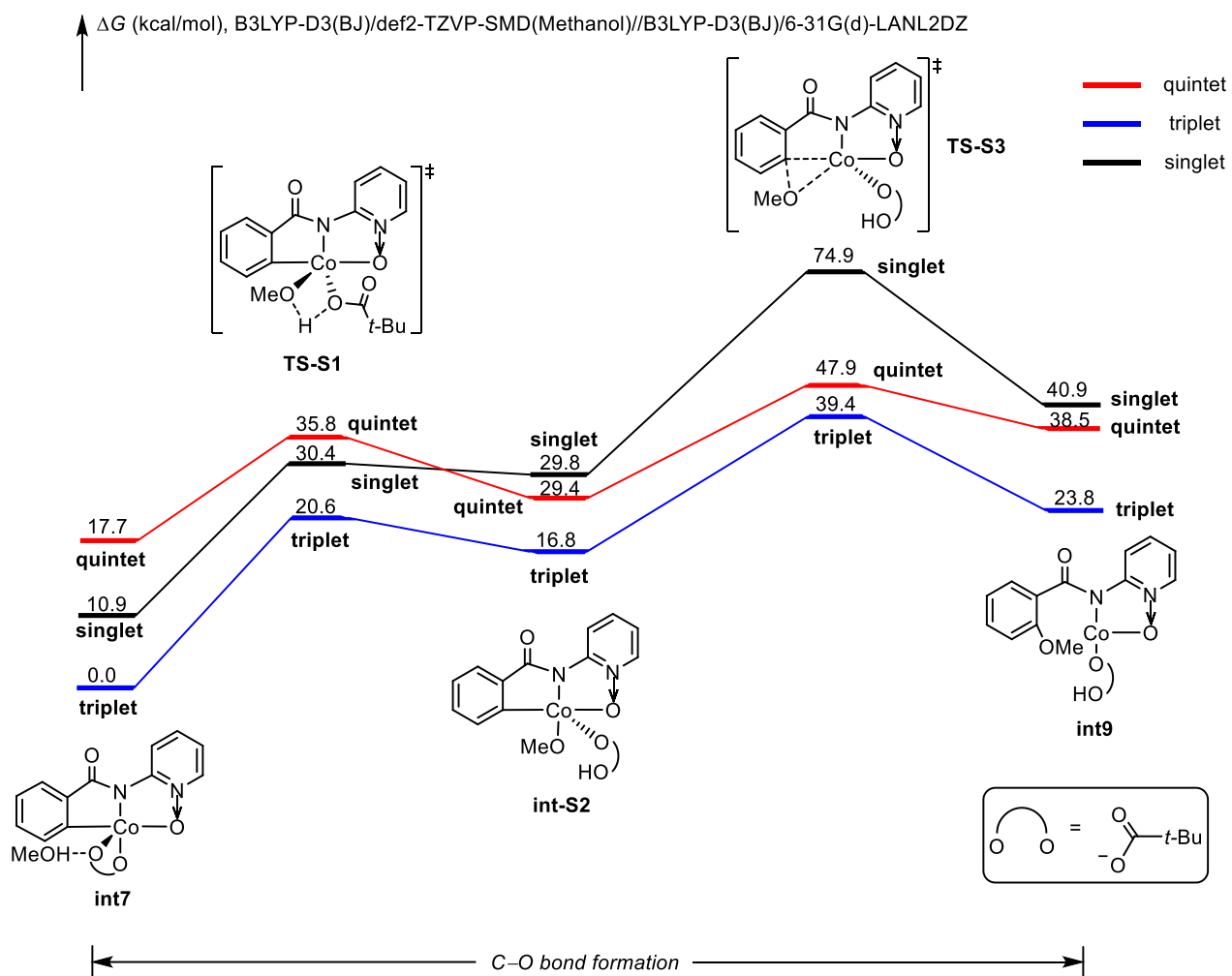


Figure S1. Reductive elimination of arylcobalt(III)(OMe) species. All free energies are compared to triplet **int7**.

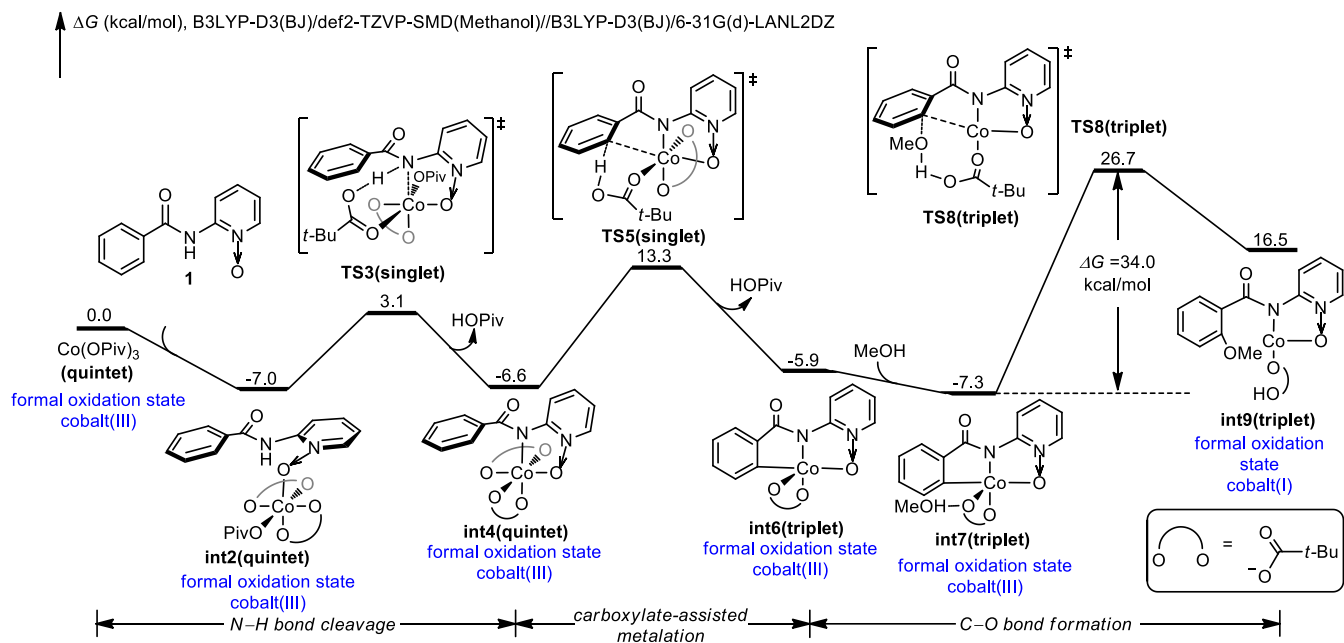


Figure S2. DFT-computed free energy changes of mechanism A and formal oxidation state of cobalt before C–O bond formation.

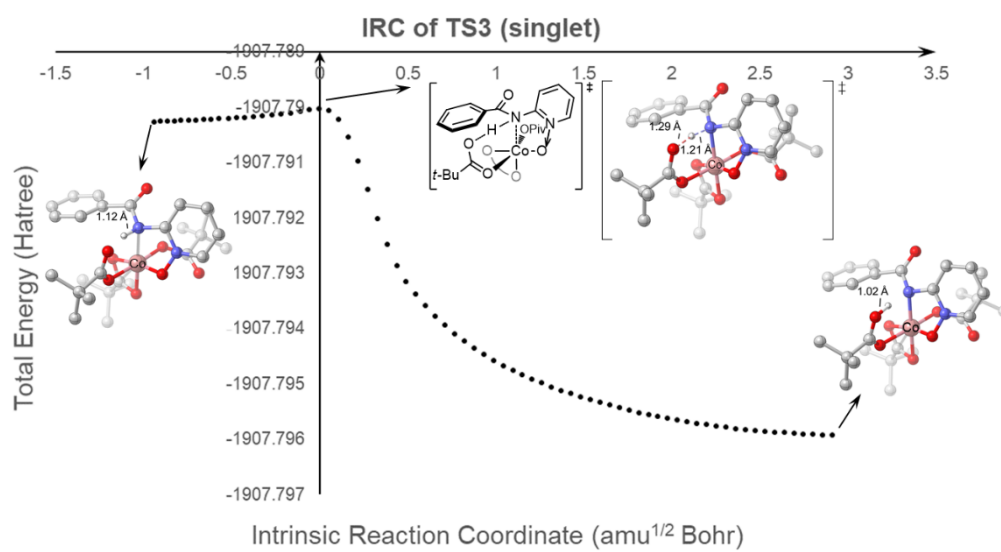


Figure S4. IRC confirmations of TS3(singlet).

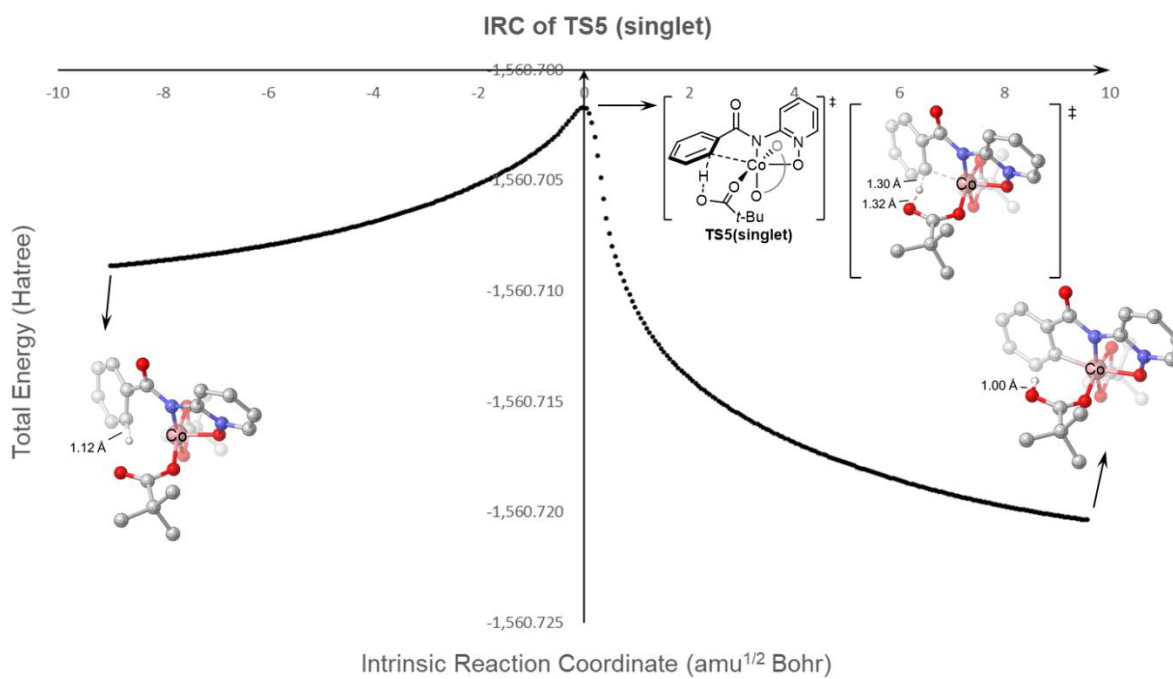


Figure S5. IRC confirmations of TS5(singlet).

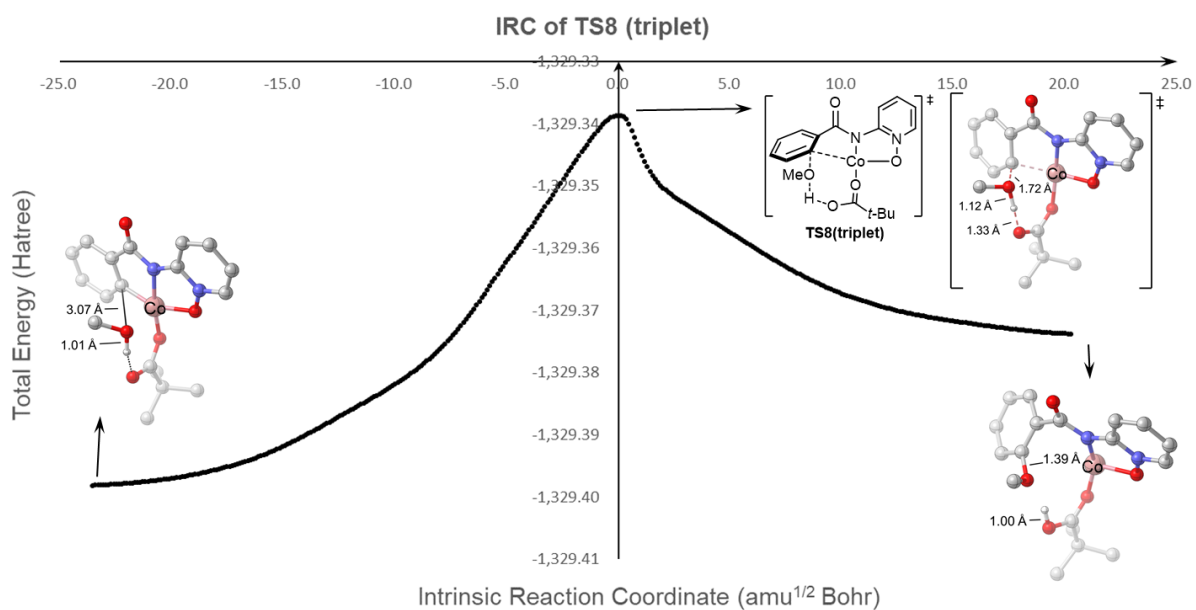


Figure S6. IRC confirmations of **TS8(triplet)**.

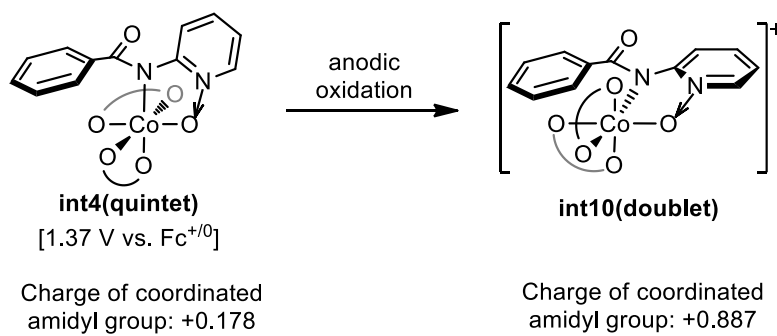


Figure S7. Charge of the coordinated amidyl group in **int4** and **int10**.

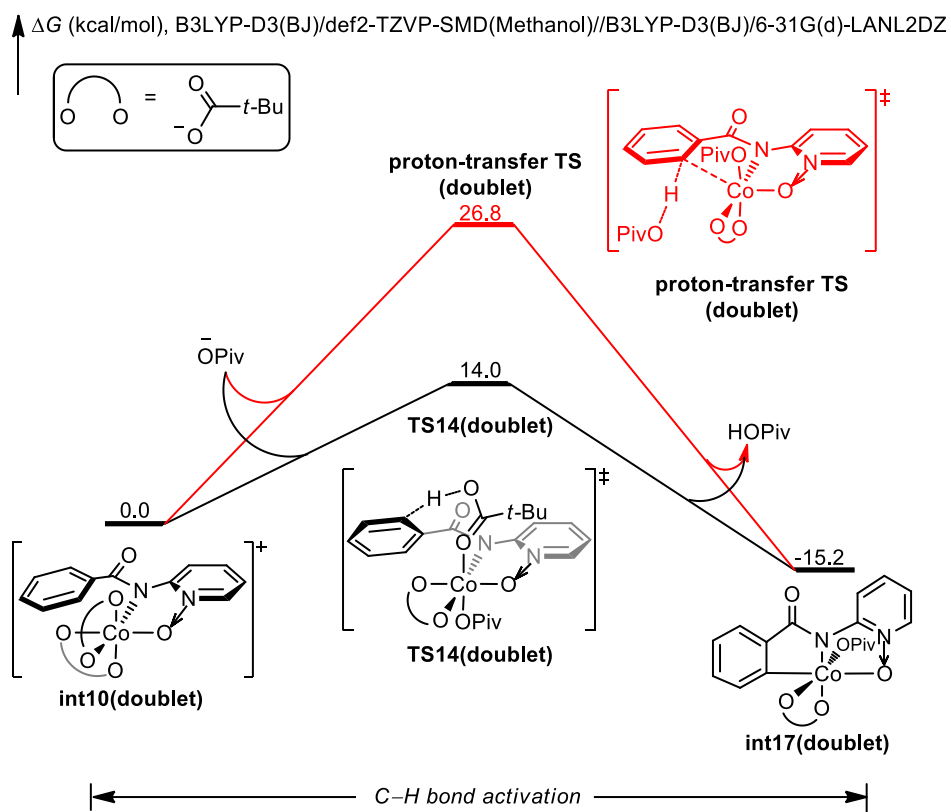


Figure S8. Proton transfer process for the arene C–H bond cleavage of cobalt(IV) intermediate.

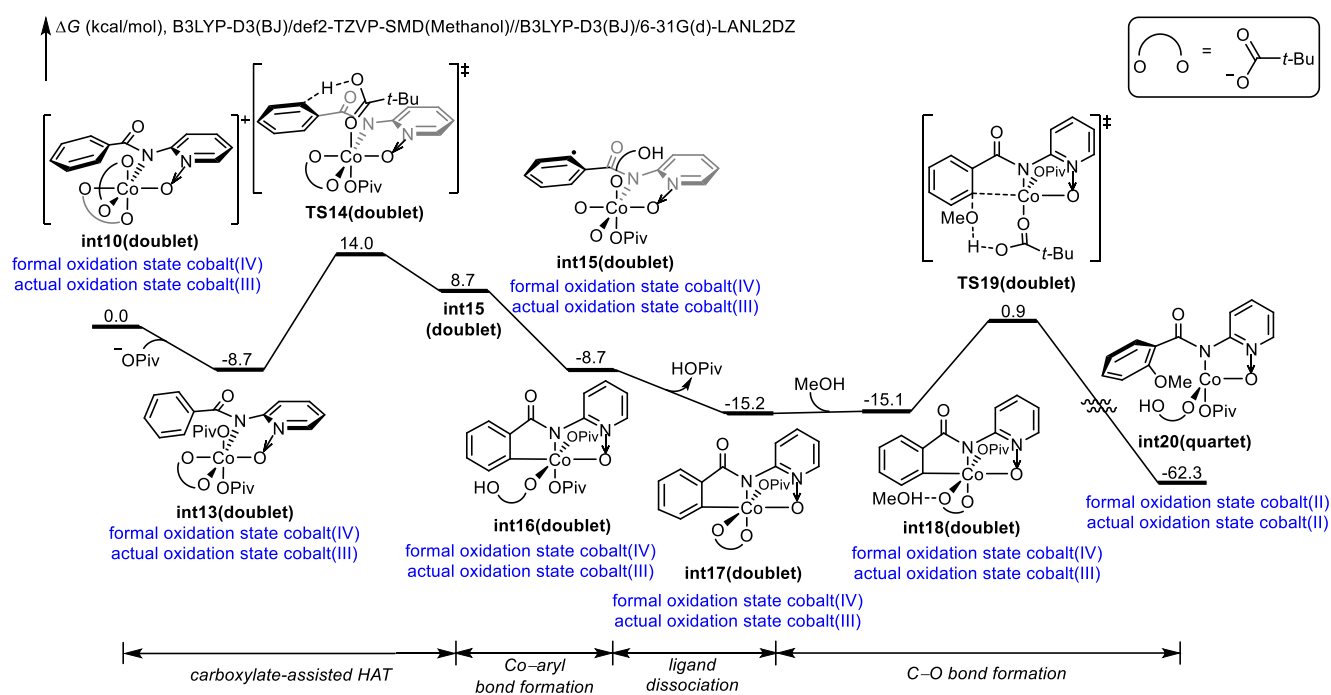


Figure S9. DFT-computed free energy changes of the pathway from int10, formal oxidation state of cobalt and actual oxidation state of cobalt.

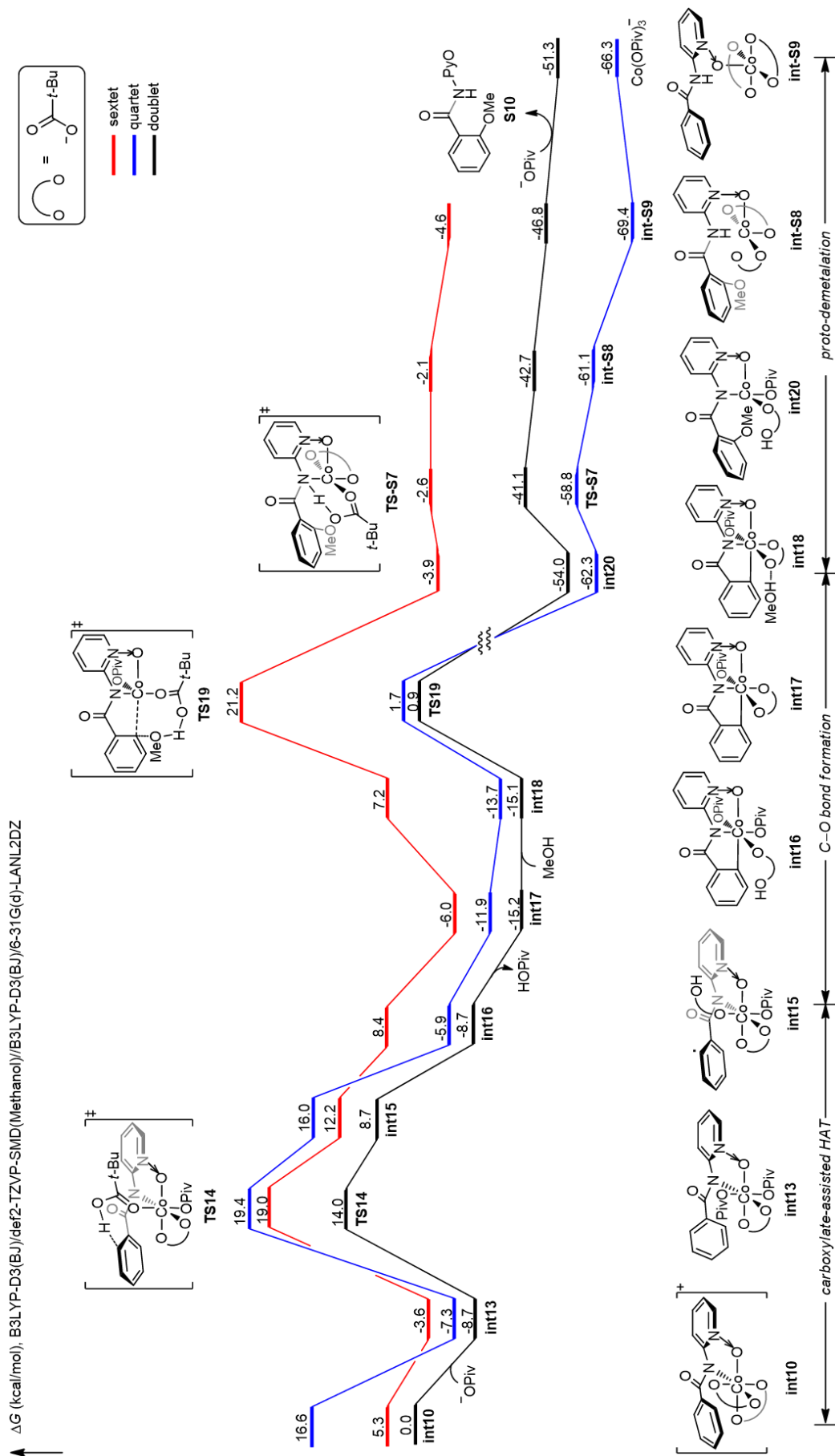


Figure S10. Free energy diagram of the pathway from formal Co(IV) intermediate **int10** including all spin states.

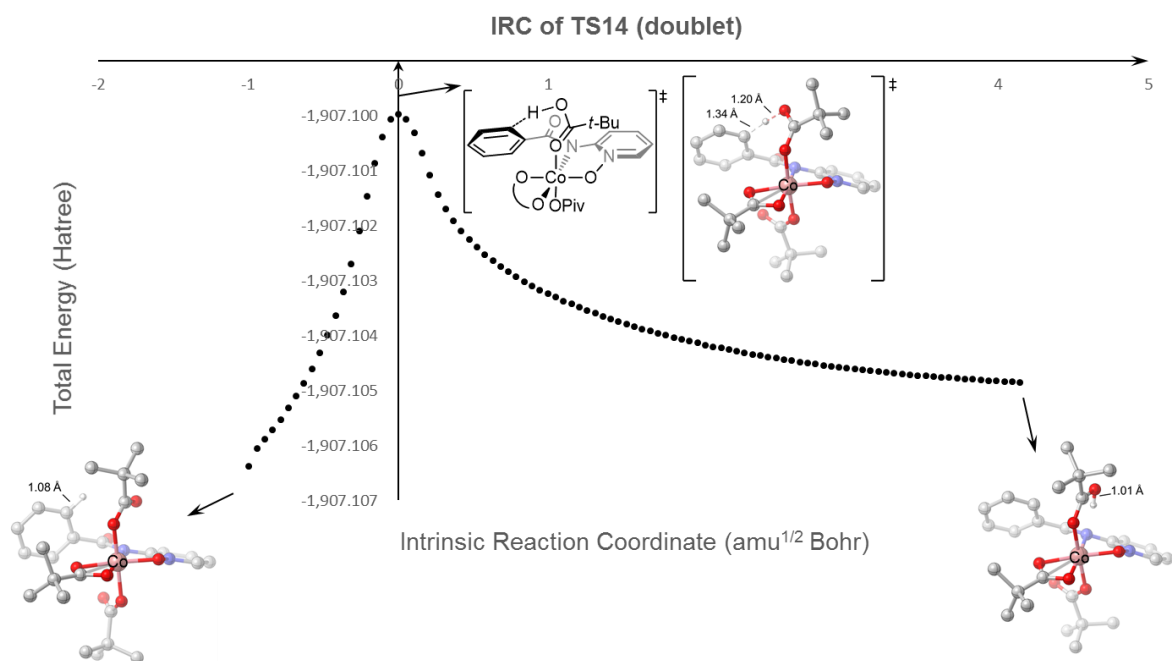


Figure S11. IRC confirmations of **TS14**(doublet).

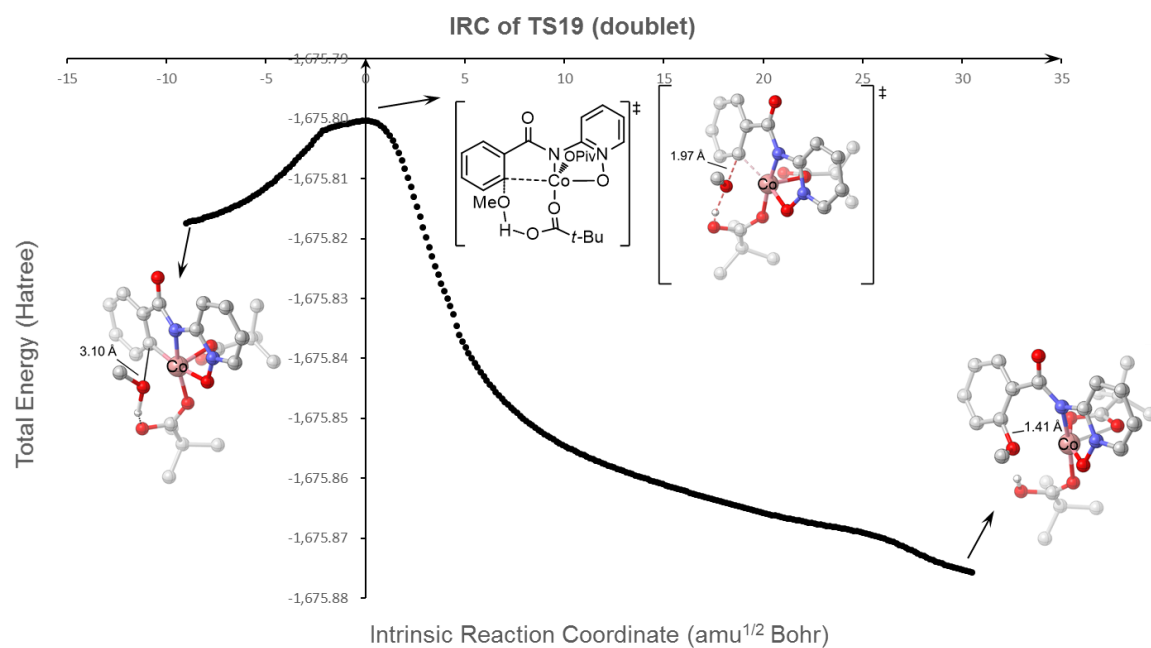
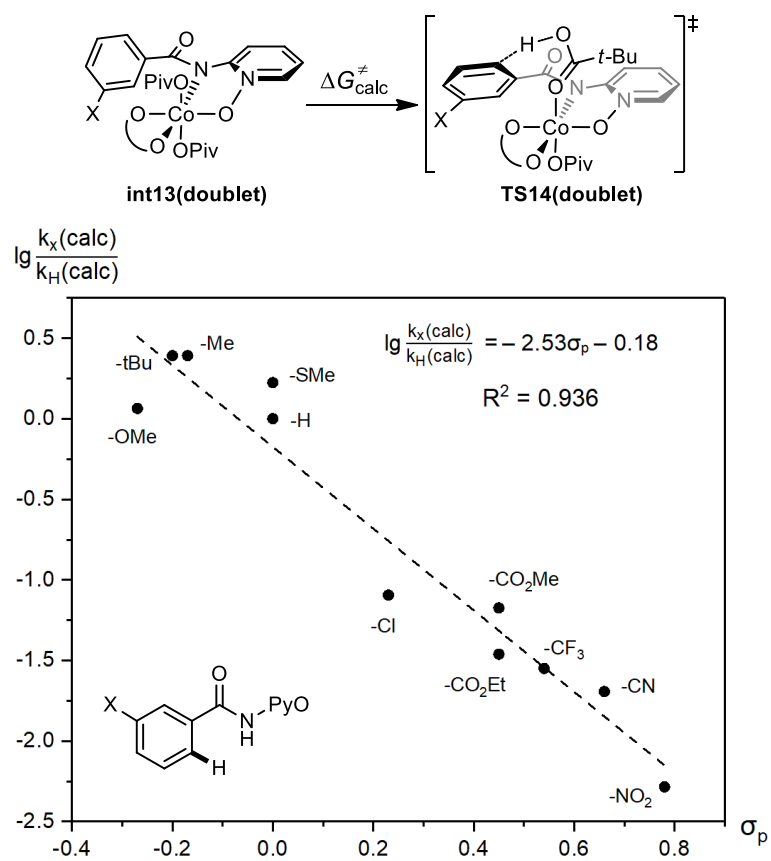


Figure S12. IRC confirmations of **TS19**(doublet).



Scheme S1. Computed Hammett analysis of C–H bond activation rate.

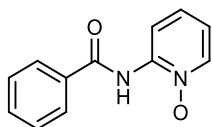
II. Experimental studies

General remarks

Nuclear magnetic resonance (NMR) spectra were recorded at ambient temperature using Agilent DD2 600 spectrometers, with working frequencies of 600 and 150 MHz for ^1H and ^{13}C , respectively. Chemical shifts are reported in ppm relative to the residual internal non deuterated solvent signals (CDCl_3 : $\delta = 7.26$ ppm). MS data were recorded using Q-TOF detection (Agilent 6545) equipped with an electrospray ionization source (ESI). Single-crystal X-ray diffraction studies were performed on Bruker D8 Venture (Ims 3.0 Photon II) and using $\text{Mo K}\alpha$ radiation. The cyclic voltammetry studies was carried out with a CHI630C electrochemical workstation (CH Instruments Inc. Shanghai China) using 2 mm glassy carbon electrode as working electrode, a Pt wire as counter electrode and a Ag/Ag^+ electrode was used as a quasi-reference electrode with ferrocene as internal reference. UV-vis is performed by UV-3150 (Shimadzu, Japan). Benzoic acid, N,N-dimethyl-4-aminopyridine, EDCI, $\text{Co}(\text{acac})_3$, AgOAc , $\text{NaOPiv}\cdot\text{H}_2\text{O}$, Ag_2O were purchased from Adamas and used without further purification. 2-aminopyridine 1-oxide was purchased from TCI and used without further purification.

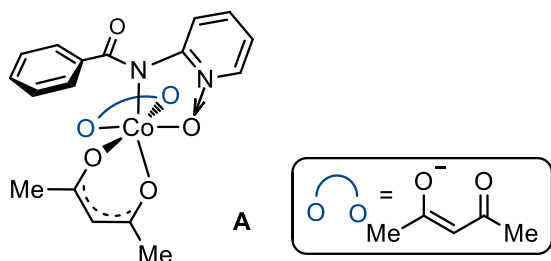
Preparation procedures

Preparation of substrate **1**^[9]



The benzoic acid (6 mmol), 2-aminopyridine 1-oxide (660 mg, 6 mmol), N,N-dimethyl-4-aminopyridine (73.3 mg, 0.6 mmol) were dissolved in anhydrous CH₂Cl₂ (20 mL) in a 100 mL two-necked reaction flask and the flask was flushed with argon. EDCI (1.14 g, 7.2 mmol) in CH₂Cl₂ (30 mL) was dropwise added to the solution through dropping funnel at 0 °C. The reaction mixture was gradually warmed to room temperature, and stirred for overnight. The reaction was quenched with water (20 mL) and extracted with CH₂Cl₂ (3 × 20 mL). The mixture was dried by MgSO₄ and filtered. Concentration in vacuo and purification by column chromatography afforded pure substrate **1**. ¹H NMR (600 MHz, CDCl₃) δ 10.93 (s, 1H), 8.61 (dd, J = 8.4, 1.9 Hz, 1H), 8.30 (dd, J = 6.5, 1.5 Hz, 1H), 8.01 (dt, J = 7.2, 1.4 Hz, 2H), 7.64 – 7.58 (m, 1H), 7.53 (dd, J = 8.5, 7.0 Hz, 2H), 7.39 (ddd, J = 8.7, 7.6, 1.5 Hz, 1H), 7.02 (ddd, J = 8.1, 6.5, 1.9 Hz, 1H). ¹³C NMR (150 MHz, CDCl₃) δ 165.44 , 144.71 , 137.19 , 133.05 , 129.10 , 128.29 , 127.79 , 118.78 , 114.92 .

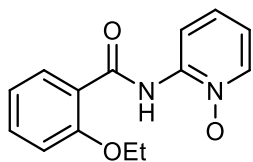
Preparation of **A**



The substrate **1** (214.1 mg, 1 mmol), Co(acac)₃ (356.3 mg, 1 mmol), AgOAc (333.8 mg, 2 mmol) and NaOPiv·H₂O (248.2 mg, 2 mmol) were dissolved in chloroform (30 mL) in a 100 mL reaction flask. The reaction was carried out at 50 °C under air and stirred for 24 hours. The reaction mixture was then filtered by Celite, concentrated in vacuo purified by column chromatography with CH₂Cl₂/acetone (3:1). **A** was obtained as green solid (142 mg, 30% yield). The crystal was prepared using evaporation method under air at room temperature in dichloromethane. ¹H NMR of **A**. (600 MHz, CDCl₃) δ 8.32 (d, J = 6.7 Hz, 1H), 8.17 – 8.09 (m, 1H), 7.99 (d, J = 7.6 Hz, 2H), 7.41 (t, J = 7.6 Hz, 1H), 7.30 (t, J = 7.3 Hz, 3H), 6.70 (t, J = 6.9 Hz, 1H), 5.52 (s, 1H), 5.19 (s, 1H), 2.21 (s, 3H), 2.13 (s, 3H), 2.01 (s, 3H), 1.29 (s, 3H). ¹³C NMR of **A**. (150 MHz, CDCl₃) δ 189.84 , 189.36 , 189.01 , 188.95 , 181.37 , 157.11 , 138.86 , 136.02 , 132.27 , 130.98 , 130.33 , 127.16 , 120.31 , 114.21 , 97.30 , 97.21 , 26.46 , 25.91 , 25.84 , 24.99. MS (positive ESI, M + Na⁺): 493.0778 found (493.0780 calculated). CCDC 1969391 contains the

supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via <https://www.ccdc.cam.ac.uk/>.

Preparation of **12**^[10]



The electrochemical oxidation was performed in a undivided cell equipped with a RVC anode (3 mm × 3 mm × 10 mm) and a platinum cathode (10 mm × 10 mm × 0.25 mm). To a 25 mL tube were sequentially added **A** (47.0 mg, 0.1 mmol), NaOPiv·H₂O (25.6 mg, 0.20 mmol, 2.0 equiv), Bu₄NPF₆ (774.9 g, 0.20 mmol, 2.0 equiv), and alcohol (8.0 mL). The electrolysis was carried out at room temperature and under air using at a constant current of 8.0 mA for 6 hours. Upon completion, the reaction mixture was subjected to flash chromatography on silica gel eluting with CH₂Cl₂/MeOH to afford the desired product **12** (22.0 mg, 85% yield). ¹H NMR of product **12**. (600 MHz, CDCl₃) δ 12.29 (s, 1H), 8.73 (dd, J = 8.5, 1.9 Hz, 1H), 8.28 (dt, J = 7.9, 1.7 Hz, 2H), 7.52 (ddd, J = 8.8, 7.2, 1.9 Hz, 1H), 7.34 (ddd, J = 8.8, 7.5, 1.5 Hz, 1H), 7.13 – 7.09 (m, 1H), 7.06 (d, J = 8.3 Hz, 1H), 6.98 (ddd, J = 8.0, 6.5, 1.9 Hz, 1H), 4.35 (q, J = 7.0 Hz, 2H), 1.71 (t, J = 7.0 Hz, 3H). ¹³C NMR of product **12**. (150 MHz, CDCl₃) δ 157.64 , 145.59 , 137.47 , 134.43 , 132.82 , 127.85 , 121.22 , 120.71 , 118.59 , 115.99 , 112.55 , 65.52 , 14.89.

Other procedures for mechanistic experiments

Procedure for the synthesis of **A** without AgOAc.

The substrate **1** (21.4 mg, 0.1 mmol), Co(acac)₃ (35.6 mg, 0.1 mmol) and NaOPiv·H₂O (24.8 mg, 0.2mmol) were dissolved in chloroform (3 mL) in a 25 mL reaction flask. The reaction was carried out at 50 °C under air and stirred for 24 hours. The transformation was not productive, **A** was not found.

Procedure for the synthesis of **A** using *t*-BuOH as solution.

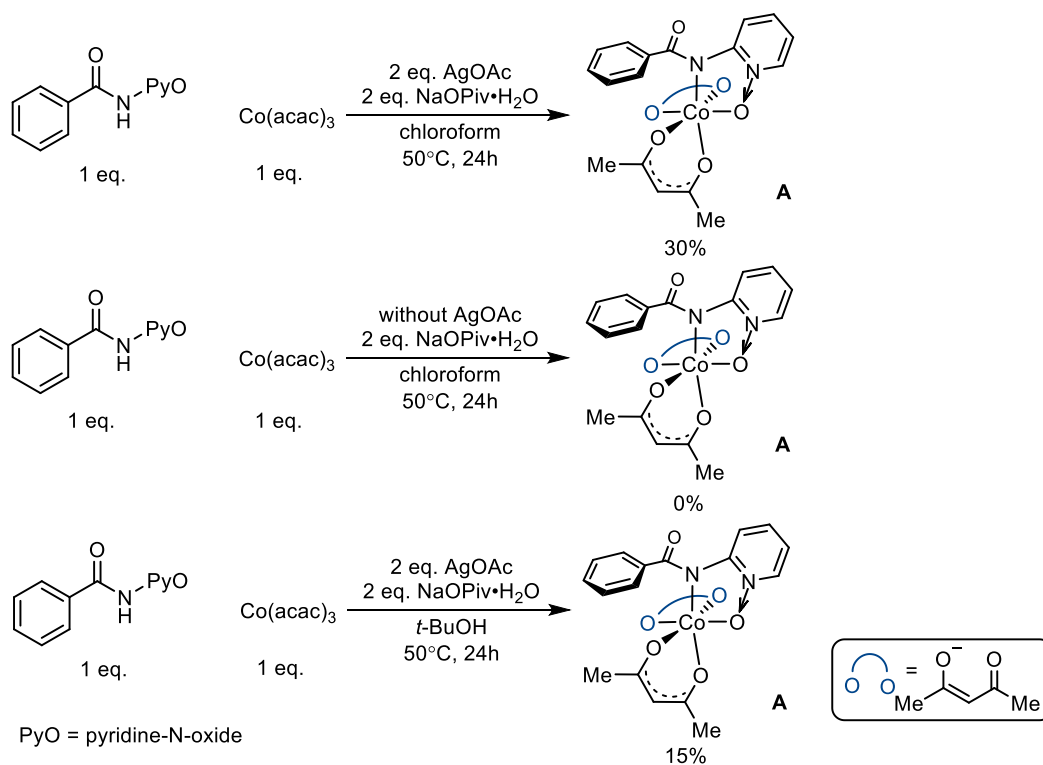
The substrate **1** (21.4 mg, 0.1 mmol), Co(acac)₃ (35.6 mg, 0.1 mmol), AgOAc (33.4 mg, 0.2 mmol) and NaOPiv·H₂O (24.8 mg, 0.2mmol) were dissolved in *t*-BuOH (3 mL) in a 25 mL reaction flask. The reaction was carried out at 50 °C under air and stirred for 24 hours. The reaction mixture was then filtered by Celite, concentrated in vacuo purified by column chromatography with CH₂Cl₂/acetone (3:1). **A** was obtained as green solid (7.2 mg, 15% yield).

Procedure for the experiment of **A** in basic solution without additional oxidant

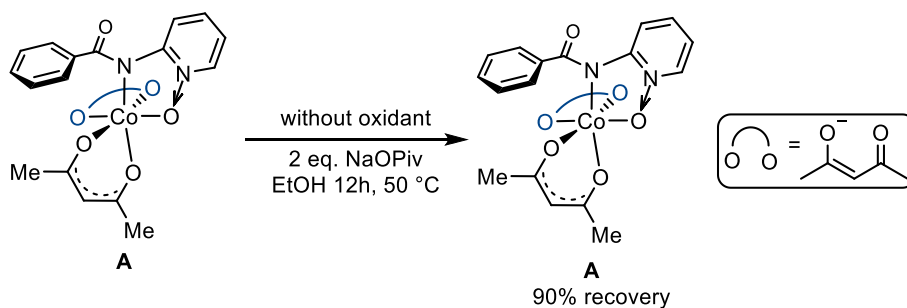
To a 25 mL tube were added **A** (47.0 mg, 0.1 mmol), NaOPiv·H₂O (24.8 mg, 0.20 mmol, 2.0 equiv) and alcohol (8.0 mL). The reaction was carried out at 50 °C under air for 12 hours. Then the reaction mixture was concentrated in vacuo and purified by column chromatography with CH₂Cl₂/acetone (3:1) to get the recovered **A** (42.3 mg, 90% recovery).

Procedure for the experiment of C–H oxygenation of **A** under chemical oxidation conditions

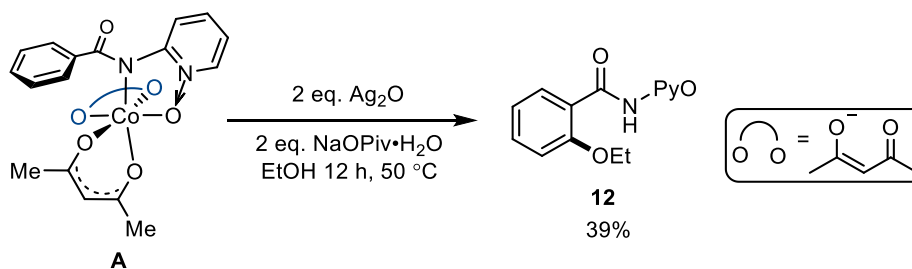
To a 25 mL tube were added **A** (47.0 mg, 0.1 mmol), Ag₂O (46.3 mg, 0.20 mmol, 2.0equiv), NaOPiv·H₂O (24.8 mg, 0.20 mmol, 2.0equiv) and alcohol (8.0 mL). Then the reaction mixture was concentrated in vacuo and purified by column chromatography with CH₂Cl₂/acetone (3:1) to get **12** (10.1 mg, 39% yield).



Scheme S2. Change of conditions for amidylcobalt(III) synthesis.



Scheme S3. Recovery of **A** in basic solution without additional oxidant.



Scheme S4. C-H oxygenation of **A** under chemical oxidation conditions.

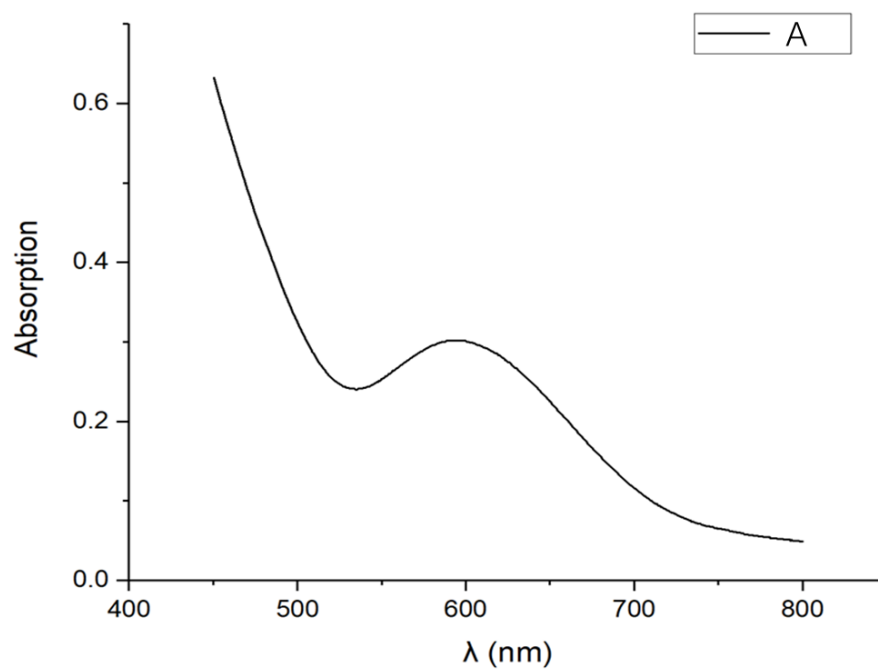


Figure S13. UV-vis spectrum of **A**.

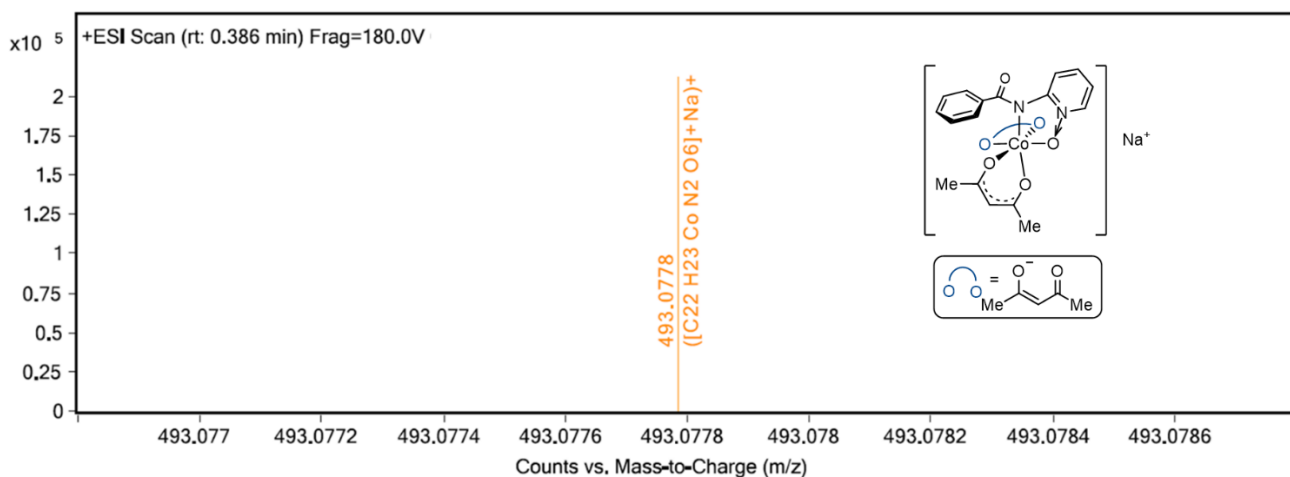
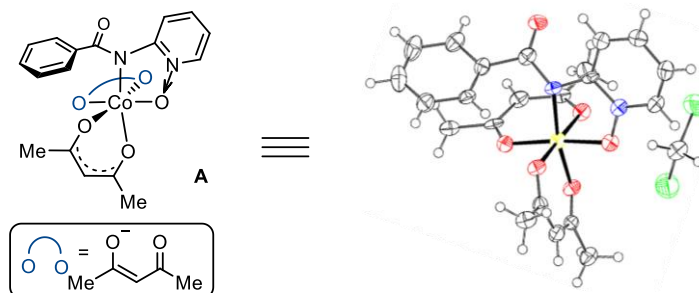


Figure S14. Q-TOF MS data of A.

Table S1. X-Ray Crystallographic Data of A



| | | | |
|---|--|--|------------|
| Bond precision: | C–C = 0.0133 Å | Wavelength = 0.71073 | |
| Cell: | a=18.880(14) | b=7.915(8) | c=30.41(6) |
| | alpha=90 | beta=98.22(4) | gamma=90 |
| Temperature: | 170 K | | |
| | Calculated | Reported | |
| Volume | 4498(11) | 4498(11) | |
| Space group | C 2/c | C 1 2/c 1 | |
| Hall group | -C 2yc | -C 2yc | |
| Moiety formula | 2(C ₂₂ H ₂₃ Co N ₂ O ₆), C H ₂ Cl ₂ | | |
| Sum formula | C ₄₅ H ₄₈ Cl ₂ Co ₂ N ₄ O ₁₂ | C ₄₅ H ₄₈ Cl ₂ Co ₂ N ₄ O ₁₂ | |
| Mr | 1025.63 | 1025.63 | |
| Dx, g cm ⁻³ | 1.515 | 1.515 | |
| Z | 4 | 4 | |
| Mu (mm ⁻¹) | 0.924 | 0.924 | |
| F000 | 2120.0 | 2120.0 | |
| F000' | 2124.85 | | |
| h,k,lmax | 24,10,39 | 24,10,38 | |
| Nref | 4974 | 4907 | |
| Tmin,Tmax | 0.839,0.946 | 0.612,0.746 | |
| Tmin' | 0.839 | | |
| Correction method= # Reported T Limits: Tmin=0.612 Tmax=0.746 AbsCorr = MULTI-SCAN | | | |
| Data completeness= 0.987 | Theta(max)= 27.121 | | |
| R(reflections)= 0.1113(4089) | wR2(reflections)= 0.2562(4907) | | |
| S = 1.279 | Npar= 298 | | |

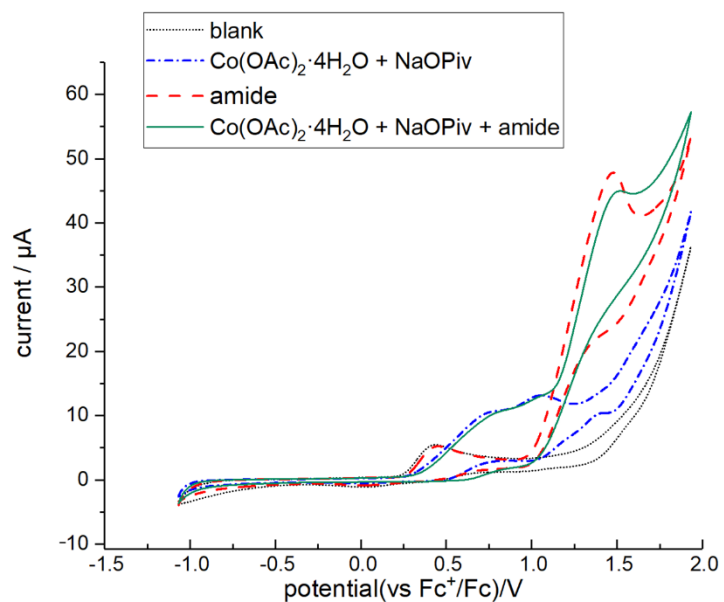


Figure S15. Cyclic voltammetry studies at 0.1 V/s. The measurements were carried out in a solvent mixture of DCM and MeOH (4:1), with electrolyte $n\text{-Bu}_4\text{NPF}_6$ (0.05 M). Amide (substrate **1**) (0.5 mM), NaOPiv·H₂O (2 mM), $\text{Co}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$ (0.5 mM). The oxidation peak in the blank CV may due to the water impurity in the solvent mixture, as the CV experiments were conducted in open air.

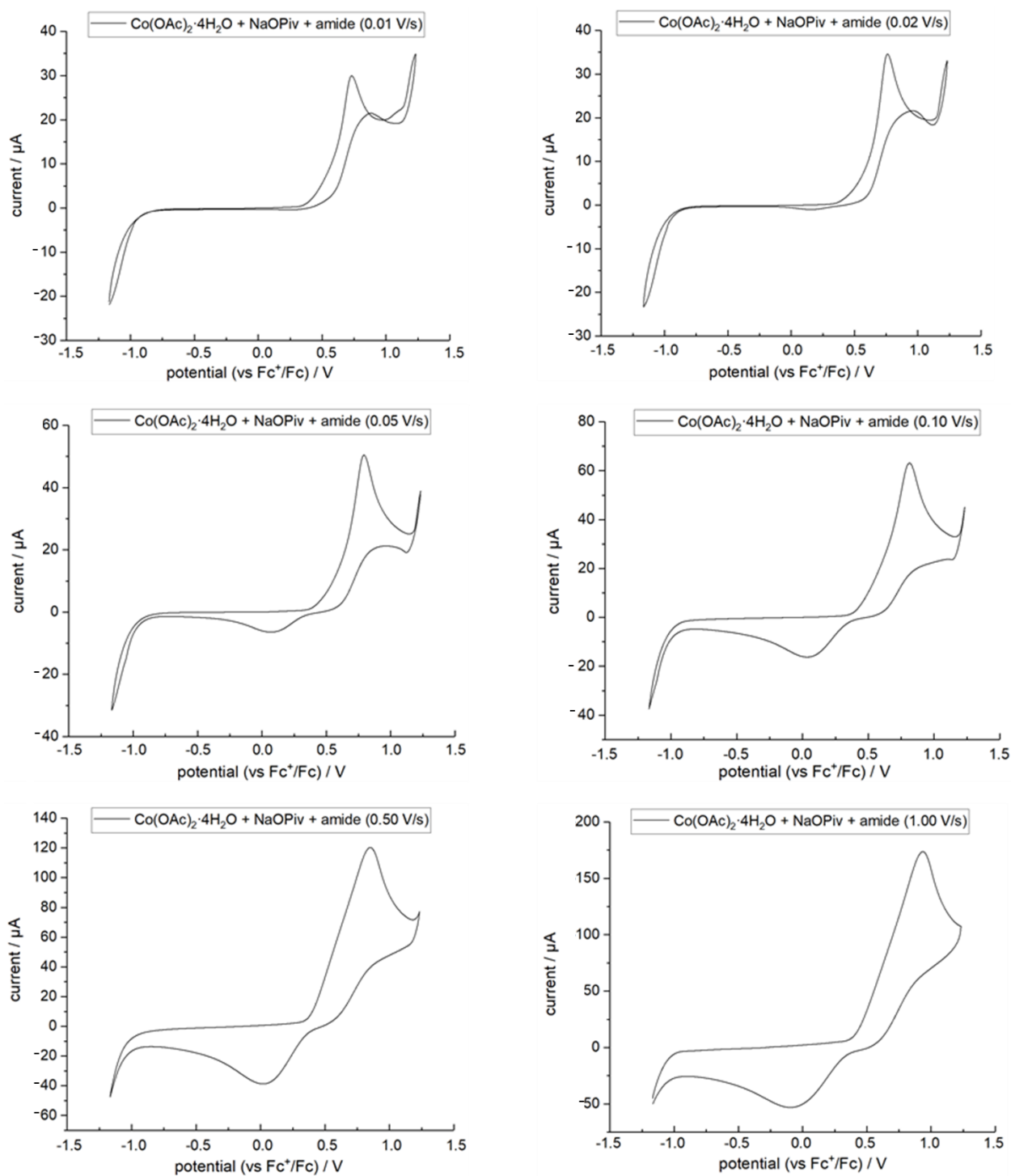


Figure S16. Cyclic voltammety studies with varying scan rates. The measurements were carried out at a scan rate of 0.01 V/s, 0.02 V/s, 0.05 V/s, 0.10 V/s, 0.50 V/s, 1.00 V/s respectively in a solvent mixture of DCM and MeOH (4:1), with electrolyte $n\text{-Bu}_4\text{NPF}_6$ (0.05M). Amide (substrate **1**) (0.5 mM), $\text{NaOPiv} \cdot \text{H}_2\text{O}$ (2 mM), $\text{Co(OAc)}_2 \cdot 4\text{H}_2\text{O}$ (0.5 mM).

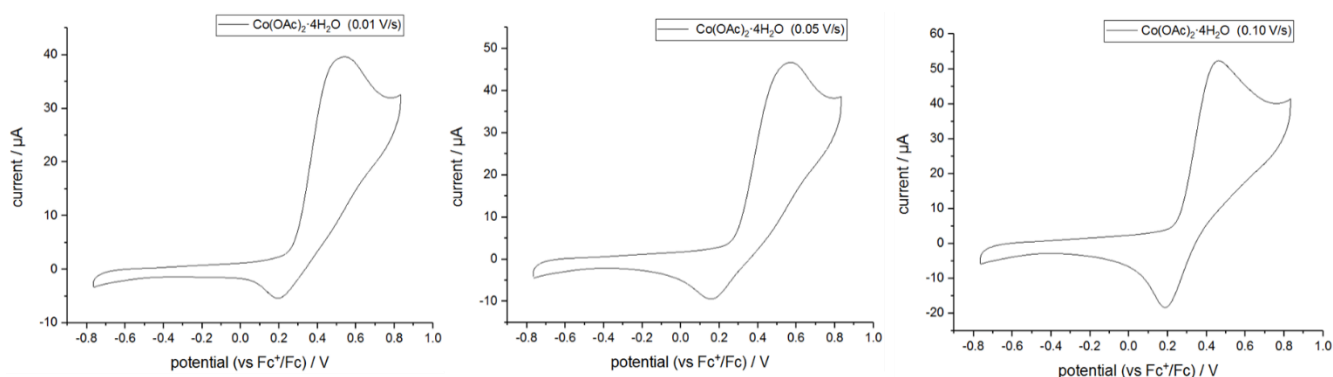


Figure S17. Cyclic voltammetry studies with varying scan rates of $\text{Co}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$. The measurements were carried out at a scan rate of 0.01 V/s, 0.05 V/s, 0.10 V/s respectively in a solvent mixture of DCM and MeOH (4:1), with electrolyte $n\text{-Bu}_4\text{NPF}_6$ (0.05M), $\text{Co}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$ (0.5 mM).

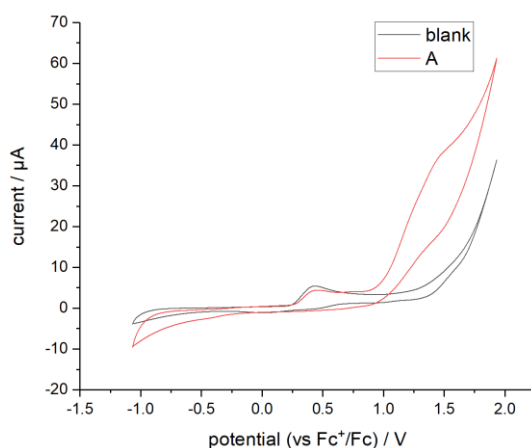


Figure S18. Cyclic voltammetry studies of A. The measurements were carried out at a scan rate of 0.10 V/s in a solvent mixture of DCM and MeOH (4:1), with electrolyte $n\text{-Bu}_4\text{NPF}_6$ (0.05M), A (0.5 mM).

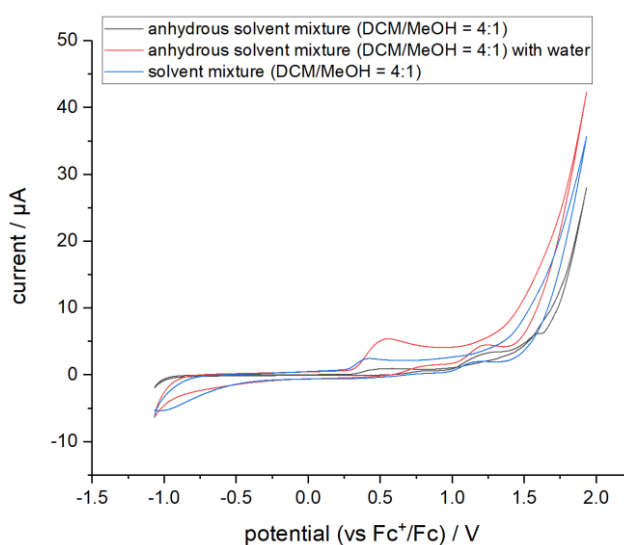
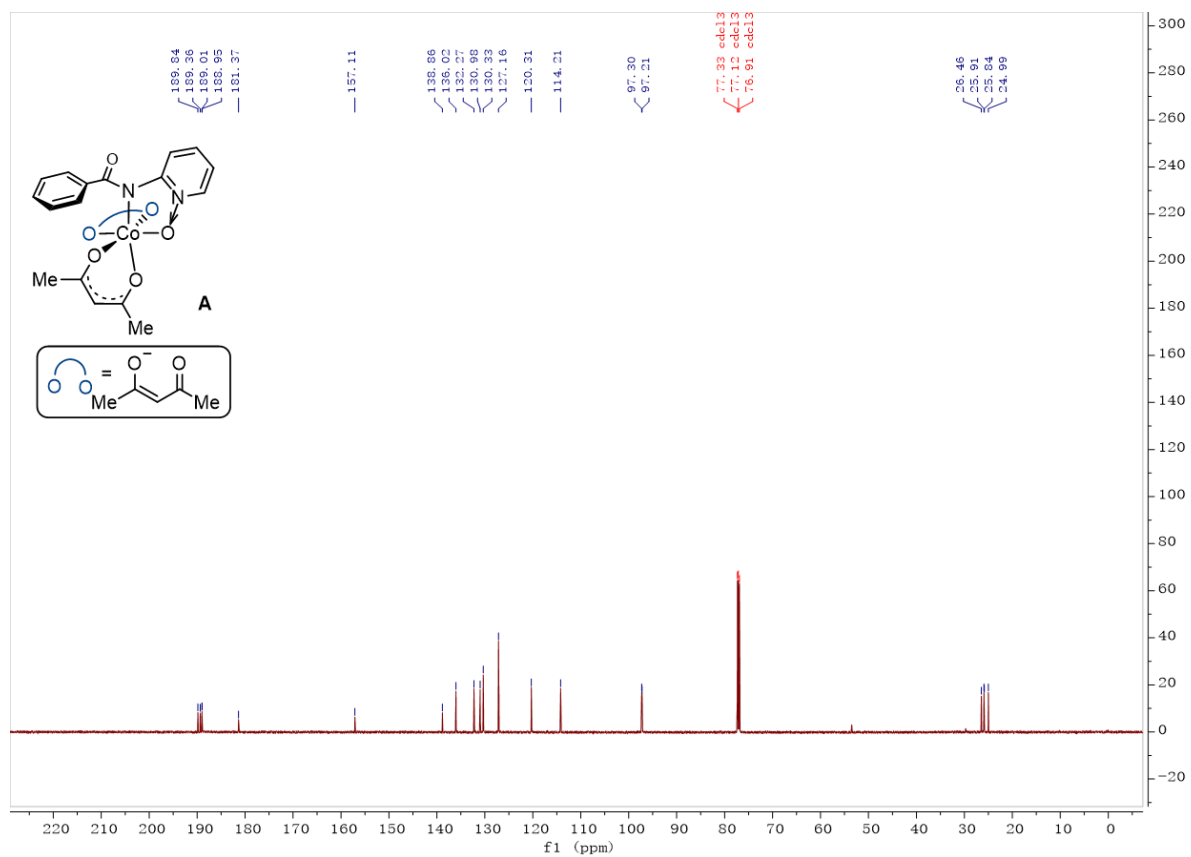
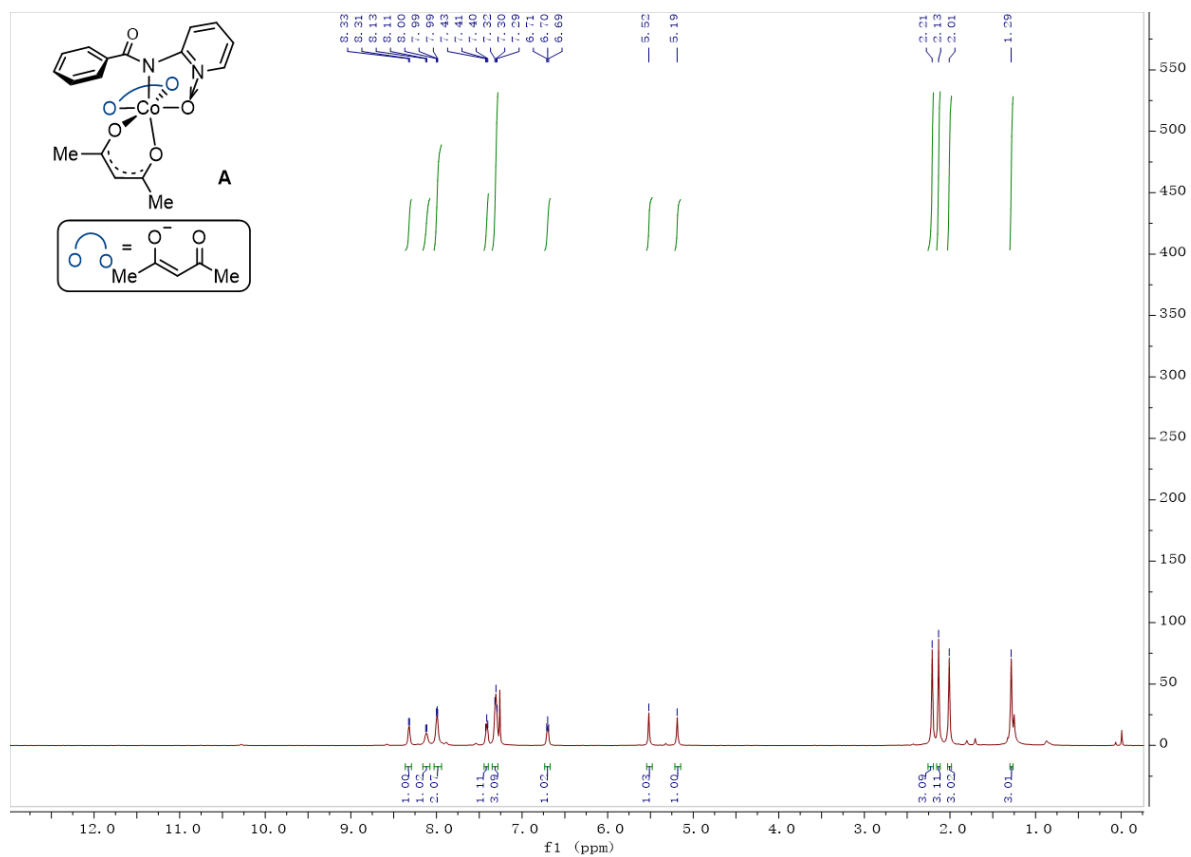


Figure S19. Cyclic voltammetry studies of solvent mixtures to confirm the water oxidation peak. The measurements were carried out at a scan rate of 0.10 V/s with electrolyte $n\text{-Bu}_4\text{NPF}_6$ (0.05M). Black line is the anhydrous solvent mixture of DCM and MeOH (4:1). Red line is an anhydrous solvent mixture of DCM and MeOH (4:1) with water (0.2 M). Blue line is the solvent mixture of DCM and MeOH (4:1), blank in Figure S15 and S18.

III. References

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IV. NMR Spectra



V. Table of Energies

Zero-point correction (*ZPE*) thermal correction to enthalpy (*TCH*) thermal correction to Gibbs free energy (*TCG*) energies (*E*) enthalpies (*H*) and Gibbs free energy (*G*) (in Hartree) of the structures calculated at the B3LYP-D3(BJ)/def2TZVP-SMD(Methanol)//B3LYP-D3(BJ)/6-31G(d)-LANL2DZ level of theory.

Table S2. Energies in Figure 1, Figure 3, Figure S1, Figure S3, Figure S8 and Figure S10.

| Structures | <i>ZPE</i> | <i>TCH</i> | <i>TCG</i> | <i>E</i> | <i>H</i> | <i>G</i> | Imaginary Frequency |
|------------------------------------|------------|------------|------------|--------------|--------------|--------------|---------------------|
| Co(OPiv) ₃ (singlet) | 0.411801 | 0.440545 | 0.351575 | -2422.676192 | -2422.235647 | -2422.324617 | |
| Co(OPiv) ₃ (triplet) | 0.409535 | 0.439200 | 0.345726 | -2422.682778 | -2422.243578 | -2422.337052 | |
| Co(OPiv) ₃ (quintet) | 0.410474 | 0.439814 | 0.346067 | -2422.711172 | -2422.271358 | -2422.365105 | |
| 1 | 0.202059 | 0.215467 | 0.161681 | -723.570507 | -723.355040 | -723.408826 | |
| int2(singlet) | 0.618500 | 0.659858 | 0.544742 | -3146.32237 | -3145.662512 | -3145.777628 | |
| int2(triplet) | 0.616549 | 0.659228 | 0.536186 | -3146.306506 | -3145.647278 | -3145.77032 | |
| int2(quintet) | 0.614998 | 0.657920 | 0.535096 | -3146.317187 | -3145.659267 | -3145.78209 | |
| TS3(singlet) | 0.613226 | 0.654198 | 0.538920 | -3146.304926 | -3145.650728 | -3145.766006 | 734.90 <i>i</i> |
| TS3(triplet) | 0.611025 | 0.652958 | 0.534682 | -3146.293888 | -3145.640930 | -3145.759206 | 1186.53 <i>i</i> |
| TS3(quintet) | 0.609714 | 0.652252 | 0.529919 | -3146.291513 | -3145.639261 | -3145.761594 | 1092.65 <i>i</i> |
| int4(singlet) | 0.468281 | 0.500228 | 0.405298 | -2799.091574 | -2798.591346 | -2798.686276 | |
| int4(triplet) | 0.467317 | 0.498966 | 0.403305 | -2799.091157 | -2798.592191 | -2798.687852 | |
| int4(quintet) | 0.464602 | 0.498212 | 0.395686 | -2799.087530 | -2798.589318 | -2798.691844 | |
| TS5(singlet) | 0.462793 | 0.494266 | 0.400588 | -2799.060694 | -2798.566428 | -2798.660106 | 938.47 <i>i</i> |
| TS5(triplet) | 0.493602 | 0.461493 | 0.397694 | -2799.052397 | -2798.558795 | -2798.654703 | 773.24 <i>i</i> |
| TS5(quintet) | 0.459753 | 0.492568 | 0.392991 | -2799.040555 | -2798.547987 | -2798.647564 | 1161.19 <i>i</i> |
| int6(singlet) | 0.318496 | 0.341092 | 0.267817 | -2451.846368 | -2451.505276 | -2451.578551 | |

| | | | | | | | |
|-----------------------|----------|----------|----------|--------------|--------------|--------------|----------|
| int6(triplet) | 0.317232 | 0.340475 | 0.263313 | -2451.864407 | -2451.523932 | -2451.601094 | |
| int6(quintet) | 0.315654 | 0.339463 | 0.259872 | -2451.820002 | -2451.480539 | -2451.560130 | |
| int7(singlet) | 0.371973 | 0.398035 | 0.316251 | -2567.656886 | -2567.258851 | -2567.340635 | |
| int7(triplet) | 0.371786 | 0.398698 | 0.313553 | -2567.671523 | -2567.272825 | -2567.357970 | |
| int7(quintet) | 0.369627 | 0.397126 | 0.310231 | -2567.640007 | -2567.242881 | -2567.329776 | |
| TS8(singlet) | 0.369198 | 0.395069 | 0.314049 | -2567.586367 | -2567.191298 | -2567.272318 | 345.82i |
| TS8(triplet) | 0.367441 | 0.393989 | 0.310055 | -2567.613826 | -2567.219837 | -2567.303771 | 422.06i |
| TS8(quintet) | 0.368906 | 0.395636 | 0.310724 | -2567.599400 | -2567.203764 | -2567.288676 | 274.95i |
| int9(singlet) | 0.374447 | 0.400692 | 0.318082 | -2567.610827 | -2567.210135 | -2567.292745 | |
| int9(triplet) | 0.372825 | 0.399791 | 0.314082 | -2567.63414 | -2567.234349 | -2567.320058 | |
| int9(quintet) | 0.371491 | 0.398262 | 0.313060 | -2567.609662 | -2567.211400 | -2567.296602 | |
| int10(doublet) | 0.467515 | 0.499707 | 0.403053 | -2798.87795 | -2798.378243 | -2798.474897 | |
| int10(quartet) | 0.463919 | 0.497663 | 0.394789 | -2798.843159 | -2798.345496 | -2798.448370 | |
| int10(sextet) | 0.464148 | 0.497804 | 0.395169 | -2798.861550 | -2798.363746 | -2798.466381 | |
| int13(doublet) | 0.603985 | 0.645375 | 0.529530 | -3145.651897 | -3145.006522 | -3145.122367 | |
| int13(quartet) | 0.602029 | 0.644486 | 0.523507 | -3145.643659 | -3144.999173 | -3145.120152 | |
| int13(sextet) | 0.601014 | 0.643991 | 0.521267 | -3145.635573 | -3144.991582 | -3145.114306 | |
| TS14(doublet) | 0.597078 | 0.638447 | 0.522752 | -3145.608861 | -3144.970414 | -3145.086109 | 1379.59i |
| TS14(quartet) | 0.593077 | 0.635940 | 0.515485 | -3145.593067 | -3144.957127 | -3145.077582 | 1417.28i |
| TS14(sextet) | 0.593167 | 0.636009 | 0.515288 | -3145.593396 | -3144.957387 | -3145.078108 | 1410.53i |
| int15(doublet) | 0.604253 | 0.645634 | 0.529669 | -3145.624288 | -3144.978654 | -3145.094619 | |
| int15(quartet) | 0.601553 | 0.643906 | 0.523787 | -3145.610934 | -3144.967028 | -3145.087147 | |
| int15(sextet) | 0.600264 | 0.643240 | 0.521291 | -3145.616343 | -3144.973103 | -3145.095052 | |
| int16(doublet) | 0.603660 | 0.644829 | 0.530701 | -3145.653067 | -3145.008238 | -3145.122366 | |
| int16(quartet) | 0.600893 | 0.643470 | 0.523226 | -3145.641201 | -3144.997731 | -3145.117975 | |
| int16(sextet) | 0.600126 | 0.642819 | 0.523163 | -3145.618202 | -3144.975383 | -3145.095039 | |
| int17(doublet) | 0.454876 | 0.486692 | 0.391568 | -2798.434587 | -2797.947895 | -2798.043019 | |
| int17(quartet) | 0.453439 | 0.486202 | 0.386551 | -2798.424321 | -2797.938119 | -2798.03777 | |
| int17(sextet) | 0.450777 | 0.484346 | 0.383159 | -2798.392374 | -2797.908028 | -2798.009215 | |
| int18(doublet) | 0.509091 | 0.544426 | 0.441314 | -2914.238842 | -2913.694416 | -2913.797528 | |
| int18(quartet) | 0.506732 | 0.544230 | 0.432127 | -2914.227452 | -2913.683222 | -2913.795325 | |
| int18(sextet) | 0.505709 | 0.542674 | 0.434305 | -2914.196262 | -2913.653588 | -2913.761957 | |

| | | | | | | | |
|--|----------|----------|----------|--------------|--------------|--------------|------------------|
| TS19(doublet) | 0.508347 | 0.543469 | 0.441819 | -2914.214137 | -2913.670668 | -2913.772318 | 208.55 <i>i</i> |
| TS19(quartet) | 0.505163 | 0.541203 | 0.436000 | -2914.207009 | -2913.665806 | -2913.771009 | 194.71 <i>i</i> |
| TS19(sextet) | 0.502877 | 0.539209 | 0.431976 | -2914.174580 | -2913.635371 | -2913.742604 | 248.92 <i>i</i> |
| int20(doublet) | 0.512390 | 0.547646 | 0.445081 | -2914.304880 | -2913.757234 | -2913.859799 | |
| int20(quartet) | 0.511100 | 0.547171 | 0.441727 | -2914.314730 | -2913.767559 | -2913.873003 | |
| int20(sextet) | 0.506408 | 0.542831 | 0.437177 | -2914.217066 | -2913.674235 | -2913.779889 | |
| TS-S1 (singlet) | 0.368250 | 0.394380 | 0.313161 | -2567.622642 | -2567.228262 | -2567.309481 | 1017.57 <i>i</i> |
| TS-S1 (triplet) | 0.366598 | 0.393403 | 0.308540 | -2567.633679 | -2567.240276 | -2567.325139 | 927.41 <i>i</i> |
| TS-S1 (quintet) | 0.365071 | 0.392447 | 0.305369 | -2567.606300 | -2567.213853 | -2567.300931 | 936.94 <i>i</i> |
| int-S2 (singlet) | 0.372215 | 0.398898 | 0.316262 | -2567.626610 | -2567.227712 | -2567.310348 | |
| int-S2 (triplet) | 0.372121 | 0.398962 | 0.314868 | -2567.646003 | -2567.247041 | -2567.331135 | |
| int-S2 (quintet) | 0.369716 | 0.397675 | 0.309337 | -2567.620314 | -2567.222639 | -2567.310977 | |
| TS-S3 (singlet) | 0.371207 | 0.396854 | 0.315617 | -2567.554336 | -2567.157482 | -2567.238719 | 423.80 <i>i</i> |
| TS-S3 (triplet) | 0.369340 | 0.395974 | 0.311684 | -2567.606939 | -2567.210965 | -2567.295255 | 321.48 <i>i</i> |
| TS-S3 (quintet) | 0.368568 | 0.395284 | 0.310681 | -2567.592338 | -2567.197054 | -2567.281657 | 368.80 <i>i</i> |
| int-S4 (singlet) | 0.617178 | 0.658907 | 0.540412 | -3146.314544 | -3145.655637 | -3145.774132 | |
| int-S4 (triplet) | 0.615344 | 0.657816 | 0.537120 | -3146.307243 | -3145.649427 | -3145.770123 | |
| int-S4 (quintet) | 0.613416 | 0.656529 | 0.532001 | -3146.305718 | -3145.649189 | -3145.773717 | |
| int-S5 (singlet) | 0.468303 | 0.500139 | 0.406402 | -2799.087735 | -2798.587596 | -2798.681333 | |
| int-S5 (triplet) | 0.467471 | 0.499841 | 0.403029 | -2799.088478 | -2798.588637 | -2798.685449 | |
| int-S5 (quintet) | 0.464698 | 0.498199 | 0.396502 | -2799.086815 | -2798.588616 | -2798.690313 | |
| int-S6 (singlet) | 0.467885 | 0.499660 | 0.404901 | -2799.092347 | -2798.592687 | -2798.687446 | |
| int-S6 (triplet) | 0.466574 | 0.499391 | 0.400769 | -2799.090327 | -2798.590936 | -2798.689558 | |
| int-S6 (quintet) | 0.463994 | 0.497717 | 0.394828 | -2799.053975 | -2798.556279 | -2798.659488 | |
| proton-transfer TS(doublet) | 0.598319 | 0.639200 | 0.526875 | -3145.592668 | -3144.953468 | -3145.065793 | 1145.27 <i>i</i> |
| proton-transfer TS(quartet) | 0.593888 | 0.636523 | 0.517109 | -3145.573412 | -3144.936889 | -3145.056303 | 1536.01 <i>i</i> |
| proton-transfer TS(sextet) | 0.593701 | 0.636450 | 0.514896 | -3145.570377 | -3144.933927 | -3145.055481 | 1682.25 <i>i</i> |
| TS-S7 (doublet) | 0.507134 | 0.542114 | 0.440597 | -2914.279724 | -2913.737610 | -2913.839127 | 995.63 <i>i</i> |

| | | | | | | | |
|--|----------|----------|----------|--------------|--------------|--------------|----------|
| TS-S7 (quartet) | 0.506856 | 0.542079 | 0.439179 | -2914.306488 | -2913.764409 | -2913.867309 | 691.57i |
| TS-S7 (sextet) | 0.502824 | 0.538861 | 0.433649 | -2914.211443 | -2913.672582 | -2913.777794 | 1077.75i |
| int-S8 (doublet) | 0.512338 | 0.548008 | 0.443223 | -2914.294386 | -2913.746378 | -2913.851163 | |
| int-S8 (quartet) | 0.511561 | 0.547737 | 0.439631 | -2914.326795 | -2913.779058 | -2913.887164 | |
| int-S8 (sextet) | 0.507248 | 0.544283 | 0.435874 | -2914.219701 | -2913.675418 | -2913.783827 | |
| int-S9 (doublet) | 0.510596 | 0.545832 | 0.443301 | -2914.282614 | -2913.736782 | -2913.839313 | |
| int-S9 (quartet) | 0.510455 | 0.546253 | 0.441215 | -2914.31229 | -2913.766037 | -2913.871075 | |
| int-S9 (sextet) | 0.506720 | 0.543165 | 0.436679 | -2914.215241 | -2913.672076 | -2913.778562 | |
| S10 | 0.235038 | 0.250986 | 0.191347 | -838.148849 | -837.897863 | -837.957502 | |
| Co(OPiv)₃⁻ (doublet) | 0.410003 | 0.439320 | 0.346632 | -2422.884155 | -2422.444835 | -2422.537523 | |
| Co(OPiv)₃⁻ (quartet) | 0.409643 | 0.439147 | 0.346077 | -2422.907470 | -2422.468323 | -2422.561393 | |
| HOPiv | 0.147586 | 0.156785 | 0.115252 | -347.207918 | -347.051133 | -347.092666 | |
| OPiv⁻ | 0.133622 | 0.142594 | 0.101474 | -346.737837 | -346.595243 | -346.636623 | |
| MeOH | 0.051483 | 0.055717 | 0.028762 | -115.786545 | -115.730828 | -115.757783 | |

Table S3. Energies in Scheme S1.

| Structures | ZPE | TCH | TCG | E | H | G | Imaginary Frequency |
|--|------------|------------|------------|--------------|--------------|--------------|----------------------------|
| int13-tBu (doublet) | 0.717720 | 0.764408 | 0.639317 | -3302.992604 | -3302.228196 | -3302.353287 | |
| TS14-tBu (doublet) | 0.710657 | 0.757494 | 0.631077 | -3302.948886 | -3302.191392 | -3302.317809 | 1346.10i |
| int13-Me (doublet) | 0.631861 | 0.674989 | 0.555087 | -3184.989808 | -3184.314819 | -3184.434721 | |
| TS14-Me (doublet) | 0.624902 | 0.668132 | 0.548200 | -3184.947448 | -3184.279316 | -3184.399248 | 1351.49 |
| int13-OMe (doublet) | 0.637145 | 0.680960 | 0.560101 | -3260.231123 | -3259.550163 | -3259.671022 | |
| TS14-OMe (doublet) | 0.631070 | 0.674922 | 0.554183 | -3260.189083 | -3259.514161 | -3259.634900 | 1232.57i |
| int13-SMe (doublet) | 0.633315 | 0.677846 | 0.555275 | -3583.214614 | -3582.536768 | -3582.659339 | |
| TS14-SMe (doublet) | 0.626995 | 0.671537 | 0.549054 | -3583.172587 | -3582.50105 | -3582.623533 | 1302.03i |
| int13-Cl (doublet) | 0.594840 | 0.637220 | 0.519329 | -3605.283485 | -3605.237783 | -3604.764156 | |
| TS14-Cl (doublet) | 0.587911 | 0.630361 | 0.512065 | -3605.237783 | -3604.607422 | -3604.725718 | 1396.38i |
| int13-CO₂Me (doublet) | 0.647802 | 0.693451 | 0.568808 | -3373.642013 | -3372.948562 | -3373.073205 | |
| TS14-CO₂Me (doublet) | 0.640360 | 0.686268 | 0.560093 | -3373.594704 | -3372.908436 | -3373.034611 | 1397.05i |

| | | | | | | | |
|---------------------------------------|----------|----------|----------|--------------|--------------|--------------|------------------|
| int13-CO ₂ Et (doublet) | 0.676138 | 0.723208 | 0.593834 | -3412.981217 | -3412.258009 | -3412.387383 | |
| TS14-CO ₂ Et (doublet) | 0.668834 | 0.716060 | 0.585705 | -3412.93391 | -3412.217850 | -3412.348205 | 1398.20 <i>i</i> |
| int13-CF ₃ (doublet) | 0.609349 | 0.654107 | 0.530839 | -3482.853035 | -3482.198928 | -3482.322196 | |
| TS14-CF ₃ (doublet) | 0.602155 | 0.646975 | 0.523958 | -3482.806801 | -3482.159826 | -3482.282843 | 1416.25 <i>i</i> |
| int13-CN (doublet) | 0.603121 | 0.646083 | 0.527481 | -3237.938197 | -3237.292114 | -3237.410716 | |
| TS14-CN (doublet) | 0.595900 | 0.638967 | 0.519979 | -3237.891059 | -3237.252092 | -3237.37108 | 1420.87 <i>i</i> |
| int13-NO ₂ (doublet) | 0.607258 | 0.650885 | 0.530683 | -3350.249969 | -3349.599084 | -3349.719286 | |
| TS14-NO ₂ (doublet) | 0.599847 | 0.643658 | 0.522125 | -3350.200604 | -3349.556946 | -3349.678479 | 1435.64 <i>i</i> |

VI. Cartesian coordinates of the structures

Co(OPiv)₃ (singlet)

| | | | |
|----|-------------|-------------|-------------|
| Co | 0.26690800 | -0.74882300 | -1.00622700 |
| O | -1.40882400 | -1.25628700 | -0.85347100 |
| O | 1.33713900 | -1.24505500 | 0.41510500 |
| O | 0.22116200 | 1.02941300 | -0.83984200 |
| C | -2.10132800 | -1.58811000 | 0.26896100 |
| O | -1.57971300 | -2.17529800 | 1.18840900 |
| C | 2.40884500 | -0.94682600 | -0.24542000 |
| O | 2.19053500 | -0.59701300 | -1.44717100 |
| C | -0.33292400 | 1.59713000 | 0.23518000 |
| O | -0.76065800 | 0.98827700 | 1.19548400 |
| C | 3.75652300 | -0.93084900 | 0.42478300 |
| C | 3.80341000 | 0.40656200 | 1.20833000 |
| C | 3.86306600 | -2.11689600 | 1.39968500 |
| C | 4.86711600 | -0.97297000 | -0.63384300 |
| H | 3.69331200 | 1.26163300 | 0.53321100 |
| H | 3.00655900 | 0.44797600 | 1.95676800 |
| H | 4.76924900 | 0.48882300 | 1.71787000 |
| H | 3.82678200 | -3.07230600 | 0.86528300 |
| H | 4.81666500 | -2.06170100 | 1.93501700 |
| H | 3.05013700 | -2.10213200 | 2.13019300 |
| H | 5.84202100 | -0.91347700 | -0.13871600 |
| H | 4.83201000 | -1.90431300 | -1.20857500 |
| H | 4.78070900 | -0.13823500 | -1.33451800 |
| C | -0.33819000 | 3.13375500 | 0.10532400 |
| C | -1.00837000 | 3.72694700 | 1.35066400 |
| C | 1.12135200 | 3.61912800 | -0.00239800 |
| C | -1.12222600 | 3.52577800 | -1.16222300 |
| H | -2.04337500 | 3.38512800 | 1.44246100 |
| H | -0.48006300 | 3.43285800 | 2.26167800 |
| H | -1.00782400 | 4.82084500 | 1.28119300 |
| H | 1.61059500 | 3.20108400 | -0.88649100 |
| H | 1.14525300 | 4.71257500 | -0.07395000 |
| H | 1.69809700 | 3.32692700 | 0.88309800 |
| H | -1.16176300 | 4.61753800 | -1.25066100 |
| H | -0.64961300 | 3.12107300 | -2.06118700 |
| H | -2.15180100 | 3.15285900 | -1.11683800 |
| C | -3.58109700 | -1.20543800 | 0.19047000 |
| C | -3.70481700 | 0.31171600 | -0.05360300 |
| C | -4.21584300 | -1.97410500 | -0.98818600 |

| | | | |
|---|-------------|-------------|-------------|
| C | -4.26499100 | -1.58999400 | 1.50793100 |
| H | -3.24752600 | 0.87601300 | 0.76358400 |
| H | -3.21174900 | 0.60018300 | -0.98691700 |
| H | -4.76380200 | 0.58669700 | -0.12189000 |
| H | -4.13307300 | -3.05731600 | -0.84342800 |
| H | -5.28012800 | -1.72253400 | -1.06223300 |
| H | -3.73264800 | -1.71392200 | -1.93458500 |
| H | -5.32858400 | -1.32837300 | 1.46489500 |
| H | -4.17703800 | -2.66334600 | 1.69933800 |
| H | -3.80919500 | -1.06357900 | 2.35149200 |

Co(OPiv)₃ (triplet)

| | | | |
|----|-------------|-------------|-------------|
| Co | -0.56689000 | -0.22467700 | -0.20876800 |
| O | 0.85379100 | 1.05808200 | -0.41440600 |
| O | -2.19440600 | -0.28060000 | 1.01137100 |
| O | 0.71353600 | -1.72059500 | -0.09779200 |
| C | 0.77314400 | 2.35211900 | -0.12503800 |
| O | -0.34684100 | 2.84097100 | -0.03857900 |
| C | -2.92548900 | -0.34006500 | -0.03858500 |
| O | -2.34392400 | -0.36927100 | -1.17871700 |
| C | 1.96733300 | -1.53077900 | -0.05286200 |
| O | 2.54893800 | -0.41093600 | -0.10423300 |
| C | -4.43990900 | -0.35458900 | 0.08827600 |
| C | -4.83261200 | -1.51814800 | 1.02142400 |
| C | -4.85575900 | 0.98766200 | 0.73019600 |
| C | -5.09979300 | -0.51848200 | -1.28643200 |
| H | -4.54587600 | -2.48386900 | 0.58943900 |
| H | -4.34611000 | -1.41788600 | 1.99503900 |
| H | -5.91849500 | -1.52156000 | 1.16793100 |
| H | -4.57619800 | 1.83265300 | 0.09130100 |
| H | -5.94282800 | 1.00725700 | 0.86712100 |
| H | -4.37591800 | 1.11873700 | 1.70381000 |
| H | -6.18982300 | -0.51932600 | -1.17327000 |
| H | -4.82045400 | 0.29734600 | -1.95891200 |
| H | -4.80028900 | -1.45856100 | -1.75964200 |
| C | 2.87037800 | -2.77850700 | 0.08190000 |
| C | 4.35599600 | -2.39783600 | 0.11793900 |
| C | 2.46173300 | -3.48606600 | 1.38890000 |
| C | 2.57148800 | -3.68165700 | -1.13046100 |
| H | 4.65943500 | -1.88312400 | -0.79852600 |
| H | 4.57978700 | -1.74138500 | 0.96411700 |
| H | 4.96133900 | -3.30535000 | 0.21855400 |
| H | 1.40101700 | -3.74847900 | 1.37754400 |
| H | 3.05114200 | -4.40296300 | 1.50252200 |
| H | 2.65414900 | -2.85013600 | 2.26023200 |
| H | 3.15917900 | -4.60315100 | -1.04872800 |
| H | 1.51131800 | -3.94313500 | -1.17159300 |
| H | 2.84570700 | -3.18786000 | -2.06933800 |
| C | 2.07797500 | 3.10861300 | 0.07359400 |
| C | 2.70892900 | 2.60542800 | 1.39192000 |
| C | 3.02416400 | 2.81481600 | -1.10690200 |
| C | 1.77889300 | 4.61110000 | 0.16737300 |
| H | 2.04532900 | 2.79785200 | 2.24266400 |
| H | 2.91785800 | 1.53437900 | 1.34313000 |
| H | 3.65021300 | 3.13757800 | 1.56998900 |
| H | 2.58423100 | 3.14465000 | -2.05490300 |
| H | 3.96388700 | 3.36007600 | -0.96341900 |
| H | 3.24535700 | 1.74812400 | -1.17836300 |
| H | 2.71118500 | 5.16222300 | 0.33251300 |
| H | 1.31802900 | 4.98049600 | -0.75406300 |
| H | 1.09529700 | 4.82883400 | 0.99295000 |

Co(OPiv)₃ (quintet)

| | | | |
|----|-------------|-------------|-------------|
| Co | -0.03744100 | -0.23633300 | -0.17913600 |
|----|-------------|-------------|-------------|

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|---|-------------|-------------|-------------|
| O | 1.32785400 | -1.41722100 | -0.75315000 |
| O | -0.47485100 | 1.45844100 | 0.83106700 |
| O | -1.82613800 | -0.50707600 | -1.04003800 |
| C | 2.25311800 | -1.09769700 | 0.12773600 |
| O | 1.95284600 | -0.23283900 | 0.97057000 |
| C | 0.03022700 | 2.17890100 | -0.10595200 |
| O | 0.48753600 | 1.56344800 | -1.11649800 |
| C | -2.23130300 | -1.16817300 | -0.01184600 |
| O | -1.39163800 | -1.34427900 | 0.92685300 |
| C | 0.09027900 | 3.68713700 | 0.03997100 |
| C | -1.30850300 | 4.19898000 | 0.43697900 |
| C | 1.09851000 | 3.98573400 | 1.17314600 |
| C | 0.55294100 | 4.32992200 | -1.27404700 |
| H | -2.04286800 | 3.98795300 | -0.34845200 |
| H | -1.64950000 | 3.72735800 | 1.36231400 |
| H | -1.27329700 | 5.28351600 | 0.58764900 |
| H | 2.09657800 | 3.61250500 | 0.91913100 |
| H | 1.16490500 | 5.06861600 | 1.32589600 |
| H | 0.78421300 | 3.51673000 | 2.10958600 |
| H | 0.60448800 | 5.41753500 | -1.15182100 |
| H | 1.54162600 | 3.96565300 | -1.56671000 |
| H | -0.14115900 | 4.10644600 | -2.09011200 |
| C | -3.66311000 | -1.66044100 | 0.06672900 |
| C | -3.84475900 | -2.58796000 | 1.27527200 |
| C | -4.55573600 | -0.40568100 | 0.21057300 |
| C | -4.00395400 | -2.39471700 | -1.24481600 |
| H | -3.20442600 | -3.47208200 | 1.19520800 |
| H | -3.59396800 | -2.07627800 | 2.20830200 |
| H | -4.88710800 | -2.92123400 | 1.32816100 |
| H | -4.42503500 | 0.26606300 | -0.64259100 |
| H | -5.60679000 | -0.71082700 | 0.25941000 |
| H | -4.31572200 | 0.14529700 | 1.12646800 |
| H | -5.05118200 | -2.71549700 | -1.22234400 |
| H | -3.85438500 | -1.74341500 | -2.10967700 |
| H | -3.37812300 | -3.28510100 | -1.37202900 |
| C | 3.59317100 | -1.79989600 | 0.04373700 |
| C | 3.34661200 | -3.31594400 | 0.20205300 |
| C | 4.19270800 | -1.51177700 | -1.34988300 |
| C | 4.52197300 | -1.28424900 | 1.15028900 |
| H | 2.91085300 | -3.54451600 | 1.18099600 |
| H | 2.67008300 | -3.68693700 | -0.57274400 |
| H | 4.29931500 | -3.85050300 | 0.12011800 |
| H | 4.36067500 | -0.43856500 | -1.49267400 |
| H | 5.15656800 | -2.02370500 | -1.44466000 |
| H | 3.52920100 | -1.86482000 | -2.14393800 |
| H | 5.48842800 | -1.79602200 | 1.08565700 |
| H | 4.69239900 | -0.20789200 | 1.05396200 |
| H | 4.09723100 | -1.46792500 | 2.14148800 |

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|---|-------------|-------------|-------------|
| C | -2.32283300 | 1.06100900 | -0.31454700 |
| C | -2.02547700 | -0.28017500 | -0.03348400 |
| C | -3.06804700 | -1.17157300 | 0.25104000 |
| C | -4.38611400 | -0.72626800 | 0.27513800 |
| C | -4.67667700 | 0.61272300 | 0.00382300 |
| C | -3.64432100 | 1.50274000 | -0.29635000 |
| H | -1.53832100 | 1.76311400 | -0.58145200 |
| H | -2.81846700 | -2.20798700 | 0.44996300 |
| H | -5.18796400 | -1.42214500 | 0.50401600 |
| H | -5.70560200 | 0.96064000 | 0.02015100 |
| H | -3.86708800 | 2.54127900 | -0.52221100 |
| C | -0.63734200 | -0.83716000 | -0.03865600 |
| O | -0.41400500 | -2.04180400 | -0.09691800 |
| N | 0.36662200 | 0.10506800 | 0.03723200 |

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|---|------------|-------------|-------------|
| H | 0.17561500 | 1.09777700 | 0.18265400 |
| C | 1.72585500 | -0.10992300 | 0.00547800 |
| C | 2.40874100 | -1.31590300 | -0.12864400 |
| C | 3.80062000 | -1.31862100 | -0.14735100 |
| H | 1.81939800 | -2.21776600 | -0.21119900 |
| C | 3.78365700 | 1.07042300 | 0.10485400 |
| C | 4.49033500 | -0.11094900 | -0.02897800 |
| H | 4.33716000 | -2.25531400 | -0.25195100 |
| H | 4.22436200 | 2.05294300 | 0.20346800 |
| H | 5.57385700 | -0.07182400 | -0.03823500 |
| N | 2.42292800 | 1.08307200 | 0.12305400 |
| O | 1.76023400 | 2.18985000 | 0.24802600 |

int2(singlet)

| | | | |
|----|-------------|-------------|-------------|
| C | -5.09363600 | 1.16840000 | 2.13127100 |
| C | -3.71220300 | 1.01846400 | 2.25926200 |
| C | -3.01464500 | 0.14062100 | 1.42822600 |
| C | -3.72049400 | -0.60160800 | 0.47075700 |
| C | -5.11406700 | -0.47924600 | 0.36695000 |
| C | -5.79625100 | 0.41594500 | 1.18459800 |
| H | -5.62676000 | 1.86275500 | 2.77492800 |
| H | -3.16686400 | 1.57979200 | 3.01210500 |
| H | -1.94333000 | 0.02754000 | 1.55422800 |
| H | -5.64126700 | -1.08628000 | -0.36174300 |
| H | -6.87274200 | 0.52460100 | 1.09008700 |
| C | -3.05098800 | -1.57829500 | -0.43066400 |
| O | -3.57045800 | -2.62901000 | -0.77975500 |
| C | -0.92249200 | -1.96568400 | -1.60214300 |
| C | -1.02273700 | -3.35227000 | -1.80352500 |
| C | -0.02257900 | -4.01991200 | -2.49081900 |
| H | -1.89171000 | -3.85713100 | -1.41061600 |
| C | 1.14868100 | -1.96134800 | -2.79017100 |
| C | 1.08998500 | -3.32345700 | -2.98186200 |
| H | -0.10181600 | -5.09264600 | -2.63311300 |
| H | 1.94855400 | -1.31016200 | -3.11487100 |
| H | 1.89659800 | -3.82516200 | -3.50226700 |
| N | 0.14716700 | -1.31402700 | -2.15153400 |
| O | 0.20291000 | 0.01914400 | -2.07106900 |
| N | -1.78463200 | -1.18465100 | -0.88162400 |
| H | -1.47822400 | -0.22471700 | -0.70049200 |
| Co | 1.05245700 | 0.73439400 | -0.50894800 |
| O | 2.92611700 | 0.52510000 | -0.96300400 |
| O | 1.14833700 | -0.95965400 | 0.27169900 |
| O | 0.66592700 | 2.52194900 | -1.27394700 |
| C | 3.21537900 | 1.07764300 | 0.15445700 |
| O | 2.21719900 | 1.48321300 | 0.83951900 |
| C | -0.46736400 | 2.47506700 | -0.70429700 |
| O | -0.69674800 | 1.41297900 | -0.01454600 |
| C | 0.67066900 | -1.18107300 | 1.47183500 |
| O | 0.06287400 | -0.37120800 | 2.16446200 |
| C | -1.50527800 | 3.57229000 | -0.79029400 |
| C | -1.01655100 | 4.69084700 | -1.71904000 |
| C | -2.81356300 | 2.94914300 | -1.32355900 |
| C | -1.73293500 | 4.10841000 | 0.63991700 |
| H | -0.07879200 | 5.12274100 | -1.35744100 |
| H | -0.84427600 | 4.31713700 | -2.73299700 |
| H | -1.76989700 | 5.48497400 | -1.76500200 |
| H | -3.18121700 | 2.16709000 | -0.65427000 |
| H | -3.58160300 | 3.72659800 | -1.40004500 |
| H | -2.66672500 | 2.51687900 | -2.32002800 |
| H | -2.49820300 | 4.89233000 | 0.61773000 |
| H | -2.06909400 | 3.30887600 | 1.30478400 |
| H | -0.81266800 | 4.53773900 | 1.05092500 |
| C | 0.90006400 | -2.62388900 | 1.98152700 |

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|---|-------------|-------------|-------------|
| C | 1.78095400 | -3.45473600 | 1.04061600 |
| C | 1.55970300 | -2.51902000 | 3.36880000 |
| C | -0.49284700 | -3.27051500 | 2.11856000 |
| H | 1.32199900 | -3.56381000 | 0.05497700 |
| H | 2.76072900 | -2.98742500 | 0.90063200 |
| H | 1.93353200 | -4.45673700 | 1.46095100 |
| H | 0.95853400 | -1.88997200 | 4.02968300 |
| H | 1.66239100 | -3.51438400 | 3.81733400 |
| H | 2.56064200 | -2.07701200 | 3.29353600 |
| H | -0.40717200 | -4.27249400 | 2.55563200 |
| H | -1.13592500 | -2.66111500 | 2.75958600 |
| H | -0.98075500 | -3.37231500 | 1.14205600 |
| C | 4.62908300 | 1.15390900 | 0.68543800 |
| C | 4.79501800 | -0.08367500 | 1.60086600 |
| C | 5.63355600 | 1.09770500 | -0.47408300 |
| C | 4.80193000 | 2.44240600 | 1.50611900 |
| H | 4.06835500 | -0.06156000 | 2.41889200 |
| H | 4.64979500 | -1.01030700 | 1.03549400 |
| H | 5.80390600 | -0.09136900 | 2.02815900 |
| H | 5.51246400 | 1.95616100 | -1.14321100 |
| H | 6.65473000 | 1.11317200 | -0.07753600 |
| H | 5.50276800 | 0.18740100 | -1.06524800 |
| H | 5.80613800 | 2.46907800 | 1.94348600 |
| H | 4.67987900 | 3.32978900 | 0.87536400 |
| H | 4.06633600 | 2.49521200 | 2.31269700 |

int2(triplet)

| | | | |
|----|-------------|-------------|-------------|
| C | -5.47586300 | 1.50891400 | 1.18728600 |
| C | -4.09680300 | 1.36602800 | 1.34836300 |
| C | -3.39922400 | 0.40185400 | 0.62030300 |
| C | -4.09333100 | -0.43354700 | -0.26734400 |
| C | -5.48165300 | -0.30614800 | -0.40726500 |
| C | -6.16808600 | 0.67073800 | 0.30816200 |
| H | -6.01337000 | 2.26518700 | 1.75243400 |
| H | -3.55996200 | 1.99775000 | 2.05003600 |
| H | -2.33459300 | 0.27842400 | 0.77694000 |
| H | -6.00195500 | -0.98126800 | -1.07843200 |
| H | -7.24223000 | 0.77629800 | 0.18716200 |
| C | -3.41426500 | -1.52162900 | -1.02922700 |
| O | -3.98208800 | -2.55481600 | -1.35779200 |
| C | -1.13395900 | -2.18823400 | -1.66396200 |
| C | -1.31475700 | -3.56361100 | -1.84766800 |
| C | -0.21193000 | -4.36766400 | -2.09279000 |
| H | -2.32068100 | -3.95064400 | -1.77858400 |
| C | 1.21169300 | -2.44239800 | -2.00956600 |
| C | 1.06856600 | -3.80550500 | -2.16465000 |
| H | -0.34891000 | -5.43600300 | -2.22383300 |
| H | 2.14595500 | -1.89835500 | -2.02892400 |
| H | 1.94841100 | -4.41139600 | -2.34549500 |
| N | 0.12692000 | -1.66429100 | -1.78083900 |
| O | 0.25469000 | -0.34333300 | -1.68496000 |
| N | -2.08955800 | -1.25796900 | -1.35666100 |
| H | -1.67619200 | -0.36478400 | -1.10141500 |
| Co | 1.28875900 | 0.49607900 | -0.09167300 |
| O | 2.94984900 | -0.30793500 | -0.58901500 |
| O | 1.25591400 | -0.46477300 | 1.48967100 |
| O | 1.14055000 | 2.17847900 | -1.22266600 |
| C | 3.75154000 | 0.51783500 | 0.02642800 |
| O | 3.25674000 | 1.46160900 | 0.66939200 |
| C | 0.02288700 | 2.40672400 | -0.66815700 |
| O | -0.31716100 | 1.57272400 | 0.25578700 |
| C | 0.13378800 | -1.04687700 | 1.86021600 |
| O | -0.71153200 | -1.46760200 | 1.07670700 |
| C | -0.90101600 | 3.52607700 | -1.09179000 |

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|---|-------------|-------------|-------------|
| C | -0.12074500 | 4.56001200 | -1.91618900 |
| C | -2.00923300 | 2.87683800 | -1.95626300 |
| C | -1.52568800 | 4.17421400 | 0.15670700 |
| H | 0.68225800 | 5.01181700 | -1.32499800 |
| H | 0.33037000 | 4.10233300 | -2.80058000 |
| H | -0.79976000 | 5.35556700 | -2.24200400 |
| H | -2.60088200 | 2.16661000 | -1.37151300 |
| H | -2.68258000 | 3.65673600 | -2.32833700 |
| H | -1.57963800 | 2.35257300 | -2.81656500 |
| H | -2.23007400 | 4.95504700 | -0.15031900 |
| H | -2.06693000 | 3.43531500 | 0.75198200 |
| H | -0.75872800 | 4.63392800 | 0.78945900 |
| C | -0.04066300 | -1.11518200 | 3.38661700 |
| C | 1.23076000 | -1.68944100 | 4.03645500 |
| C | -0.26750400 | 0.33377900 | 3.87006700 |
| C | -1.26060800 | -1.98160300 | 3.72165600 |
| H | 1.42042000 | -2.71283700 | 3.69209500 |
| H | 2.10395900 | -1.07890900 | 3.79335600 |
| H | 1.11279500 | -1.71655300 | 5.12610500 |
| H | -1.15725300 | 0.76852000 | 3.39958200 |
| H | -0.41728700 | 0.34414500 | 4.95601500 |
| H | 0.59144400 | 0.96561300 | 3.62741700 |
| H | -1.40427500 | -2.01618900 | 4.80798800 |
| H | -2.16697600 | -1.57937500 | 3.26072300 |
| H | -1.13013200 | -3.00561900 | 3.35755200 |
| C | 5.24870400 | 0.24946700 | -0.08195000 |
| C | 5.52740100 | -1.12358700 | 0.56498200 |
| C | 5.63328000 | 0.21384000 | -1.57450000 |
| C | 6.02639800 | 1.35271900 | 0.64655700 |
| H | 5.23888200 | -1.12469300 | 1.62195700 |
| H | 4.96901100 | -1.91575300 | 0.05807400 |
| H | 6.59719200 | -1.35295900 | 0.50219900 |
| H | 5.41942600 | 1.17320300 | -2.05887200 |
| H | 6.70563100 | 0.01181600 | -1.67655300 |
| H | 5.08013600 | -0.56653500 | -2.10480400 |
| H | 7.10196400 | 1.15382900 | 0.57618600 |
| H | 5.82453800 | 2.33381000 | 0.20655300 |
| H | 5.74817200 | 1.39855400 | 1.70320400 |

int2(quintet)

| | | | |
|---|-------------|-------------|-------------|
| C | -6.00879200 | 0.45477200 | 0.78280000 |
| C | -5.37241300 | 0.74537800 | -0.42462000 |
| C | -4.24834600 | 0.02051900 | -0.81681300 |
| C | -3.76510600 | -1.01128400 | -0.00312800 |
| C | -4.42467400 | -1.31914500 | 1.19626500 |
| C | -5.53260100 | -0.57909300 | 1.59461000 |
| H | -6.87811500 | 1.02946800 | 1.08996300 |
| H | -5.74631000 | 1.54056600 | -1.06217800 |
| H | -3.75421600 | 0.26016600 | -1.74908800 |
| H | -4.05275500 | -2.13911100 | 1.80055400 |
| H | -6.02872100 | -0.80899800 | 2.53286400 |
| C | -2.61398800 | -1.87003200 | -0.38664900 |
| O | -2.51471100 | -3.02919500 | 0.00128200 |
| C | -0.59733800 | -1.96913200 | -1.74917600 |
| C | -0.52258400 | -3.35725500 | -1.95134600 |
| C | 0.61784000 | -3.91525400 | -2.50372500 |
| H | -1.35880800 | -3.96162300 | -1.63742200 |
| C | 1.59889100 | -1.74567400 | -2.67054500 |
| C | 1.70133100 | -3.10388200 | -2.86539100 |
| H | 0.66634300 | -4.98929800 | -2.64958100 |
| H | 2.36822500 | -1.01397000 | -2.87568600 |
| H | 2.61234000 | -3.51591500 | -3.28203200 |
| N | 0.47146400 | -1.21369200 | -2.14248600 |
| O | 0.41642900 | 0.10983300 | -1.96498600 |

| | | | |
|----|-------------|-------------|-------------|
| N | -1.65555500 | -1.27682400 | -1.21804400 |
| H | -1.57685400 | -0.24251500 | -1.20138100 |
| Co | 1.08328900 | 0.74373400 | -0.21779900 |
| O | 2.96572900 | 0.83111600 | -0.94918700 |
| O | -0.04855100 | -0.16354200 | 1.23250700 |
| O | 0.12532900 | 2.35504200 | -0.13832800 |
| C | 3.47251300 | 1.08968000 | 0.21019200 |
| O | 2.67049900 | 1.28451000 | 1.16093500 |
| C | -1.14580400 | 2.46395100 | -0.44532100 |
| O | -1.83411100 | 1.54645600 | -0.89522600 |
| C | 0.69611900 | -1.20499300 | 1.27354700 |
| O | 1.62089000 | -1.30019100 | 0.41238000 |
| C | -1.73248300 | 3.85503200 | -0.16957200 |
| C | -1.64587000 | 4.10118600 | 1.35130300 |
| C | -0.89343200 | 4.90861300 | -0.91791300 |
| C | -3.19393200 | 3.90505500 | -0.63078000 |
| H | -2.22643500 | 3.35233700 | 1.90220000 |
| H | -0.60936300 | 4.05236700 | 1.69541900 |
| H | -2.05156600 | 5.09113400 | 1.59110700 |
| H | -0.92599000 | 4.74100400 | -2.00096000 |
| H | -1.28999000 | 5.91114200 | -0.71891900 |
| H | 0.15111600 | 4.87552300 | -0.59722800 |
| H | -3.61502200 | 4.89593800 | -0.42413800 |
| H | -3.27558400 | 3.71233200 | -1.70544500 |
| H | -3.79477000 | 3.15332200 | -0.11167900 |
| C | 0.51886000 | -2.25904000 | 2.35542800 |
| C | 1.72698300 | -2.10277700 | 3.30725300 |
| C | -0.79418600 | -2.04215400 | 3.11916900 |
| C | 0.54043900 | -3.65482700 | 1.70434800 |
| H | 2.66653700 | -2.25932500 | 2.76878100 |
| H | 1.74938100 | -1.10247700 | 3.75333200 |
| H | 1.65696000 | -2.84063300 | 4.11439000 |
| H | -1.65421200 | -2.15044800 | 2.45286900 |
| H | -0.88332400 | -2.78838700 | 3.91711200 |
| H | -0.83259800 | -1.04544400 | 3.56690000 |
| H | 0.51413400 | -4.42442800 | 2.48441000 |
| H | -0.33059900 | -3.79332900 | 1.05694900 |
| H | 1.44750400 | -3.79171200 | 1.10894900 |
| C | 4.97958000 | 1.06471600 | 0.39471100 |
| C | 5.39205100 | -0.42508700 | 0.34806300 |
| C | 5.65067900 | 1.83074600 | -0.75928300 |
| C | 5.35584400 | 1.67730000 | 1.75020200 |
| H | 4.89098100 | -0.99358000 | 1.13873500 |
| H | 5.12452600 | -0.87161100 | -0.61415500 |
| H | 6.47534900 | -0.51287400 | 0.48856900 |
| H | 5.36993400 | 2.88986700 | -0.74511400 |
| H | 6.74041100 | 1.76643000 | -0.66274800 |
| H | 5.35986700 | 1.41457800 | -1.72749100 |
| H | 6.44170400 | 1.62793500 | 1.89007900 |
| H | 5.04835500 | 2.72641300 | 1.80841700 |
| H | 4.87189100 | 1.14180200 | 2.57117900 |

TS3(singlet)

| | | | |
|---|-------------|-------------|------------|
| C | -2.90731000 | 1.95012000 | 3.43166700 |
| C | -3.20108400 | 0.72311900 | 2.83535600 |
| C | -2.17212800 | -0.12469300 | 2.43032500 |
| C | -0.83932600 | 0.24899600 | 2.63782500 |
| C | -0.54734700 | 1.46751800 | 3.26675100 |
| C | -1.57733100 | 2.31985000 | 3.64962900 |
| H | -3.71231200 | 2.61474400 | 3.73256300 |
| H | -4.23376400 | 0.42300500 | 2.68259000 |
| H | -2.41248600 | -1.07665400 | 1.97516700 |
| H | 0.49102100 | 1.73645800 | 3.42480500 |
| H | -1.34561900 | 3.27180700 | 4.11831800 |

| | | | |
|----|-------------|-------------|-------------|
| C | 0.32536900 | -0.57981400 | 2.23071300 |
| O | 1.36929800 | -0.57787600 | 2.85848900 |
| C | 1.24721800 | -2.16838500 | 0.64855400 |
| C | 2.09384700 | -2.89920300 | 1.47553600 |
| C | 3.09919500 | -3.68229900 | 0.91455900 |
| H | 1.97073600 | -2.81531400 | 2.54449900 |
| C | 2.39592000 | -2.99321300 | -1.27015600 |
| C | 3.25578500 | -3.72413500 | -0.47218200 |
| H | 3.76580400 | -4.24340300 | 1.56040700 |
| H | 2.43605900 | -2.91665000 | -2.34690600 |
| H | 4.04569500 | -4.30011400 | -0.93924000 |
| N | 1.40818900 | -2.26979200 | -0.70233300 |
| O | 0.57110100 | -1.61320600 | -1.50041100 |
| N | 0.17498200 | -1.32648000 | 1.01539900 |
| H | -0.87132600 | -1.88377000 | 0.75529400 |
| Co | -0.03629900 | -0.06882700 | -0.59657500 |
| O | 1.64569800 | 0.57392800 | -0.11997400 |
| O | -0.74611500 | 1.61656100 | 0.04022900 |
| O | -1.85497400 | -0.60816900 | -1.01592100 |
| C | 2.74747600 | 0.51076100 | -0.83495800 |
| O | 2.88105700 | -0.02657500 | -1.92644700 |
| C | -2.41792800 | -1.66422100 | -0.61394500 |
| O | -1.93641200 | -2.44033700 | 0.28115600 |
| C | -0.63329000 | 2.06718500 | -1.14839900 |
| O | -0.19445700 | 1.22688400 | -2.00511100 |
| C | -3.79279700 | -2.01560100 | -1.18665600 |
| C | -4.81221700 | -1.85640000 | -0.03784600 |
| C | -4.15418200 | -1.08247400 | -2.34892600 |
| C | -3.76467700 | -3.48109800 | -1.66042100 |
| H | -4.57026800 | -2.52336800 | 0.79487900 |
| H | -4.82526700 | -0.82473900 | 0.33317500 |
| H | -5.81804600 | -2.10004200 | -0.39781600 |
| H | -3.41516500 | -1.14918700 | -3.15284100 |
| H | -5.13454500 | -1.35986000 | -2.75278900 |
| H | -4.19499000 | -0.03972800 | -2.02195600 |
| H | -4.75376200 | -3.76749500 | -2.03539000 |
| H | -3.04165000 | -3.61640200 | -2.47282500 |
| H | -3.49157100 | -4.15152400 | -0.84165900 |
| C | -0.92487100 | 3.50767200 | -1.49565800 |
| C | 0.42473300 | 4.25478300 | -1.37443100 |
| C | -1.45280900 | 3.59447400 | -2.93619700 |
| C | -1.94071800 | 4.07855300 | -0.49393500 |
| H | 0.82520200 | 4.17387700 | -0.35899700 |
| H | 1.16240700 | 3.84148200 | -2.06946000 |
| H | 0.27902400 | 5.31512000 | -1.60903300 |
| H | -2.40411600 | 3.06113500 | -3.03888300 |
| H | -1.61608200 | 4.64363200 | -3.20638300 |
| H | -0.74177900 | 3.15701200 | -3.64181600 |
| H | -2.11062800 | 5.13985400 | -0.70643400 |
| H | -2.90015700 | 3.55513400 | -0.56628800 |
| H | -1.58131900 | 3.97703600 | 0.53350300 |
| C | 3.94304700 | 1.14151700 | -0.07826600 |
| C | 3.52625400 | 2.46098500 | 0.59178900 |
| C | 4.37303800 | 0.12368100 | 0.99977300 |
| C | 5.09373600 | 1.38128700 | -1.06308300 |
| H | 3.20325300 | 3.19461200 | -0.15623900 |
| H | 2.69998500 | 2.30003500 | 1.28801400 |
| H | 4.37359600 | 2.89035300 | 1.14057700 |
| H | 4.65303200 | -0.83204900 | 0.53976200 |
| H | 5.24513000 | 0.50190700 | 1.54731600 |
| H | 3.56487000 | -0.05948500 | 1.71310000 |
| H | 5.96548600 | 1.78220700 | -0.53179800 |
| H | 5.37995200 | 0.45207900 | -1.56191100 |
| H | 4.80428600 | 2.09706000 | -1.83980500 |

TS3(triplet)

| | | | |
|----|-------------|-------------|-------------|
| C | 1.54081600 | -1.81958500 | 4.05935600 |
| C | 2.03526600 | -0.67144300 | 3.44114400 |
| C | 1.17860900 | 0.16728600 | 2.73286600 |
| C | -0.18631800 | -0.13383000 | 2.64671900 |
| C | -0.68446600 | -1.27012100 | 3.30090600 |
| C | 0.17679200 | -2.11454600 | 3.99227400 |
| H | 2.21434400 | -2.48063800 | 4.59740600 |
| H | 3.09196900 | -0.42849700 | 3.50308300 |
| H | 1.57480800 | 1.06622000 | 2.28232100 |
| H | -1.74475500 | -1.48165900 | 3.24231600 |
| H | -0.21379700 | -3.00360300 | 4.47852800 |
| C | -1.17223900 | 0.69765600 | 1.90488600 |
| O | -2.34967300 | 0.74413200 | 2.21596900 |
| C | -1.52997700 | 2.29674900 | 0.11221200 |
| C | -2.43237200 | 3.15995100 | 0.72793500 |
| C | -3.15235300 | 4.07205400 | -0.03300100 |
| H | -2.56892600 | 3.08114500 | 1.79631200 |
| C | -2.04721900 | 3.25680700 | -1.99472000 |
| C | -2.95454600 | 4.12011600 | -1.41469600 |
| H | -3.86026800 | 4.73850100 | 0.44763100 |
| H | -1.83041400 | 3.19271400 | -3.05173900 |
| H | -3.50005900 | 4.81212600 | -2.04544000 |
| N | -1.35225700 | 2.37766200 | -1.23775500 |
| O | -0.53041800 | 1.53976700 | -1.84743600 |
| N | -0.66511000 | 1.38898700 | 0.75525800 |
| H | 0.44366200 | 1.99559200 | 0.80779800 |
| Co | 0.05212900 | 0.02459800 | -0.64200400 |
| O | -1.41297400 | -1.07368500 | -0.38690800 |
| O | 1.21282600 | -1.80079200 | 0.16938600 |
| O | 1.86916700 | 0.76887100 | -0.58312200 |
| C | -2.67738300 | -0.77659700 | -0.62139200 |
| O | -3.09909600 | 0.30303400 | -1.00651800 |
| C | 2.25505300 | 1.85785700 | -0.07592700 |
| O | 1.51179300 | 2.59928600 | 0.65593400 |
| C | 1.30289100 | -2.03940700 | -1.05049900 |
| O | 0.74374400 | -1.22945300 | -1.89885300 |
| C | 3.71857900 | 2.24090000 | -0.28067500 |
| C | 4.52563100 | 1.32871300 | 0.67355900 |
| C | 4.11858000 | 1.95144600 | -1.73802400 |
| C | 3.95366300 | 3.71611500 | 0.06746800 |
| H | 4.26755900 | 1.52685700 | 1.72039100 |
| H | 4.32860300 | 0.27351500 | 0.46147900 |
| H | 5.59688700 | 1.52009100 | 0.54674100 |
| H | 3.54437200 | 2.57337600 | -2.43385400 |
| H | 5.18194000 | 2.17360400 | -1.87985500 |
| H | 3.93810600 | 0.90461700 | -1.99316600 |
| H | 5.01376200 | 3.95980700 | -0.06454000 |
| H | 3.36849200 | 4.37407500 | -0.58344300 |
| H | 3.67276200 | 3.93018300 | 1.10184500 |
| C | 2.07250600 | -3.22663900 | -1.62358500 |
| C | 1.14842400 | -3.99640300 | -2.58646100 |
| C | 3.28398800 | -2.66008400 | -2.39384000 |
| C | 2.54127400 | -4.13578700 | -0.48079200 |
| H | 0.26671300 | -4.37969700 | -2.06012300 |
| H | 0.80439700 | -3.35076200 | -3.39869600 |
| H | 1.68569500 | -4.84936200 | -3.01700600 |
| H | 3.93747700 | -2.08672500 | -1.72578700 |
| H | 3.87046300 | -3.48038900 | -2.82352700 |
| H | 2.95726200 | -1.99990900 | -3.20221800 |
| H | 3.10718300 | -4.98143400 | -0.88863600 |
| H | 3.18028400 | -3.59008400 | 0.21905800 |
| H | 1.68988700 | -4.52689300 | 0.08452700 |

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|---|-------------|-------------|-------------|
| C | -3.59329100 | -1.99681400 | -0.37524000 |
| C | -3.39013300 | -2.49074300 | 1.06831200 |
| C | -5.05223700 | -1.58004700 | -0.59454500 |
| C | -3.19307200 | -3.10369800 | -1.37045500 |
| H | -2.35307800 | -2.79502100 | 1.23204800 |
| H | -3.63602200 | -1.69928200 | 1.78494100 |
| H | -4.04452700 | -3.34833000 | 1.26543900 |
| H | -5.20884100 | -1.21322100 | -1.61285000 |
| H | -5.71195800 | -2.43970600 | -0.42629700 |
| H | -5.33871100 | -0.78051000 | 0.09504600 |
| H | -3.83208800 | -3.98352700 | -1.22842800 |
| H | -3.31014400 | -2.76303800 | -2.40571700 |
| H | -2.15067500 | -3.39955200 | -1.22434900 |

TS3(quintet)

| | | | |
|----|-------------|-------------|-------------|
| C | -2.31369700 | 1.35192500 | 3.75061200 |
| C | -2.69686600 | 0.18321800 | 3.09154800 |
| C | -1.73179700 | -0.67424200 | 2.56725800 |
| C | -0.37329300 | -0.37190300 | 2.71489200 |
| C | 0.00803800 | 0.78622900 | 3.40520700 |
| C | -0.95842900 | 1.65055500 | 3.90916800 |
| H | -3.06899000 | 2.02636300 | 4.14444600 |
| H | -3.74945600 | -0.06057400 | 2.97942300 |
| H | -2.03880000 | -1.58303900 | 2.06502600 |
| H | 1.06545500 | 0.99914300 | 3.51738200 |
| H | -0.65670200 | 2.55843700 | 4.42330100 |
| C | 0.72762900 | -1.20673000 | 2.14957500 |
| O | 1.80563500 | -1.31534600 | 2.71371900 |
| C | 1.48463000 | -2.47929000 | 0.26093600 |
| C | 2.36439800 | -3.37518900 | 0.87467200 |
| C | 3.30503300 | -4.06327100 | 0.12175100 |
| H | 2.29582500 | -3.49483400 | 1.94549900 |
| C | 2.49795500 | -2.96558800 | -1.84369100 |
| C | 3.37135600 | -3.85705300 | -1.25966800 |
| H | 3.98407300 | -4.75563800 | 0.60800600 |
| H | 2.47635500 | -2.70356900 | -2.89176400 |
| H | 4.09971500 | -4.36596300 | -1.87961100 |
| N | 1.58216700 | -2.30965700 | -1.09475300 |
| O | 0.79013700 | -1.44312500 | -1.72496500 |
| N | 0.46795100 | -1.74843300 | 0.86893900 |
| H | -0.66879100 | -2.24261100 | 0.52534600 |
| Co | 0.13198400 | 0.00805400 | -0.55085200 |
| O | 1.74282600 | 0.63032100 | 0.07416100 |
| O | -0.89883500 | 1.69630500 | 0.27611200 |
| O | -1.76435400 | -0.64581000 | -0.79072400 |
| C | 2.93620200 | 0.81257200 | -0.49597700 |
| O | 3.51748000 | -0.06986800 | -1.10132100 |
| C | -2.27906500 | -1.77590100 | -0.58675300 |
| O | -1.69689600 | -2.70104100 | 0.08394700 |
| C | -0.92186800 | 2.17607300 | -0.89480100 |
| O | -0.33407500 | 1.52777500 | -1.83450000 |
| C | -3.70338600 | -2.01551300 | -1.08033000 |
| C | -3.89420000 | -1.33012400 | -2.44370100 |
| C | -4.00486300 | -3.51690000 | -1.17797900 |
| C | -4.62497900 | -1.35320200 | -0.02855500 |
| H | -3.67637100 | -0.26159600 | -2.37953100 |
| H | -3.22989700 | -1.76527700 | -3.19850000 |
| H | -4.92797800 | -1.46128200 | -2.78192500 |
| H | -3.86742400 | -4.01386600 | -0.21439900 |
| H | -5.04119800 | -3.66389300 | -1.50225300 |
| H | -3.34772400 | -4.00470900 | -1.90575900 |
| H | -5.67023000 | -1.44932200 | -0.34239800 |
| H | -4.51734900 | -1.83675400 | 0.94899300 |
| H | -4.38871400 | -0.29024500 | 0.08198800 |

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|---|-------------|------------|-------------|
| C | -1.70186900 | 3.44667900 | -1.20346400 |
| C | -1.77225900 | 4.33094600 | 0.05073100 |
| C | -1.05438000 | 4.20300700 | -2.37274900 |
| C | -3.12155600 | 2.97473500 | -1.59814700 |
| H | -2.19554900 | 3.78011500 | 0.89433600 |
| H | -0.77435300 | 4.67668400 | 0.34241700 |
| H | -2.39375500 | 5.21149900 | -0.14876700 |
| H | -0.97674600 | 3.56578100 | -3.25717500 |
| H | -1.65528600 | 5.08447700 | -2.62467400 |
| H | -0.04642300 | 4.54261700 | -2.11071800 |
| H | -3.75284000 | 3.84277800 | -1.81990400 |
| H | -3.08517700 | 2.33445900 | -2.48555400 |
| H | -3.58217300 | 2.40809900 | -0.78188000 |
| C | 3.50498700 | 2.21260200 | -0.23563100 |
| C | 2.42855100 | 3.26971600 | -0.54794600 |
| C | 3.87637700 | 2.27912400 | 1.26171100 |
| C | 4.74738300 | 2.42668900 | -1.10753900 |
| H | 2.08791300 | 3.19323300 | -1.58591800 |
| H | 1.56031200 | 3.14431200 | 0.10445000 |
| H | 2.84110500 | 4.27348000 | -0.39280000 |
| H | 4.63735300 | 1.53187800 | 1.51251500 |
| H | 4.27793100 | 3.27082000 | 1.50065400 |
| H | 2.99772400 | 2.09831200 | 1.88798000 |
| H | 5.18130800 | 3.41219700 | -0.90241700 |
| H | 5.50329100 | 1.66220700 | -0.90884800 |
| H | 4.49366100 | 2.37679300 | -2.17146800 |

int4(singlet)

| | | | |
|----|-------------|-------------|-------------|
| C | 0.36572800 | 3.79815700 | -2.85958700 |
| C | 0.87124200 | 2.49723000 | -2.87181800 |
| C | 0.14235500 | 1.45424600 | -2.30261400 |
| C | -1.10098800 | 1.71053100 | -1.71368900 |
| C | -1.61984500 | 3.01313700 | -1.73135400 |
| C | -0.88562100 | 4.05424900 | -2.29092900 |
| H | 0.93958300 | 4.60980600 | -3.29867200 |
| H | 1.83643400 | 2.29097200 | -3.32596900 |
| H | 0.54053600 | 0.44906500 | -2.30972500 |
| H | -2.59956100 | 3.18630500 | -1.29994900 |
| H | -1.28759700 | 5.06353800 | -2.28917300 |
| C | -1.95115100 | 0.63706400 | -1.12347800 |
| O | -3.16687300 | 0.79674200 | -1.01341600 |
| N | -1.30292100 | -0.54251400 | -0.74363100 |
| C | -2.00803600 | -1.70093500 | -0.62115600 |
| C | -3.33135900 | -2.00235300 | -1.01677000 |
| C | -3.82858800 | -3.28511900 | -0.87903000 |
| H | -3.93184000 | -1.19498200 | -1.40527600 |
| C | -1.75081700 | -3.99258300 | 0.05883500 |
| C | -3.03321800 | -4.30426800 | -0.33213700 |
| H | -4.84717400 | -3.49597400 | -1.18872400 |
| H | -1.04170100 | -4.68048900 | 0.49915500 |
| H | -3.40115400 | -5.31443200 | -0.20034200 |
| N | -1.27626400 | -2.73542000 | -0.09380300 |
| O | -0.00093600 | -2.50570000 | 0.27956200 |
| Co | 0.30576100 | -0.66562000 | 0.33917500 |
| C | 2.56983500 | -0.93010400 | 0.00567600 |
| O | 1.75020100 | -0.81835600 | -0.96778000 |
| O | 2.04257800 | -0.93463400 | 1.16932500 |
| C | 4.06902400 | -0.97761900 | -0.19341800 |
| C | 4.58858900 | 0.44575400 | 0.11901400 |
| C | 4.67771400 | -1.98910800 | 0.79339800 |
| C | 4.39713300 | -1.35682700 | -1.64415000 |
| H | 4.14275900 | 1.18200800 | -0.55850500 |
| H | 4.34595600 | 0.73244200 | 1.14661800 |
| H | 5.67678900 | 0.47466900 | -0.00548600 |

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|---|-------------|-------------|-------------|
| H | 4.32172100 | -3.00420900 | 0.58594900 |
| H | 5.76932200 | -1.98375300 | 0.70014200 |
| H | 4.41240700 | -1.73945200 | 1.82389600 |
| H | 5.48342500 | -1.36028500 | -1.78661500 |
| H | 4.01425100 | -2.35307400 | -1.88806900 |
| H | 3.95552200 | -0.64569800 | -2.34749100 |
| C | -0.35832400 | 0.99299300 | 1.78403000 |
| O | -0.73014900 | -0.22473500 | 1.90926300 |
| O | 0.40396600 | 1.22795700 | 0.78536600 |
| C | -0.82638000 | 2.09445500 | 2.70755100 |
| C | 0.39651200 | 2.92695100 | 3.13741100 |
| C | -1.79848000 | 2.97320400 | 1.88700000 |
| C | -1.54051100 | 1.49554500 | 3.92653900 |
| H | 1.10555100 | 2.31920400 | 3.71041300 |
| H | 0.91745400 | 3.33246000 | 2.26608300 |
| H | 0.06994600 | 3.75949700 | 3.77008400 |
| H | -2.64719600 | 2.38676500 | 1.51850800 |
| H | -2.18349700 | 3.77923200 | 2.52150000 |
| H | -1.29059300 | 3.41485500 | 1.02568200 |
| H | -1.88078400 | 2.30308200 | 4.58402800 |
| H | -2.40925300 | 0.90413800 | 3.62426000 |
| H | -0.87171600 | 0.84379300 | 4.49747800 |

int4(triplet)

| | | | |
|----|-------------|-------------|-------------|
| C | -0.76655000 | -3.49745700 | -3.08597000 |
| C | -0.78457800 | -2.10204300 | -3.11478800 |
| C | 0.08442300 | -1.37303400 | -2.30623500 |
| C | 0.97692100 | -2.04152600 | -1.45905900 |
| C | 1.00813900 | -3.44416900 | -1.45008100 |
| C | 0.13455600 | -4.16898700 | -2.25372500 |
| H | -1.45038800 | -4.06293400 | -3.71314000 |
| H | -1.47962800 | -1.57575100 | -3.76200500 |
| H | 0.05247400 | -0.29221700 | -2.32796000 |
| H | 1.71852900 | -3.94300500 | -0.80024300 |
| H | 0.15350700 | -5.25481200 | -2.23353100 |
| C | 1.95275200 | -1.32934800 | -0.59554500 |
| O | 2.93075900 | -1.89817500 | -0.12398000 |
| N | 1.71493000 | 0.04673500 | -0.37119300 |
| C | 2.75606000 | 0.88851900 | -0.15277700 |
| C | 4.14968400 | 0.66283600 | -0.25459400 |
| C | 5.03270900 | 1.70998300 | -0.08608900 |
| H | 4.48404700 | -0.34534300 | -0.44517400 |
| C | 3.21199800 | 3.20867900 | 0.30816800 |
| C | 4.56654400 | 3.00748200 | 0.19879500 |
| H | 6.09879500 | 1.52357200 | -0.16577200 |
| H | 2.72604400 | 4.14845500 | 0.53331300 |
| H | 5.24383800 | 3.83990100 | 0.34459300 |
| N | 2.36027600 | 2.16925900 | 0.13696200 |
| O | 1.03800800 | 2.41443800 | 0.24491400 |
| Co | 0.05589600 | 0.83832400 | 0.20954900 |
| C | -2.08450300 | 1.74888800 | -0.47856600 |
| O | -1.40308700 | 1.27749900 | -1.42607200 |
| O | -1.54927400 | 1.78769200 | 0.69450900 |
| C | -3.52937800 | 2.19901200 | -0.63640400 |
| C | -4.39695500 | 1.07269200 | -0.02799800 |
| C | -3.74906900 | 3.50833000 | 0.14175100 |
| C | -3.86420200 | 2.38349700 | -2.12217800 |
| H | -4.23310200 | 0.12644600 | -0.55491800 |
| H | -4.15397500 | 0.92291100 | 1.02805000 |
| H | -5.45741900 | 1.33644300 | -0.11148800 |
| H | -3.13236000 | 4.31706600 | -0.26644900 |
| H | -4.79969400 | 3.81158200 | 0.06826100 |
| H | -3.49204600 | 3.38447000 | 1.19678000 |
| H | -4.91496800 | 2.67528400 | -2.23109500 |

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|---|-------------|-------------|-------------|
| H | -3.24206200 | 3.16338200 | -2.57350500 |
| H | -3.69803100 | 1.45832700 | -2.68033700 |
| C | -0.51716100 | -0.95323900 | 1.78400100 |
| O | 0.21575700 | -0.07539600 | 2.29566800 |
| O | -0.85583000 | -0.83213900 | 0.53874600 |
| C | -1.02132500 | -2.17710600 | 2.53859300 |
| C | -2.55767700 | -2.22035100 | 2.41695700 |
| C | -0.40753200 | -3.42405400 | 1.86756600 |
| C | -0.59660400 | -2.09573200 | 4.01008300 |
| H | -3.01281400 | -1.33026800 | 2.86633000 |
| H | -2.86408100 | -2.26913300 | 1.36868000 |
| H | -2.94599700 | -3.10224600 | 2.93918000 |
| H | 0.68746400 | -3.39023800 | 1.90453800 |
| H | -0.73913100 | -4.32687700 | 2.39329000 |
| H | -0.71032800 | -3.49523700 | 0.81999400 |
| H | -0.96117300 | -2.97805900 | 4.54854800 |
| H | 0.49230800 | -2.05534600 | 4.10387700 |
| H | -1.00562200 | -1.20167900 | 4.49026300 |

int4(quintet)

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|----|-------------|-------------|-------------|
| C | -1.39239800 | -2.89945900 | -3.35588300 |
| C | -1.34711500 | -1.51518900 | -3.18401300 |
| C | -0.33164500 | -0.93507700 | -2.42678500 |
| C | 0.64645700 | -1.74547600 | -1.83648000 |
| C | 0.61014600 | -3.13510100 | -2.02852600 |
| C | -0.40976800 | -3.71004700 | -2.77844700 |
| H | -2.19090300 | -3.34849700 | -3.94015300 |
| H | -2.10698000 | -0.88314400 | -3.63409700 |
| H | -0.31858300 | 0.13690700 | -2.28226700 |
| H | 1.38502500 | -3.74189900 | -1.57337600 |
| H | -0.44251700 | -4.78718000 | -2.91404400 |
| C | 1.76271600 | -1.19446600 | -1.03033800 |
| O | 2.74854500 | -1.86026400 | -0.73440200 |
| N | 1.61264200 | 0.14262700 | -0.58462500 |
| C | 2.70138900 | 0.90694500 | -0.40360300 |
| C | 4.02031600 | 0.70763600 | -0.88546500 |
| C | 5.00041800 | 1.64615900 | -0.65351400 |
| H | 4.22428200 | -0.20845600 | -1.42001300 |
| C | 3.43273700 | 3.00116800 | 0.55105100 |
| C | 4.70737100 | 2.81590700 | 0.07702600 |
| H | 6.00324400 | 1.48062100 | -1.03324400 |
| H | 3.09049800 | 3.85139300 | 1.12511200 |
| H | 5.46232200 | 3.56695900 | 0.27568100 |
| N | 2.46853900 | 2.07108600 | 0.31581700 |
| O | 1.25878500 | 2.29366000 | 0.79981100 |
| Co | 0.01926400 | 0.79958100 | 0.49025900 |
| C | -2.13783000 | 1.86033900 | 0.07142500 |
| O | -1.26376100 | 1.58614400 | -0.84190700 |
| O | -1.80520500 | 1.71036000 | 1.27455500 |
| C | -3.53902100 | 2.27083500 | -0.35512900 |
| C | -4.20456200 | 0.99524200 | -0.92188500 |
| C | -4.33126300 | 2.79385100 | 0.84970400 |
| C | -3.44517200 | 3.34296400 | -1.45555200 |
| H | -3.63274800 | 0.60300400 | -1.76804600 |
| H | -4.26009200 | 0.21230500 | -0.15811200 |
| H | -5.22181700 | 1.22585000 | -1.25853900 |
| H | -3.85842900 | 3.68420600 | 1.27699200 |
| H | -5.34834900 | 3.05924400 | 0.53879200 |
| H | -4.39116000 | 2.03875900 | 1.63786800 |
| H | -4.44971100 | 3.60696500 | -1.80538000 |
| H | -2.96713500 | 4.25430500 | -1.07826900 |
| H | -2.86195300 | 2.97890400 | -2.30543800 |
| C | -0.39595400 | -1.25483300 | 1.75665800 |
| O | 0.40815000 | -0.32425300 | 2.13735100 |

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|---|-------------|-------------|------------|
| O | -1.03617700 | -1.08806200 | 0.68182200 |
| C | -0.50670100 | -2.55451300 | 2.54148700 |
| C | -1.99725900 | -2.89901900 | 2.71464700 |
| C | 0.18281700 | -3.63760000 | 1.67983500 |
| C | 0.18696000 | -2.43435100 | 3.90436500 |
| H | -2.50716700 | -2.14328600 | 3.32271800 |
| H | -2.49674900 | -2.95099200 | 1.74389400 |
| H | -2.09853700 | -3.86737000 | 3.21798400 |
| H | 1.23596100 | -3.39040000 | 1.50397200 |
| H | 0.13744500 | -4.60395400 | 2.19506800 |
| H | -0.31211100 | -3.73150000 | 0.70911000 |
| H | 0.09963200 | -3.38202100 | 4.44826800 |
| H | 1.24790000 | -2.19642500 | 3.78782700 |
| H | -0.26829000 | -1.64513300 | 4.51104800 |

TS5(singlet)

| | | | |
|----|-------------|-------------|-------------|
| C | 2.91362800 | -2.63558000 | -1.63086600 |
| C | 2.11474900 | -2.18056400 | -0.58254500 |
| C | 0.96433400 | -1.41750600 | -0.84181400 |
| C | 0.65661500 | -1.10129200 | -2.18716600 |
| C | 1.44096700 | -1.56570600 | -3.23899600 |
| C | 2.57322500 | -2.33182800 | -2.95494300 |
| H | 3.79732900 | -3.23356600 | -1.42474100 |
| H | 2.36320100 | -2.43336600 | 0.44429400 |
| H | -0.05157200 | -1.91872200 | -0.19737200 |
| H | 1.17332100 | -1.30232700 | -4.25760500 |
| H | 3.19782500 | -2.69256400 | -3.76757700 |
| C | -0.48200100 | -0.16501500 | -2.43138700 |
| O | -1.03681000 | 0.00293000 | -3.51418500 |
| N | -0.76395600 | 0.51567300 | -1.26516300 |
| C | -1.64318400 | 1.53475600 | -1.12230800 |
| C | -2.67303100 | 1.94973700 | -1.98520500 |
| C | -3.50507300 | 2.99231000 | -1.61044000 |
| H | -2.77011100 | 1.42334800 | -2.92432600 |
| C | -2.28964700 | 3.22048200 | 0.44407500 |
| C | -3.32082300 | 3.63232600 | -0.37616200 |
| H | -4.30491500 | 3.30581700 | -2.27343500 |
| H | -2.04487800 | 3.64916900 | 1.40652900 |
| H | -3.96315500 | 4.44207700 | -0.05141200 |
| N | -1.46806600 | 2.21787700 | 0.05988300 |
| O | -0.43218500 | 1.89910700 | 0.85155700 |
| Co | 0.27302500 | 0.19663900 | 0.26984300 |
| C | -1.68182100 | -1.69954000 | 1.00083200 |
| O | -1.10183100 | -2.55957400 | 0.27624300 |
| O | -1.23933600 | -0.52327100 | 1.18422600 |
| C | -3.00667200 | -2.04315400 | 1.68774200 |
| C | -2.85080000 | -1.78265100 | 3.19837800 |
| C | -4.07260500 | -1.09325700 | 1.09984400 |
| C | -3.39108600 | -3.50458800 | 1.42826600 |
| H | -2.09045900 | -2.44059900 | 3.63425900 |
| H | -2.55586400 | -0.74720600 | 3.38649200 |
| H | -3.80106400 | -1.97868700 | 3.70780100 |
| H | -4.17770700 | -1.23999200 | 0.01862600 |
| H | -5.04409600 | -1.29354800 | 1.56542200 |
| H | -3.80448600 | -0.04877100 | 1.28145200 |
| H | -4.34452600 | -3.72656300 | 1.92099200 |
| H | -3.49870400 | -3.70275900 | 0.35808400 |
| H | -2.63247800 | -4.18890600 | 1.81971500 |
| C | 2.41781000 | 0.74153800 | 0.92464700 |
| O | 1.95463300 | 1.06675200 | -0.21893900 |
| O | 1.63178700 | 0.06627800 | 1.67398000 |
| C | 3.82505300 | 1.09160200 | 1.36451800 |
| C | 3.74955300 | 1.74521400 | 2.75783600 |
| C | 4.61552700 | -0.23287500 | 1.44828600 |

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|---|------------|-------------|-------------|
| C | 4.47866700 | 2.04027900 | 0.35114600 |
| H | 3.18781900 | 2.68515700 | 2.72004200 |
| H | 3.25686000 | 1.08189500 | 3.47357700 |
| H | 4.76056600 | 1.96520500 | 3.11862500 |
| H | 4.65673600 | -0.72682300 | 0.47120200 |
| H | 5.64153600 | -0.02931000 | 1.77439300 |
| H | 4.15159600 | -0.91849100 | 2.16360900 |
| H | 5.49718100 | 2.28081200 | 0.67603700 |
| H | 4.52819000 | 1.58518600 | -0.64212500 |
| H | 3.91397300 | 2.97349700 | 0.26315400 |

TS5(triplet)

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|----|-------------|-------------|-------------|
| C | 2.86614200 | -3.03832500 | -0.76821800 |
| C | 2.11765900 | -2.24339500 | 0.09503500 |
| C | 0.91253700 | -1.66647000 | -0.34237900 |
| C | 0.50293500 | -1.88049500 | -1.68165700 |
| C | 1.23842400 | -2.68762600 | -2.54323700 |
| C | 2.42368400 | -3.26204200 | -2.07992000 |
| H | 3.79260300 | -3.49282400 | -0.42856900 |
| H | 2.44422300 | -2.07893500 | 1.11744300 |
| H | -0.04341900 | -1.79822000 | 0.47256500 |
| H | 0.89567400 | -2.83543300 | -3.56255300 |
| H | 3.01506600 | -3.88400100 | -2.74605800 |
| C | -0.69846300 | -1.12984800 | -2.14623000 |
| O | -1.37618100 | -1.39950300 | -3.12873500 |
| N | -0.88655100 | -0.03247000 | -1.31377900 |
| C | -1.79715100 | 0.95635900 | -1.49692100 |
| C | -2.96406800 | 0.96449700 | -2.27960700 |
| C | -3.78852100 | 2.07739800 | -2.26123600 |
| H | -3.17462300 | 0.08332000 | -2.86893500 |
| C | -2.29163100 | 3.16990900 | -0.73660500 |
| C | -3.45627700 | 3.19179800 | -1.47517600 |
| H | -4.69936600 | 2.07985900 | -2.85081500 |
| H | -1.92873900 | 3.97136600 | -0.10746700 |
| H | -4.09083600 | 4.06886700 | -1.43473600 |
| N | -1.48796500 | 2.08268300 | -0.77261600 |
| O | -0.32517800 | 2.11563900 | -0.10356500 |
| Co | 0.34167300 | 0.31867100 | 0.08019500 |
| C | -1.67688800 | -1.09229600 | 1.64627300 |
| O | -1.19106800 | -2.16649200 | 1.17625300 |
| O | -1.11344000 | 0.03753600 | 1.54318000 |
| C | -3.04577000 | -1.13336100 | 2.34173200 |
| C | -3.56528500 | -2.57079300 | 2.45758900 |
| C | -2.90407400 | -0.49383900 | 3.73536000 |
| C | -4.00319200 | -0.28594100 | 1.47579800 |
| H | -3.67255800 | -3.03370900 | 1.47252300 |
| H | -2.88035100 | -3.19168600 | 3.04288400 |
| H | -4.54347600 | -2.57350100 | 2.95292800 |
| H | -2.50147200 | 0.51931500 | 3.65741100 |
| H | -3.88200800 | -0.45035200 | 4.22892400 |
| H | -2.23085800 | -1.08177800 | 4.36975400 |
| H | -5.00247500 | -0.27090200 | 1.92605700 |
| H | -3.64110200 | 0.74289000 | 1.39332500 |
| H | -4.09332600 | -0.70237000 | 0.46534900 |
| C | 2.67978100 | 1.00019100 | 0.41173900 |
| O | 2.39895200 | 0.86923700 | -0.80105300 |
| O | 1.76508000 | 0.75487800 | 1.29770000 |
| C | 4.06200800 | 1.40789300 | 0.91303800 |
| C | 4.63678900 | 0.21639800 | 1.70825800 |
| C | 4.97334600 | 1.74349900 | -0.27376300 |
| C | 3.90760700 | 2.62780600 | 1.84195900 |
| H | 3.98881200 | -0.03862000 | 2.55192900 |
| H | 4.73841000 | -0.66804800 | 1.06818700 |
| H | 5.63042900 | 0.47025300 | 2.09484500 |

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|---|------------|------------|-------------|
| H | 4.56732100 | 2.57398500 | -0.85888100 |
| H | 5.96736000 | 2.02755800 | 0.09089200 |
| H | 5.07864200 | 0.88568800 | -0.94411100 |
| H | 4.88604200 | 2.91914100 | 2.24136800 |
| H | 3.49381300 | 3.48393600 | 1.29704900 |
| H | 3.23978400 | 2.40032700 | 2.67694700 |

TS5(quintet)

| | | | |
|----|-------------|-------------|-------------|
| C | 2.79630400 | -1.32863700 | -2.71335300 |
| C | 1.89677900 | -1.53025100 | -1.66589000 |
| C | 0.79409900 | -0.67907800 | -1.49978500 |
| C | 0.64793400 | 0.40247700 | -2.38513100 |
| C | 1.53026700 | 0.60093100 | -3.45107400 |
| C | 2.60894300 | -0.26617200 | -3.60837900 |
| H | 3.64110500 | -2.00051700 | -2.84318600 |
| H | 2.03745600 | -2.36438800 | -0.98414500 |
| H | -0.38440900 | -1.41037100 | -1.24374500 |
| H | 1.37502300 | 1.44379000 | -4.11736300 |
| H | 3.31282500 | -0.11367700 | -4.42183100 |
| C | -0.42916400 | 1.39094400 | -2.12317800 |
| O | -0.81924100 | 2.21079300 | -2.94807200 |
| N | -0.88460600 | 1.29797900 | -0.80211700 |
| C | -1.67348800 | 2.24176300 | -0.25330800 |
| C | -2.42564400 | 3.27269900 | -0.86420700 |
| C | -3.20421800 | 4.11456400 | -0.09444800 |
| H | -2.36034500 | 3.35521000 | -1.93858900 |
| C | -2.50372700 | 2.96828400 | 1.88877400 |
| C | -3.25242900 | 3.96222900 | 1.30267600 |
| H | -3.78540700 | 4.89441100 | -0.57589700 |
| H | -2.44880900 | 2.76405200 | 2.94943400 |
| H | -3.85823300 | 4.60797400 | 1.92700900 |
| N | -1.73796100 | 2.14817300 | 1.12618800 |
| O | -1.00017400 | 1.22881300 | 1.72762700 |
| Co | 0.03471100 | 0.03255500 | 0.54214300 |
| C | -1.67063200 | -2.25542500 | 0.05809500 |
| O | -1.32927700 | -2.16842600 | -1.17415400 |
| O | -1.18096900 | -1.52601300 | 0.96139000 |
| C | -2.71788100 | -3.31198100 | 0.41284800 |
| C | -2.12088500 | -4.69280400 | 0.06839400 |
| C | -3.07077400 | -3.23880800 | 1.90335200 |
| C | -3.96921700 | -3.05543500 | -0.45090000 |
| H | -1.85425300 | -4.74947100 | -0.99039700 |
| H | -1.22258000 | -4.89253700 | 0.66371100 |
| H | -2.85419800 | -5.47675000 | 0.28849200 |
| H | -3.47992700 | -2.25829400 | 2.16517000 |
| H | -3.81960700 | -4.00251500 | 2.14198600 |
| H | -2.18924200 | -3.40763400 | 2.52805000 |
| H | -4.72762400 | -3.81649900 | -0.23594300 |
| H | -4.40382000 | -2.07310800 | -0.23184700 |
| H | -3.72500400 | -3.09339900 | -1.51556700 |
| C | 2.39465900 | 0.20855200 | 1.19565700 |
| O | 1.89949600 | 1.21324400 | 0.62351700 |
| O | 1.62966600 | -0.81459700 | 1.39756700 |
| C | 3.84895900 | 0.14469800 | 1.64052600 |
| C | 3.87252300 | -0.10829700 | 3.16187900 |
| C | 4.51749800 | -1.03629400 | 0.90656400 |
| C | 4.56529900 | 1.45769300 | 1.30039400 |
| H | 3.40144700 | 0.71889400 | 3.70514300 |
| H | 3.34061700 | -1.03040500 | 3.41197300 |
| H | 4.90889000 | -0.19562200 | 3.50769800 |
| H | 4.48311900 | -0.89185800 | -0.17865200 |
| H | 5.56769300 | -1.11365100 | 1.21040500 |
| H | 4.01391500 | -1.97751800 | 1.14412800 |
| H | 5.61039300 | 1.40489600 | 1.62676100 |

| | | | |
|---|------------|------------|------------|
| H | 4.54577100 | 1.64866100 | 0.22341200 |
| H | 4.08874100 | 2.30784000 | 1.79738200 |

int6(singlet)

| | | | |
|----|-------------|-------------|-------------|
| C | -2.47669500 | 3.32628300 | -0.53137400 |
| C | -1.59270500 | 4.22967800 | 0.06736300 |
| C | -0.30153500 | 3.82083300 | 0.39982800 |
| C | 0.08154700 | 2.50490200 | 0.13316600 |
| C | -0.80300000 | 1.58807400 | -0.46004400 |
| C | -2.08812400 | 2.00540300 | -0.79555200 |
| H | -3.48092200 | 3.65183600 | -0.79285500 |
| H | -1.91085300 | 5.24877800 | 0.26765700 |
| H | 0.41456700 | 4.50087600 | 0.85247300 |
| H | -2.78802200 | 1.31738400 | -1.26085700 |
| C | 1.44678800 | 1.99982400 | 0.41838300 |
| O | 2.36494500 | 2.62809200 | 0.92856900 |
| N | 1.53448100 | 0.67083500 | -0.02681300 |
| C | 2.61907100 | -0.13081500 | 0.07980400 |
| C | 3.88654400 | 0.13559700 | 0.63531100 |
| C | 3.34523600 | -2.34509200 | -0.47719400 |
| C | 4.85928700 | -0.84818200 | 0.62523800 |
| H | 4.04491600 | 1.11938100 | 1.05347900 |
| C | 4.59029700 | -2.10766400 | 0.06369700 |
| H | 3.02593200 | -3.27092500 | -0.93652300 |
| H | 5.83319300 | -0.64258000 | 1.05756900 |
| H | 5.33427200 | -2.89503700 | 0.04696900 |
| O | 1.20775500 | -1.62204500 | -1.02858100 |
| N | 2.39838300 | -1.37702300 | -0.46638600 |
| Co | -0.01361400 | -0.14404200 | -0.64051400 |
| O | -1.66589100 | -1.05350400 | -1.21681200 |
| C | -1.89298900 | -1.26851300 | 0.01363100 |
| O | -1.00225700 | -0.79870200 | 0.81698000 |
| C | -3.12639400 | -1.96389400 | 0.54321300 |
| C | -3.98126800 | -0.88193100 | 1.24336300 |
| C | -3.90580700 | -2.59844500 | -0.61580100 |
| C | -2.69233200 | -3.03136000 | 1.56611900 |
| H | -3.42936700 | -0.41874300 | 2.06602500 |
| H | -4.27261300 | -0.09390100 | 0.54080600 |
| H | -4.89218000 | -1.34000200 | 1.64408500 |
| H | -3.30194200 | -3.34866100 | -1.13559500 |
| H | -4.80581100 | -3.08700900 | -0.22689100 |
| H | -4.20758300 | -1.84528900 | -1.34894400 |
| H | -3.57859700 | -3.51420500 | 1.99198300 |
| H | -2.07751600 | -3.80431200 | 1.09179500 |
| H | -2.11389300 | -2.58406200 | 2.37893300 |

int6(triplet)

| | | | |
|---|-------------|-------------|-------------|
| C | -1.83944200 | 3.72050300 | -0.24248200 |
| C | -0.72007300 | 4.51531100 | 0.03424900 |
| C | 0.53553400 | 3.92960300 | 0.18626400 |
| C | 0.65323700 | 2.54389800 | 0.06376600 |
| C | -0.46957900 | 1.74556700 | -0.20203300 |
| C | -1.72166900 | 2.33109600 | -0.36109300 |
| H | -2.81267300 | 4.18834100 | -0.36744200 |
| H | -0.83204400 | 5.59180700 | 0.12582700 |
| H | 1.42295500 | 4.52028000 | 0.39447500 |
| H | -2.59236100 | 1.72603800 | -0.58931300 |
| C | 1.95206300 | 1.83708100 | 0.19206100 |
| O | 3.03821600 | 2.35260100 | 0.41625600 |
| N | 1.73147800 | 0.46666900 | 0.00396200 |
| C | 2.68568900 | -0.49693800 | 0.03184700 |
| C | 4.07431500 | -0.38331700 | 0.23559300 |
| C | 2.92520200 | -2.86929100 | -0.19018200 |
| C | 4.86282600 | -1.52118300 | 0.22419400 |

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|----|-------------|-------------|-------------|
| H | 4.47138500 | 0.60808900 | 0.39992200 |
| C | 4.28646600 | -2.78326100 | 0.00954300 |
| H | 2.37088000 | -3.78160000 | -0.36464400 |
| H | 5.93233800 | -1.43196400 | 0.38464900 |
| H | 4.88209600 | -3.68802900 | -0.00272300 |
| O | 0.84020600 | -1.86837500 | -0.37753900 |
| N | 2.16248900 | -1.75155000 | -0.17835100 |
| Co | -0.02815200 | -0.13438800 | -0.30071700 |
| O | -1.74553500 | -0.72415200 | -1.08270300 |
| C | -2.24810500 | -0.98320300 | 0.06949600 |
| O | -1.54738000 | -0.73137900 | 1.09075500 |
| C | -3.65300200 | -1.55985100 | 0.20207300 |
| C | -4.49756900 | -0.54198600 | 0.99698900 |
| C | -4.27455100 | -1.81016100 | -1.17791900 |
| C | -3.55041200 | -2.87778600 | 0.99571100 |
| H | -4.04498200 | -0.33919200 | 1.97137400 |
| H | -4.58657200 | 0.40722200 | 0.45545700 |
| H | -5.50776300 | -0.93781800 | 1.15155800 |
| H | -3.67748300 | -2.52075300 | -1.75707200 |
| H | -5.28456000 | -2.21960700 | -1.06031300 |
| H | -4.34196500 | -0.88417400 | -1.75678300 |
| H | -4.55088300 | -3.29838800 | 1.14854500 |
| H | -2.94936100 | -3.61633000 | 0.45322700 |
| H | -3.08631300 | -2.70733400 | 1.97071700 |

int6(quintet)

| | | | |
|----|-------------|-------------|-------------|
| C | -2.47631600 | 3.39203400 | -0.44534300 |
| C | -1.57550700 | 4.24519000 | 0.20292200 |
| C | -0.28859300 | 3.80742600 | 0.51224200 |
| C | 0.08854100 | 2.50773600 | 0.16063700 |
| C | -0.81157400 | 1.66484100 | -0.49359300 |
| C | -2.10318400 | 2.08746800 | -0.79723000 |
| H | -3.47951400 | 3.74151700 | -0.67649700 |
| H | -1.88378500 | 5.25192800 | 0.47059900 |
| H | 0.42719000 | 4.44652300 | 1.02080000 |
| H | -2.81516500 | 1.42396300 | -1.27929100 |
| C | 1.44237200 | 1.97978300 | 0.47404000 |
| O | 2.32964400 | 2.62445300 | 1.02223400 |
| N | 1.54784800 | 0.65676500 | 0.04443600 |
| C | 2.67811700 | -0.06500900 | 0.11828700 |
| C | 3.94702300 | 0.25472400 | 0.65288700 |
| C | 3.52470400 | -2.23538000 | -0.49517400 |
| C | 4.97063700 | -0.67229500 | 0.60183000 |
| H | 4.06173600 | 1.23673000 | 1.08851000 |
| C | 4.76480400 | -1.93746400 | 0.02246900 |
| H | 3.24690000 | -3.16981700 | -0.96404700 |
| H | 5.94160800 | -0.41829900 | 1.01505800 |
| H | 5.55334000 | -2.67846300 | -0.02631900 |
| O | 1.33193900 | -1.63713400 | -0.94963000 |
| N | 2.53029300 | -1.31856600 | -0.44250400 |
| Co | -0.05019900 | -0.28059000 | -0.83794100 |
| O | -3.80501300 | -0.77782900 | -1.00602600 |
| C | -2.80710700 | -1.26511100 | -0.50836400 |
| O | -1.61328600 | -1.16972100 | -1.09970100 |
| C | -2.80175700 | -1.99852500 | 0.84309800 |
| C | -2.10765600 | -1.08320200 | 1.87669400 |
| C | -4.25071600 | -2.25714000 | 1.27626500 |
| C | -2.03082000 | -3.32607600 | 0.72220300 |
| H | -1.04534900 | -0.94161600 | 1.64787600 |
| H | -2.58013600 | -0.09583100 | 1.91476300 |
| H | -2.17442000 | -1.53477700 | 2.87305000 |
| H | -4.77321500 | -2.88044600 | 0.54402800 |
| H | -4.26501900 | -2.77237000 | 2.24368900 |
| H | -4.80620300 | -1.32024700 | 1.36855100 |

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|---|-------------|-------------|-------------|
| H | -2.02665700 | -3.84141800 | 1.68977100 |
| H | -2.50254100 | -3.98948200 | -0.01137000 |
| H | -0.99447600 | -3.16148100 | 0.41349400 |

int7(singlet)

| | | | |
|----|-------------|-------------|-------------|
| C | -1.52348600 | 3.78140600 | -0.40059400 |
| C | -0.33803900 | 4.52357800 | -0.39009700 |
| C | 0.89088200 | 3.86694600 | -0.33771400 |
| C | 0.91249600 | 2.47164000 | -0.28765900 |
| C | -0.27511700 | 1.71742800 | -0.29081900 |
| C | -1.49749400 | 2.38054800 | -0.35374600 |
| H | -2.47969900 | 4.29759200 | -0.44279300 |
| H | -0.37612200 | 5.60849500 | -0.42690000 |
| H | 1.83097500 | 4.41138200 | -0.34024500 |
| H | -2.42951000 | 1.82526100 | -0.36119300 |
| C | 2.18104500 | 1.70015600 | -0.23672500 |
| O | 3.31250200 | 2.17098600 | -0.21033500 |
| N | 1.87476300 | 0.33671500 | -0.23507800 |
| C | 2.76903600 | -0.67808900 | -0.19633000 |
| C | 4.17254600 | -0.63633300 | -0.08463900 |
| C | 2.86125300 | -3.06999300 | -0.26576500 |
| C | 4.89494000 | -1.81691700 | -0.06251500 |
| H | 4.63386700 | 0.33907500 | -0.02350700 |
| C | 4.23505900 | -3.05319800 | -0.15057200 |
| H | 2.24859700 | -3.95797200 | -0.34452200 |
| H | 5.97588100 | -1.78204100 | 0.02732400 |
| H | 4.77645600 | -3.99141000 | -0.12966200 |
| O | 0.83308100 | -1.95701600 | -0.44755900 |
| N | 2.16074500 | -1.91167700 | -0.29421800 |
| Co | 0.07319600 | -0.16021900 | -0.15995600 |
| O | -1.69304100 | -0.72354200 | -0.53351500 |
| C | -2.64304400 | -0.90495300 | 0.30689600 |
| O | -2.52367900 | -0.73169900 | 1.54899300 |
| C | -3.97974300 | -1.36313400 | -0.28635300 |
| C | -4.43021600 | -0.31857100 | -1.32679400 |
| C | -3.74459300 | -2.71984300 | -0.98179000 |
| C | -5.03570500 | -1.50666800 | 0.81616400 |
| H | -4.61161500 | 0.65472400 | -0.85493100 |
| H | -3.67255900 | -0.18835100 | -2.10398000 |
| H | -5.36570500 | -0.64075700 | -1.79822000 |
| H | -3.41566800 | -3.47755600 | -0.26130500 |
| H | -4.67696500 | -3.06966300 | -1.43970700 |
| H | -2.98156000 | -2.63188300 | -1.75963600 |
| H | -5.98337300 | -1.84093300 | 0.37827400 |
| H | -4.72398800 | -2.23629400 | 1.56885600 |
| H | -5.20687700 | -0.55470000 | 1.32752300 |
| O | -0.12253700 | -0.22788900 | 1.71055600 |
| H | -1.17229100 | -0.43806300 | 1.77357500 |
| C | 0.21907700 | 0.86119600 | 2.57641900 |
| H | 1.26802300 | 1.11237600 | 2.41799400 |
| H | -0.40352300 | 1.73798100 | 2.38228900 |
| H | 0.07683000 | 0.51545900 | 3.60530300 |

int7(triplet)

| | | | |
|---|-------------|------------|-------------|
| C | -1.26941000 | 3.91804800 | -0.50103100 |
| C | -0.04815800 | 4.59282200 | -0.39289500 |
| C | 1.14153000 | 3.87409000 | -0.27852800 |
| C | 1.08921800 | 2.47972900 | -0.26491500 |
| C | -0.13533600 | 1.80271900 | -0.35990200 |
| C | -1.32191900 | 2.51759200 | -0.49166900 |
| H | -2.19137500 | 4.48675600 | -0.59312200 |
| H | -0.02819600 | 5.67880100 | -0.40350200 |
| H | 2.10597200 | 4.36855100 | -0.20457000 |
| H | -2.27179400 | 2.00233000 | -0.58010100 |

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|----|-------------|-------------|-------------|
| C | 2.29807000 | 1.62470900 | -0.16556000 |
| O | 3.45585700 | 2.01401700 | -0.06873500 |
| N | 1.88957000 | 0.29218400 | -0.19937500 |
| C | 2.70913700 | -0.78382100 | -0.19710200 |
| C | 4.10833400 | -0.84900200 | -0.04668000 |
| C | 2.63732000 | -3.16810700 | -0.41737900 |
| C | 4.74426200 | -2.07814100 | -0.07595200 |
| H | 4.63421200 | 0.08509900 | 0.08978100 |
| C | 4.00410800 | -3.25698400 | -0.26060700 |
| H | 1.96679000 | -4.00284500 | -0.57108400 |
| H | 5.82109200 | -2.12644900 | 0.04986400 |
| H | 4.47792000 | -4.23095200 | -0.28156700 |
| O | 0.69959100 | -1.90308100 | -0.59372800 |
| N | 2.02378000 | -1.96292100 | -0.38750800 |
| Co | 0.02728000 | -0.11705000 | -0.19366200 |
| O | -1.79242100 | -0.49453600 | -0.51865600 |
| C | -2.67805100 | -0.88410400 | 0.34358900 |
| O | -2.48905000 | -0.97930600 | 1.57092400 |
| C | -4.04402000 | -1.23265000 | -0.27030800 |
| C | -4.56238800 | -0.00248500 | -1.04055300 |
| C | -3.83965900 | -2.40728200 | -1.24839300 |
| C | -5.03565200 | -1.62518100 | 0.83132100 |
| H | -4.69911900 | 0.85384800 | -0.36863000 |
| H | -3.86472700 | 0.28589000 | -1.83142600 |
| H | -5.53358400 | -0.22738600 | -1.49636600 |
| H | -3.46229100 | -3.29261900 | -0.72375200 |
| H | -4.79404400 | -2.67307500 | -1.71792300 |
| H | -3.12452100 | -2.14212900 | -2.03168900 |
| H | -6.00488100 | -1.87849900 | 0.38587900 |
| H | -4.67522200 | -2.48959200 | 1.39590500 |
| H | -5.18372400 | -0.80533200 | 1.54056700 |
| O | -0.02266700 | -0.32833200 | 1.89881500 |
| H | -0.99078300 | -0.62179700 | 1.95742200 |
| C | 0.20763200 | 0.79116000 | 2.75294000 |
| H | 1.22200400 | 1.14861500 | 2.56484100 |
| H | -0.49853100 | 1.60416500 | 2.54818400 |
| H | 0.12421800 | 0.48336300 | 3.80114100 |

int7(quintet)

| | | | |
|----|-------------|-------------|-------------|
| C | -1.48635400 | 3.67815600 | -0.83098900 |
| C | -0.34894300 | 4.44346700 | -0.54655600 |
| C | 0.87212100 | 3.82183100 | -0.28968100 |
| C | 0.94425100 | 2.42463200 | -0.30520800 |
| C | -0.20225000 | 1.67184700 | -0.56644700 |
| C | -1.41587800 | 2.27838600 | -0.86077300 |
| H | -2.43290500 | 4.17279300 | -1.03509400 |
| H | -0.41756000 | 5.52754500 | -0.53757900 |
| H | 1.77386600 | 4.39217100 | -0.08563900 |
| H | -2.29593200 | 1.68784600 | -1.09322100 |
| C | 2.22522500 | 1.69955500 | -0.07039300 |
| O | 3.31957900 | 2.24805300 | 0.02219300 |
| N | 1.98215700 | 0.33424700 | -0.00265800 |
| C | 2.93164000 | -0.60654500 | -0.13598900 |
| C | 4.33666800 | -0.47864600 | -0.21295900 |
| C | 3.17418100 | -2.98602800 | -0.38504000 |
| C | 5.12886700 | -1.59988500 | -0.37078800 |
| H | 4.73948400 | 0.52118200 | -0.13395200 |
| C | 4.54480600 | -2.87556400 | -0.45620100 |
| H | 2.61644700 | -3.91096900 | -0.44318500 |
| H | 6.20752900 | -1.49150200 | -0.42350000 |
| H | 5.14311800 | -3.77099500 | -0.57406800 |
| O | 1.07852700 | -2.03599100 | -0.18458400 |
| N | 2.40253000 | -1.88298500 | -0.23096800 |
| Co | 0.04718800 | -0.38035900 | 0.09937500 |

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|---|-------------|-------------|-------------|
| O | -1.75511500 | -0.96113700 | -0.40002200 |
| C | -2.82642500 | -0.89185600 | 0.31983300 |
| O | -2.84919000 | -0.53951500 | 1.52033200 |
| C | -4.12539100 | -1.29745400 | -0.39194800 |
| C | -4.30899700 | -0.38909100 | -1.62377100 |
| C | -3.97234800 | -2.76191200 | -0.85169400 |
| C | -5.32461400 | -1.15909700 | 0.55294100 |
| H | -4.44489600 | 0.65735300 | -1.32409900 |
| H | -3.44189600 | -0.45071500 | -2.28707800 |
| H | -5.20078400 | -0.69210600 | -2.18468800 |
| H | -3.82870100 | -3.42883000 | 0.00631700 |
| H | -4.87620300 | -3.08337800 | -1.38229700 |
| H | -3.11392600 | -2.87185400 | -1.51957600 |
| H | -6.24415100 | -1.45439300 | 0.03405400 |
| H | -5.20527900 | -1.79239500 | 1.43657000 |
| H | -5.43800300 | -0.12732600 | 0.89903300 |
| O | -0.39356400 | -0.21119300 | 2.06456000 |
| H | -1.41545200 | -0.33107100 | 2.01506400 |
| C | -0.05245200 | 0.98138700 | 2.77900100 |
| H | 1.02889800 | 1.11101600 | 2.70779700 |
| H | -0.54914500 | 1.85712200 | 2.34785300 |
| H | -0.33793000 | 0.86855100 | 3.82967700 |

TS8(singlet)

| | | | |
|----|-------------|-------------|-------------|
| C | -1.26219200 | 3.68773600 | -0.45652100 |
| C | -0.04859700 | 4.34984900 | -0.71766900 |
| C | 1.14986700 | 3.65791400 | -0.58632500 |
| C | 1.15179000 | 2.31894400 | -0.18949800 |
| C | -0.07420000 | 1.64106600 | 0.15573200 |
| C | -1.28828400 | 2.37972300 | -0.00136100 |
| H | -2.20245800 | 4.21456900 | -0.59755600 |
| H | -0.05307800 | 5.38423900 | -1.04682100 |
| H | 2.10231800 | 4.11910400 | -0.83237800 |
| H | -2.23247000 | 1.91388600 | 0.25376400 |
| C | 2.37492200 | 1.47915400 | -0.23623000 |
| O | 3.53061200 | 1.85232600 | -0.06334200 |
| N | 1.94404800 | 0.19235900 | -0.51582400 |
| C | 2.61502500 | -0.93671000 | -0.23321100 |
| C | 3.98367800 | -1.14385500 | 0.03553500 |
| C | 2.20413200 | -3.27552300 | 0.10356500 |
| C | 4.43526400 | -2.41697000 | 0.32926600 |
| H | 4.62924900 | -0.27670300 | -0.00022200 |
| C | 3.53923500 | -3.50253700 | 0.35722600 |
| H | 1.42661600 | -4.02779100 | 0.10785600 |
| H | 5.48868600 | -2.57952500 | 0.53366900 |
| H | 3.87329400 | -4.50994700 | 0.57412700 |
| O | 0.45836400 | -1.81209500 | -0.38688000 |
| N | 1.77251100 | -2.02380000 | -0.17388800 |
| Co | 0.09145500 | -0.01462400 | -0.77758000 |
| O | -1.75688400 | -0.44673800 | -0.91531400 |
| C | -2.42424000 | -0.72839200 | 0.13242300 |
| O | -2.07114900 | -0.46196600 | 1.32118700 |
| C | -3.76948400 | -1.42957000 | -0.09800500 |
| C | -4.62626200 | -0.53092200 | -1.01205700 |
| C | -3.48356400 | -2.76775000 | -0.80941800 |
| C | -4.49404200 | -1.67835200 | 1.23027500 |
| H | -4.84172000 | 0.43048900 | -0.52980100 |
| H | -4.11189100 | -0.33416100 | -1.95615400 |
| H | -5.58340000 | -1.02002100 | -1.22689900 |
| H | -2.86536100 | -3.42007700 | -0.18200600 |
| H | -4.42499100 | -3.28894400 | -1.01918400 |
| H | -2.95495900 | -2.59935200 | -1.75117300 |
| H | -5.45062600 | -2.17999900 | 1.04281300 |
| H | -3.89599800 | -2.30837300 | 1.89492500 |

| | | | |
|---|-------------|-------------|------------|
| H | -4.69333600 | -0.73906200 | 1.75502400 |
| O | -0.05705700 | 0.91144200 | 1.70888600 |
| H | -0.92245300 | 0.24741200 | 1.57228700 |
| C | -0.26504800 | 1.83841800 | 2.78719600 |
| H | 0.56440000 | 2.54826500 | 2.77729200 |
| H | -1.21302200 | 2.37277600 | 2.67015300 |
| H | -0.26310400 | 1.27107300 | 3.72109900 |

TS8(triplet)

| | | | |
|----|-------------|-------------|-------------|
| C | -1.41604100 | 3.64531000 | -0.85352300 |
| C | -0.19816500 | 4.33170600 | -0.98065300 |
| C | 0.98941800 | 3.68623600 | -0.63940200 |
| C | 0.97344500 | 2.37337500 | -0.16938200 |
| C | -0.26636400 | 1.68886500 | 0.01240400 |
| C | -1.46790500 | 2.35727500 | -0.33283100 |
| H | -2.34286800 | 4.13274400 | -1.14570800 |
| H | -0.18132600 | 5.34783200 | -1.36162500 |
| H | 1.95506400 | 4.16585600 | -0.77423000 |
| H | -2.42281200 | 1.86745800 | -0.17643700 |
| C | 2.22701900 | 1.59144100 | -0.02327600 |
| O | 3.33221800 | 2.07137300 | 0.21597700 |
| N | 1.93990900 | 0.24687400 | -0.23890300 |
| C | 2.81857100 | -0.76633700 | -0.06511900 |
| C | 4.20188600 | -0.72005500 | 0.19984200 |
| C | 2.93272200 | -3.16009100 | -0.08110000 |
| C | 4.92691600 | -1.89317600 | 0.31746400 |
| H | 4.64725200 | 0.25999600 | 0.29694600 |
| C | 4.28797900 | -3.13411900 | 0.17098400 |
| H | 2.33743700 | -4.05493000 | -0.20335400 |
| H | 5.99223600 | -1.84842300 | 0.52032000 |
| H | 4.82912800 | -4.06925300 | 0.25349400 |
| O | 0.91069200 | -2.08346400 | -0.40729000 |
| N | 2.22451800 | -2.01025200 | -0.18554900 |
| Co | 0.10476400 | -0.25525100 | -0.66087000 |
| O | -1.74669500 | -0.84227300 | -0.70238500 |
| C | -2.60508000 | -0.86808000 | 0.23408800 |
| O | -2.44674800 | -0.31897500 | 1.36708000 |
| C | -3.92021700 | -1.59854000 | -0.05966400 |
| C | -4.59562100 | -0.87976500 | -1.24611000 |
| C | -3.58266800 | -3.04919500 | -0.45800500 |
| C | -4.84339900 | -1.58281700 | 1.16459000 |
| H | -4.83897100 | 0.15892700 | -0.99162800 |
| H | -3.94182000 | -0.87588900 | -2.12236800 |
| H | -5.52995400 | -1.38955000 | -1.50700300 |
| H | -3.09861000 | -3.58102100 | 0.36910400 |
| H | -4.50163800 | -3.58790300 | -0.71617500 |
| H | -2.90853300 | -3.06915800 | -1.31808700 |
| H | -5.77718100 | -2.10680000 | 0.93041500 |
| H | -4.37438400 | -2.07773600 | 2.02010800 |
| H | -5.08638900 | -0.55947900 | 1.46516900 |
| O | -0.41245300 | 1.02576700 | 1.59465900 |
| H | -1.32683900 | 0.38871500 | 1.52094500 |
| C | -0.57668200 | 2.04927000 | 2.59155200 |
| H | 0.32876300 | 2.65849000 | 2.59700700 |
| H | -1.44550300 | 2.67556800 | 2.36577000 |
| H | -0.70367300 | 1.55273800 | 3.55650900 |

TS8(quintet)

| | | | |
|---|-------------|------------|-------------|
| C | -1.18456600 | 4.06033400 | -0.66324400 |
| C | 0.13246700 | 4.56302200 | -0.81122900 |
| C | 1.21523300 | 3.72666900 | -0.58170300 |
| C | 1.04450500 | 2.38012500 | -0.21939800 |
| C | -0.29934100 | 1.86002900 | -0.08311300 |
| C | -1.39519400 | 2.75960100 | -0.26287300 |

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|----|-------------|-------------|-------------|
| H | -2.03494700 | 4.70861000 | -0.86125300 |
| H | 0.29088600 | 5.59820800 | -1.09751400 |
| H | 2.23395900 | 4.08151300 | -0.70614600 |
| H | -2.40785800 | 2.39682300 | -0.10446500 |
| C | 2.25647000 | 1.53431500 | -0.15846700 |
| O | 3.40257900 | 1.99713600 | -0.18410300 |
| N | 1.96263700 | 0.16956200 | -0.09913300 |
| C | 2.88524000 | -0.81067700 | -0.09807700 |
| C | 4.29687000 | -0.72705700 | -0.07678000 |
| C | 3.08239500 | -3.20928200 | -0.10424900 |
| C | 5.06734900 | -1.87407700 | -0.07104700 |
| H | 4.71804900 | 0.26788700 | -0.07413300 |
| C | 4.45759200 | -3.14024400 | -0.08449500 |
| H | 2.50394900 | -4.12330500 | -0.11776900 |
| H | 6.14976600 | -1.79165300 | -0.05833900 |
| H | 5.03626200 | -4.05618200 | -0.08101400 |
| O | 0.99306500 | -2.22375800 | -0.13540800 |
| N | 2.33048100 | -2.08371200 | -0.10960600 |
| Co | 0.09821000 | -0.47140100 | -0.08096900 |
| O | -1.81052800 | -1.23900400 | -0.31046700 |
| C | -2.89346400 | -0.86336800 | 0.16362700 |
| O | -2.99156400 | 0.08379900 | 1.07189600 |
| C | -4.22226200 | -1.46053900 | -0.27431200 |
| C | -5.05214600 | -0.32941700 | -0.92237100 |
| C | -3.97861600 | -2.58881200 | -1.28436600 |
| C | -4.95772100 | -1.99975000 | 0.97069800 |
| H | -5.23945800 | 0.47963400 | -0.21140700 |
| H | -4.53770600 | 0.08690700 | -1.79558800 |
| H | -6.01491100 | -0.73157500 | -1.25540000 |
| H | -3.37276900 | -3.38858600 | -0.84845500 |
| H | -4.93913700 | -3.01163500 | -1.59737600 |
| H | -3.45585600 | -2.22037800 | -2.17148400 |
| H | -5.92349400 | -2.41825300 | 0.66782900 |
| H | -4.38178100 | -2.79578800 | 1.45592600 |
| H | -5.13663300 | -1.20681900 | 1.70152600 |
| O | -0.55352400 | 0.96896600 | 1.27700300 |
| H | -2.07611900 | 0.48495400 | 1.25399000 |
| C | 0.04510200 | 1.49009700 | 2.47365600 |
| H | 1.13243800 | 1.52425600 | 2.37007400 |
| H | -0.33927800 | 2.49786000 | 2.65853500 |
| H | -0.22856900 | 0.82147700 | 3.29490100 |

int9(singlet)

| | | | |
|---|-------------|-------------|-------------|
| C | -4.34930700 | -2.92143000 | -0.43459800 |
| C | -5.07248900 | -1.73016500 | -0.44491400 |
| C | -4.41793900 | -0.53253300 | -0.17757900 |
| C | -3.04207100 | -0.47378700 | 0.09292000 |
| C | -2.98505800 | -2.90314600 | -0.15017700 |
| H | -4.83731500 | -3.86843300 | -0.64650900 |
| H | -6.13693900 | -1.73310600 | -0.65845700 |
| H | -4.95612300 | 0.40787500 | -0.16013500 |
| H | -2.42543400 | -3.83088700 | -0.14713000 |
| C | -2.49785600 | 0.91173800 | 0.34395900 |
| O | -3.30419300 | 1.79238200 | 0.67034000 |
| N | -1.15816000 | 1.10764900 | 0.11382500 |
| C | -0.65130900 | 2.37559600 | 0.05342400 |
| C | -1.26641300 | 3.62518400 | 0.29490200 |
| C | 1.37231700 | 3.55961700 | -0.49732200 |
| C | -0.56311200 | 4.80694800 | 0.13655400 |
| H | -2.29846100 | 3.60617700 | 0.60650700 |
| C | 0.78080300 | 4.78074800 | -0.26763000 |
| H | 2.39683900 | 3.41298500 | -0.81189800 |
| H | -1.05780800 | 5.75318100 | 0.33154800 |
| H | 1.36106500 | 5.68660600 | -0.39920800 |

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|----|-------------|-------------|-------------|
| O | 1.30175400 | 1.25468000 | -0.58538700 |
| N | 0.67653200 | 2.40694700 | -0.33659000 |
| Co | 0.19042900 | -0.20011500 | -0.16271300 |
| C | -2.33984900 | -1.69199500 | 0.11139000 |
| O | -0.99283600 | -1.67707200 | 0.42777700 |
| C | -0.42507500 | -2.85131300 | 1.01965000 |
| H | -1.12335900 | -3.26441700 | 1.75247500 |
| H | -0.18765200 | -3.59748000 | 0.25480500 |
| H | 0.48898900 | -2.52251500 | 1.50946000 |
| C | 2.79607600 | -1.68773800 | -0.55116200 |
| O | 1.58435700 | -1.49383100 | -0.62703700 |
| C | 3.78769500 | -1.01069100 | 0.38127000 |
| C | 4.35835900 | 0.20812100 | -0.38516200 |
| C | 3.07160500 | -0.54200900 | 1.65762500 |
| C | 4.92913400 | -1.98034000 | 0.74235600 |
| H | 4.87005400 | -0.10883100 | -1.30008500 |
| H | 3.55425500 | 0.90171700 | -0.64049600 |
| H | 5.08581800 | 0.72004100 | 0.25519300 |
| H | 2.68311700 | -1.39466800 | 2.22738400 |
| H | 3.78779900 | -0.01191900 | 2.29493600 |
| H | 2.23751600 | 0.12480900 | 1.42435900 |
| H | 5.61938900 | -1.47631200 | 1.42689900 |
| H | 4.54948800 | -2.87655900 | 1.24565500 |
| H | 5.48876400 | -2.29602400 | -0.14147700 |
| O | 3.35770100 | -2.57679700 | -1.39103000 |
| H | 2.64247700 | -2.88305300 | -1.98155500 |

int9(triplet)

| | | | |
|----|-------------|-------------|-------------|
| C | 2.74472600 | 4.12250300 | -0.28294300 |
| C | 3.71005900 | 3.35058600 | -0.92431600 |
| C | 3.64816600 | 1.96255700 | -0.82537100 |
| C | 2.62815700 | 1.31141700 | -0.12185200 |
| C | 1.72899800 | 3.50772000 | 0.45096100 |
| H | 2.77712000 | 5.20694700 | -0.33980600 |
| H | 4.50857300 | 3.82269900 | -1.48839700 |
| H | 4.40473600 | 1.33721300 | -1.28629500 |
| H | 0.99253800 | 4.11997600 | 0.95690700 |
| C | 2.71564000 | -0.20128000 | -0.08250400 |
| O | 3.84314400 | -0.70843600 | -0.09290800 |
| N | 1.51611400 | -0.86182100 | -0.08997000 |
| C | 1.45328300 | -2.21695900 | -0.03755500 |
| C | 2.50182500 | -3.16741200 | -0.02531200 |
| C | -0.09798200 | -4.05373900 | 0.05868500 |
| C | 2.24071200 | -4.52490500 | 0.02895100 |
| H | 3.50618300 | -2.77426900 | -0.06106800 |
| C | 0.91743700 | -4.98489400 | 0.07042100 |
| H | -1.15348400 | -4.28839900 | 0.09004600 |
| H | 3.06708700 | -5.22912000 | 0.03759800 |
| H | 0.67294000 | -6.04000400 | 0.11085700 |
| O | -0.89160100 | -1.89812400 | 0.01266900 |
| N | 0.15745200 | -2.72403600 | 0.00832700 |
| Co | -0.28444600 | 0.03153400 | -0.15160200 |
| C | 1.66868800 | 2.11396300 | 0.53166400 |
| O | 0.68489700 | 1.46955000 | 1.25962000 |
| C | -0.16130900 | 2.24268100 | 2.10505000 |
| H | 0.43330900 | 2.83001700 | 2.81322000 |
| H | -0.81051100 | 2.90358900 | 1.51977300 |
| H | -0.77341600 | 1.51606100 | 2.63961000 |
| C | -3.04910800 | 1.22665100 | -0.62719300 |
| O | -1.81950500 | 1.23065300 | -0.54029900 |
| C | -3.97745700 | 0.19505600 | -0.01183600 |
| C | -3.93205400 | -1.04970200 | -0.93392300 |
| C | -3.45813800 | -0.18048900 | 1.38910000 |
| C | -5.41627600 | 0.72956300 | 0.08033400 |

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|---|-------------|-------------|-------------|
| H | -4.26426900 | -0.79934900 | -1.94768500 |
| H | -2.92538600 | -1.47481400 | -0.97055700 |
| H | -4.61197200 | -1.80946700 | -0.53205500 |
| H | -3.43094500 | 0.69549500 | 2.04813000 |
| H | -4.13653800 | -0.91598800 | 1.83446300 |
| H | -2.46011600 | -0.62271400 | 1.33905200 |
| H | -6.05301500 | -0.03677200 | 0.53458300 |
| H | -5.47136800 | 1.62938200 | 0.70252400 |
| H | -5.82166300 | 0.97300800 | -0.90514200 |
| O | -3.65811600 | 2.17865600 | -1.35710200 |
| H | -2.94747900 | 2.72779600 | -1.74101000 |

int9(quintet)

| | | | |
|----|-------------|-------------|-------------|
| C | 3.63533500 | -2.62742300 | -0.38571600 |
| C | 2.90224700 | -3.08551800 | -1.47798000 |
| C | 1.51881700 | -2.92954200 | -1.48254400 |
| C | 0.84270000 | -2.30849600 | -0.42595700 |
| C | 2.98785100 | -2.03418900 | 0.70040300 |
| H | 4.71625500 | -2.72837300 | -0.36538700 |
| H | 3.40181300 | -3.55265100 | -2.32040000 |
| H | 0.92057600 | -3.27797800 | -2.31694000 |
| H | 3.57141200 | -1.68754500 | 1.54301000 |
| C | -0.64819000 | -2.15145800 | -0.60322400 |
| O | -1.27012300 | -3.00586700 | -1.23275200 |
| N | -1.17236000 | -0.98712300 | -0.08650900 |
| C | -2.49357000 | -0.67510200 | -0.18932600 |
| C | -3.52189800 | -1.32939400 | -0.89890200 |
| C | -4.09865500 | 0.96777600 | 0.51374500 |
| C | -4.81182300 | -0.82597000 | -0.89478600 |
| H | -3.24937600 | -2.22494500 | -1.43610200 |
| C | -5.11085100 | 0.34290500 | -0.18217700 |
| H | -4.20829800 | 1.86939100 | 1.10096400 |
| H | -5.58829400 | -1.34067500 | -1.45165200 |
| H | -6.10831900 | 0.76545900 | -0.16262900 |
| O | -1.91609200 | 1.11533400 | 1.23017200 |
| N | -2.84188400 | 0.46535600 | 0.51228100 |
| Co | -0.10797500 | 0.39881900 | 0.87912600 |
| C | 1.59939900 | -1.88652500 | 0.68715500 |
| O | 0.91270300 | -1.32460800 | 1.75509700 |
| C | 1.66141100 | -0.95898200 | 2.92847200 |
| H | 2.18718800 | -1.83287800 | 3.32282900 |
| H | 2.34763400 | -0.14289200 | 2.68963200 |
| H | 0.91429400 | -0.62099300 | 3.64746700 |
| C | 1.97555000 | 1.92037000 | -0.23343000 |
| O | 1.46784700 | 1.38395700 | 0.90018500 |
| C | 1.39723600 | 3.23381000 | -0.74362400 |
| C | -0.04354400 | 3.01295300 | -1.26724800 |
| C | 1.37208500 | 4.24482300 | 0.41298800 |
| C | 2.27509800 | 3.76960400 | -1.88756200 |
| H | -0.05604400 | 2.25457900 | -2.05735500 |
| H | -0.71837800 | 2.69185400 | -0.46371600 |
| H | -0.44958000 | 3.94540000 | -1.67897500 |
| H | 2.38427100 | 4.42546400 | 0.79258700 |
| H | 0.95590600 | 5.20180000 | 0.07524500 |
| H | 0.76302200 | 3.87321900 | 1.24239700 |
| H | 1.89537800 | 4.73625200 | -2.24093800 |
| H | 3.30741500 | 3.90948500 | -1.54726100 |
| H | 2.29002400 | 3.07343000 | -2.73094500 |
| O | 2.13479100 | 0.99237600 | -1.26834700 |
| H | 2.46994600 | 0.17947600 | -0.85517900 |

int10(doublet)

| | | | |
|---|-------------|-------------|-------------|
| C | -3.13413500 | -2.49626600 | -2.84312500 |
| C | -3.18038400 | -1.52674300 | -1.85027100 |

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|----|-------------|-------------|-------------|
| C | -2.06972100 | -0.68764000 | -1.64144900 |
| C | -0.92118200 | -0.81926500 | -2.43992300 |
| C | -0.88745800 | -1.78892200 | -3.43644700 |
| C | -1.98778300 | -2.62746400 | -3.63590400 |
| H | -3.98550900 | -3.14951200 | -3.00397300 |
| H | -4.05885500 | -1.40317600 | -1.22620000 |
| H | -0.05776100 | -0.18630800 | -2.27573400 |
| H | -0.00240900 | -1.89518700 | -4.05529600 |
| H | -1.95385700 | -3.38611900 | -4.41194900 |
| C | -2.17637500 | 0.31396300 | -0.58550200 |
| O | -3.15394500 | 0.54443000 | 0.10089500 |
| N | -0.97251000 | 1.09163300 | -0.29160500 |
| C | -1.03753500 | 2.41085400 | -0.18775900 |
| C | -2.09810600 | 3.28031700 | -0.56913300 |
| C | 0.27062700 | 4.32947600 | 0.48409300 |
| C | -1.95339900 | 4.63876900 | -0.42623200 |
| H | -3.00703300 | 2.83586800 | -0.95176000 |
| C | -0.75419000 | 5.17041500 | 0.10375000 |
| H | 1.21712400 | 4.64043600 | 0.90640200 |
| H | -2.75858600 | 5.30474500 | -0.71540800 |
| H | -0.62193600 | 6.23923400 | 0.22442800 |
| N | 0.12458900 | 2.98830700 | 0.34581900 |
| O | 1.09719200 | 2.19865300 | 0.72790100 |
| Co | 0.62985300 | 0.35699100 | 0.50627200 |
| O | -0.32584000 | 0.03815200 | 2.14441800 |
| O | 1.80669700 | 0.18481800 | -1.00143700 |
| C | -0.53511500 | -1.16561800 | 1.75351700 |
| O | -0.03626000 | -1.41498500 | 0.59392600 |
| C | 2.72255300 | -0.23207800 | -0.19819200 |
| O | 2.35730000 | -0.23765200 | 1.02967100 |
| C | 4.06171200 | -0.72339000 | -0.67297400 |
| C | 3.81616900 | -2.14821700 | -1.23261700 |
| C | 4.57089200 | 0.20297000 | -1.79351300 |
| C | 5.05031900 | -0.77090700 | 0.50191700 |
| H | 3.43394000 | -2.81804800 | -0.45555900 |
| H | 3.10141900 | -2.12913800 | -2.06086000 |
| H | 4.76415600 | -2.55340000 | -1.60010400 |
| H | 4.73961500 | 1.21923700 | -1.42157500 |
| H | 5.52278700 | -0.18135100 | -2.17256700 |
| H | 3.86199100 | 0.25138000 | -2.62444200 |
| H | 6.01068800 | -1.15848400 | 0.14828400 |
| H | 5.21783600 | 0.22585600 | 0.92203400 |
| H | 4.68905600 | -1.42141400 | 1.30283300 |
| C | -1.29524200 | -2.17889900 | 2.56185000 |
| C | -0.38082600 | -2.59230400 | 3.74079500 |
| C | -2.57907800 | -1.50818000 | 3.09370300 |
| C | -1.63250600 | -3.39352500 | 1.68312100 |
| H | 0.54423800 | -3.05523100 | 3.38181200 |
| H | -0.12283100 | -1.72989800 | 4.36198500 |
| H | -0.91100100 | -3.32192700 | 4.36069400 |
| H | -3.22460900 | -1.17908700 | 2.27271700 |
| H | -3.13375300 | -2.23090800 | 3.69999300 |
| H | -2.34462700 | -0.64065800 | 3.71605500 |
| H | -2.18686200 | -4.12433600 | 2.27983900 |
| H | -2.25200000 | -3.10670600 | 0.82723600 |
| H | -0.72839000 | -3.87560300 | 1.30106700 |

int10(quartet)

| | | | |
|---|-------------|-------------|-------------|
| C | -3.81531400 | 1.41140100 | -2.43274500 |
| C | -2.93437000 | 2.05480400 | -1.57403600 |
| C | -1.62862200 | 1.55391500 | -1.40795300 |
| C | -1.20780900 | 0.42174000 | -2.12471900 |
| C | -2.09415000 | -0.20804800 | -2.99302600 |
| C | -3.39476500 | 0.27865000 | -3.14190600 |

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|----|-------------|-------------|-------------|
| H | -4.82565900 | 1.78757200 | -2.55593700 |
| H | -3.23381900 | 2.93767800 | -1.01975100 |
| H | -0.20952700 | 0.02281000 | -1.99641400 |
| H | -1.77366300 | -1.08583600 | -3.54435600 |
| H | -4.08518300 | -0.22318700 | -3.81310000 |
| C | -0.75209800 | 2.26693800 | -0.48113300 |
| O | -1.00015800 | 3.32125400 | 0.07526200 |
| N | 0.49885400 | 1.61070200 | -0.12094600 |
| C | 1.59138900 | 2.33177700 | 0.02600600 |
| C | 1.86893100 | 3.63510000 | -0.48592100 |
| C | 3.85056100 | 2.22582300 | 0.89130100 |
| C | 3.11636600 | 4.18902200 | -0.33068000 |
| H | 1.07089300 | 4.15433700 | -0.99905800 |
| C | 4.12078600 | 3.47361500 | 0.35866700 |
| H | 4.54957600 | 1.62282200 | 1.45608300 |
| H | 3.33165400 | 5.17134100 | -0.73589100 |
| H | 5.11220000 | 3.89060200 | 0.49340100 |
| N | 2.62087700 | 1.68087300 | 0.74906100 |
| O | 2.36605900 | 0.53659800 | 1.31597900 |
| Co | 0.62309300 | -0.29412900 | 0.82416700 |
| O | -0.83612600 | 0.01795700 | 2.00284200 |
| O | 1.27924500 | -1.20800100 | -0.88475700 |
| C | -1.74461000 | -0.67699800 | 1.34467200 |
| O | -1.32134100 | -1.25125700 | 0.31837400 |
| C | 1.59982900 | -2.25094600 | -0.20092100 |
| O | 1.43877400 | -2.14442200 | 1.05803100 |
| C | 2.07672800 | -3.51524900 | -0.87359700 |
| C | 0.83483300 | -4.11861700 | -1.57724900 |
| C | 3.14802600 | -3.15299500 | -1.92124500 |
| C | 2.63279700 | -4.49514400 | 0.16893400 |
| H | 0.04841000 | -4.35785800 | -0.85415600 |
| H | 0.42711600 | -3.42573600 | -2.31902000 |
| H | 1.12771300 | -5.04262200 | -2.08564700 |
| H | 4.03547200 | -2.71935400 | -1.44710300 |
| H | 3.45759300 | -4.06009500 | -2.44964600 |
| H | 2.76160100 | -2.43992100 | -2.65460100 |
| H | 2.95075000 | -5.41437600 | -0.33314700 |
| H | 3.49738200 | -4.07342000 | 0.69093300 |
| H | 1.87807100 | -4.75276300 | 0.91670500 |
| C | -3.16533000 | -0.71460800 | 1.84298500 |
| C | -3.16294500 | -1.48284700 | 3.18660400 |
| C | -3.63922500 | 0.73791700 | 2.06940000 |
| C | -4.05368700 | -1.42197300 | 0.80937100 |
| H | -2.81788300 | -2.51358100 | 3.05328800 |
| H | -2.52173500 | -0.99134300 | 3.92380400 |
| H | -4.18373700 | -1.51336600 | 3.58028700 |
| H | -3.63823600 | 1.30251500 | 1.13123500 |
| H | -4.66293500 | 0.72324100 | 2.45615700 |
| H | -3.00334500 | 1.25794300 | 2.79067600 |
| H | -5.08214100 | -1.45832700 | 1.18217200 |
| H | -4.05081900 | -0.88884400 | -0.14644400 |
| H | -3.71693000 | -2.44645500 | 0.62752200 |

int10(sextet)

| | | | |
|---|-------------|-------------|-------------|
| C | -2.44754100 | -3.40372700 | -2.60879800 |
| C | -2.68115200 | -2.15157800 | -2.05531500 |
| C | -1.61729800 | -1.24358900 | -1.90872500 |
| C | -0.32563600 | -1.59215000 | -2.33770200 |
| C | -0.10214600 | -2.84623700 | -2.89845200 |
| C | -1.15804800 | -3.75204900 | -3.02854500 |
| H | -3.26398500 | -4.11057500 | -2.71550900 |
| H | -3.67145200 | -1.85900300 | -1.72442700 |
| H | 0.49734900 | -0.89502200 | -2.23701600 |
| H | 0.89431200 | -3.11746200 | -3.23172400 |

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|----|-------------|-------------|-------------|
| H | -0.97827400 | -4.73185200 | -3.46051300 |
| C | -1.91474100 | 0.05962500 | -1.31156600 |
| O | -3.02544500 | 0.48351000 | -1.04050100 |
| N | -0.76556900 | 0.85868900 | -0.93728700 |
| C | -0.79284000 | 2.17177500 | -1.04697200 |
| C | -1.70599500 | 2.98473200 | -1.78212700 |
| C | 0.40359800 | 4.17314000 | -0.39060700 |
| C | -1.54553500 | 4.34776400 | -1.81879000 |
| H | -2.52187100 | 2.48906800 | -2.28970100 |
| C | -0.47711300 | 4.95019000 | -1.11549600 |
| H | 1.23965600 | 4.54682000 | 0.18557800 |
| H | -2.23796700 | 4.96273400 | -2.38266600 |
| H | -0.33386000 | 6.02442000 | -1.12748200 |
| N | 0.25185500 | 2.82651300 | -0.35459600 |
| O | 1.08871900 | 2.12025800 | 0.34851300 |
| Co | 0.60347700 | 0.14513000 | 0.53271900 |
| O | -0.95494500 | 0.87180900 | 2.00622500 |
| O | 2.11799700 | -0.47186100 | -0.62458700 |
| C | -1.31823600 | -0.32386900 | 2.00466100 |
| O | -0.61414700 | -1.11898300 | 1.21374400 |
| C | 2.91686000 | -0.44385300 | 0.38987500 |
| O | 2.38010800 | -0.05779700 | 1.48237500 |
| C | 4.37548600 | -0.79965500 | 0.25909000 |
| C | 4.49474500 | -2.09320900 | -0.57279600 |
| C | 5.04607700 | 0.37555900 | -0.49625900 |
| C | 5.00700900 | -0.97518300 | 1.64771300 |
| H | 4.01646800 | -2.93704500 | -0.06404100 |
| H | 4.03604300 | -1.97626700 | -1.55828500 |
| H | 5.55311300 | -2.33576200 | -0.70922000 |
| H | 4.95786200 | 1.30975800 | 0.06851000 |
| H | 6.11021800 | 0.15377100 | -0.62369300 |
| H | 4.59970800 | 0.51609400 | -1.48518900 |
| H | 6.06812300 | -1.21759400 | 1.53314700 |
| H | 4.92273400 | -0.06223800 | 2.24313200 |
| H | 4.52888900 | -1.78837000 | 2.20262900 |
| C | -2.46214300 | -0.90409400 | 2.79204400 |
| C | -1.88115600 | -1.98404200 | 3.73561400 |
| C | -3.16004000 | 0.20412000 | 3.59173600 |
| C | -3.43980800 | -1.55611900 | 1.78492500 |
| H | -1.37152000 | -2.77137000 | 3.17337000 |
| H | -1.17459600 | -1.54839900 | 4.44987600 |
| H | -2.70111800 | -2.43695200 | 4.30140000 |
| H | -3.56538100 | 0.97631100 | 2.93097700 |
| H | -3.98806100 | -0.22995500 | 4.16056500 |
| H | -2.47261700 | 0.68241700 | 4.29532400 |
| H | -4.26404000 | -2.01370600 | 2.34080800 |
| H | -3.85814700 | -0.81193900 | 1.09988300 |
| H | -2.94385500 | -2.33359400 | 1.19685300 |

int13(doublet)

| | | | |
|---|-------------|-------------|------------|
| C | -0.22010600 | 2.58212500 | 3.29514500 |
| C | 0.36653700 | 1.36339000 | 2.96132000 |
| C | -0.43102700 | 0.31996700 | 2.48214900 |
| C | -1.81398300 | 0.48326900 | 2.37894100 |
| C | -2.39613900 | 1.70342200 | 2.71825300 |
| C | -1.59998100 | 2.75810400 | 3.16716100 |
| H | 0.40166000 | 3.39709400 | 3.65535600 |
| H | 1.43828700 | 1.22163700 | 3.03067700 |
| H | -2.42555300 | -0.34551000 | 2.04735600 |
| H | -3.47212300 | 1.82771100 | 2.63338900 |
| H | -2.05399500 | 3.71044800 | 3.42735000 |
| C | 0.19891300 | -0.99869400 | 2.16551700 |
| O | 0.55179700 | -1.76403600 | 3.04136400 |
| C | 0.82898500 | -2.51305600 | 0.36776600 |

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|----|-------------|-------------|-------------|
| C | 1.40498000 | -3.55878700 | 1.11781900 |
| C | 1.17323100 | -3.79931800 | -1.62996000 |
| C | 1.84942300 | -4.70537500 | 0.48438200 |
| H | 1.48061600 | -3.41885000 | 2.18381000 |
| C | 1.72908400 | -4.83334200 | -0.90684200 |
| H | 1.03789600 | -3.78163300 | -2.70270700 |
| H | 2.29576900 | -5.50173200 | 1.07009800 |
| H | 2.07015200 | -5.71861100 | -1.43044200 |
| O | 0.19265700 | -1.73089900 | -1.73335500 |
| N | 0.74383400 | -2.68209300 | -0.99987100 |
| Co | 0.05203100 | -0.13602800 | -0.71936200 |
| O | -1.83328900 | -0.26468000 | -0.75015500 |
| O | -0.19773000 | 1.21170500 | -2.11667000 |
| O | 1.91352000 | 0.13171700 | -0.93562500 |
| C | -0.27657100 | 2.08320000 | -1.19221200 |
| O | -0.09984500 | 1.63771400 | -0.00634400 |
| C | -2.47349500 | -1.28091700 | -0.29495000 |
| O | -1.99692100 | -2.20098600 | 0.39137700 |
| C | 2.71755300 | 0.27174000 | 0.06473800 |
| O | 2.49213300 | -0.05656800 | 1.23807900 |
| C | -0.64137500 | 3.53000800 | -1.42661300 |
| C | -0.36182500 | 3.91926100 | -2.88389500 |
| C | -2.15352600 | 3.63229800 | -1.11288600 |
| C | 0.15462900 | 4.41217500 | -0.44885100 |
| H | 0.70507900 | 3.83442100 | -3.11656900 |
| H | -0.90920900 | 3.27435800 | -3.57669100 |
| H | -0.66893800 | 4.95707500 | -3.05402200 |
| H | -2.35211200 | 3.32804400 | -0.08074300 |
| H | -2.48738700 | 4.66707400 | -1.24911400 |
| H | -2.73515200 | 2.98872100 | -1.78149100 |
| H | -0.15349700 | 5.45768300 | -0.56084000 |
| H | -0.01848600 | 4.10071800 | 0.58467100 |
| H | 1.22966400 | 4.34949900 | -0.65015200 |
| C | 4.06529600 | 0.92666000 | -0.31966200 |
| C | 3.74387000 | 2.35231400 | -0.81143400 |
| C | 4.99687700 | 0.97682800 | 0.89638200 |
| C | 4.70579800 | 0.11004100 | -1.45642400 |
| H | 3.08813700 | 2.32034700 | -1.68587100 |
| H | 3.24454000 | 2.93208400 | -0.02652300 |
| H | 4.67004700 | 2.87275800 | -1.08254200 |
| H | 5.20405300 | -0.02804100 | 1.27689400 |
| H | 5.94815800 | 1.44446700 | 0.61673400 |
| H | 4.55220300 | 1.55437800 | 1.71178200 |
| H | 5.65046400 | 0.57462500 | -1.76299800 |
| H | 4.92584400 | -0.91325500 | -1.12890700 |
| H | 4.04015700 | 0.06026100 | -2.32161100 |
| C | -3.97830700 | -1.27650000 | -0.66493500 |
| C | -4.60475400 | 0.02471000 | -0.12841400 |
| C | -4.07475800 | -1.30690900 | -2.20243700 |
| C | -4.68072100 | -2.49594800 | -0.05777900 |
| H | -4.56824800 | 0.05986700 | 0.96642000 |
| H | -4.07911100 | 0.90050900 | -0.51672000 |
| H | -5.65758700 | 0.08019100 | -0.42918300 |
| H | -3.61948100 | -2.21870700 | -2.60606900 |
| H | -5.12712500 | -1.28838000 | -2.51013900 |
| H | -3.56168900 | -0.44689000 | -2.64007400 |
| H | -5.74446200 | -2.48056400 | -0.32255300 |
| H | -4.24485800 | -3.42852100 | -0.42788000 |
| H | -4.59586200 | -2.50011700 | 1.03304400 |
| N | 0.33289300 | -1.31307000 | 0.77786900 |

int13(quartet)

| | | | |
|---|-------------|-------------|-------------|
| C | -1.24355000 | -2.58393400 | -3.75858800 |
| C | -0.16279900 | -2.60553300 | -2.88437600 |

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|----|-------------|-------------|-------------|
| C | 0.17834300 | -1.45383500 | -2.15397800 |
| C | -0.55615700 | -0.27784400 | -2.33667700 |
| C | -1.63470900 | -0.25902200 | -3.22082000 |
| C | -1.98301400 | -1.40765600 | -3.92866000 |
| H | -1.51128900 | -3.48197900 | -4.30761400 |
| H | 0.42024300 | -3.50910500 | -2.74417800 |
| H | -0.29238900 | 0.64048500 | -1.83340700 |
| H | -2.20003700 | 0.65986700 | -3.33207700 |
| H | -2.82922200 | -1.39291900 | -4.60981900 |
| C | 1.36084600 | -1.58185200 | -1.26059500 |
| O | 2.35557800 | -2.18734800 | -1.62635900 |
| C | 2.12366700 | -1.39204300 | 1.02822700 |
| C | 3.15777800 | -2.35790400 | 0.99022300 |
| C | 2.64865000 | -1.00224400 | 3.34540900 |
| C | 3.91632800 | -2.61858800 | 2.11162900 |
| H | 3.33710200 | -2.85855900 | 0.05370500 |
| C | 3.66608200 | -1.92753800 | 3.30860800 |
| H | 2.36478500 | -0.41313000 | 4.20629300 |
| H | 4.70907200 | -3.35714300 | 2.06212500 |
| H | 4.25190500 | -2.10424200 | 4.20290100 |
| O | 0.94483100 | 0.13044900 | 2.34322100 |
| N | 1.89844300 | -0.75731000 | 2.24339700 |
| Co | 0.02386500 | 0.43939200 | 0.59289900 |
| O | 1.03834200 | 1.65124500 | -0.38865800 |
| O | -1.03275200 | 1.78057700 | 1.28815100 |
| O | -1.44571100 | -0.72691900 | 0.68864000 |
| C | -1.93687800 | 2.21640900 | 0.43948100 |
| O | -1.98426400 | 1.86080300 | -0.73517200 |
| C | 2.35385600 | 1.72376100 | -0.35912700 |
| O | 3.06788800 | 1.16066400 | 0.46145000 |
| C | -1.44901100 | -2.02096600 | 0.64445300 |
| O | -0.44807500 | -2.74583500 | 0.59099100 |
| C | -2.95068600 | 3.18022000 | 1.07644200 |
| C | -3.74861600 | 2.38187000 | 2.12843500 |
| C | -2.19491200 | 4.33673800 | 1.75713200 |
| C | -3.89140800 | 3.71763800 | -0.00830800 |
| H | -4.27434400 | 1.53954800 | 1.66343000 |
| H | -3.08576000 | 1.98545300 | 2.90260100 |
| H | -4.49595500 | 3.02944700 | 2.60183000 |
| H | -1.60936200 | 4.90621100 | 1.02616300 |
| H | -2.90830600 | 5.02301100 | 2.22875600 |
| H | -1.51103800 | 3.96181300 | 2.52313100 |
| H | -4.62985700 | 4.39158000 | 0.44187200 |
| H | -3.33666600 | 4.27086400 | -0.77225800 |
| H | -4.42095200 | 2.90182900 | -0.50832900 |
| C | -2.87319400 | -2.61843900 | 0.64360800 |
| C | -3.61073100 | -2.04525800 | -0.58308800 |
| C | -2.80417000 | -4.14716900 | 0.56337600 |
| C | -3.57498000 | -2.16888700 | 1.93926900 |
| H | -3.61357900 | -0.95278900 | -0.56146600 |
| H | -3.13048400 | -2.36406200 | -1.51302500 |
| H | -4.64580200 | -2.40743900 | -0.58903700 |
| H | -2.26939500 | -4.56747300 | 1.42059500 |
| H | -3.81849300 | -4.56216700 | 0.55016600 |
| H | -2.28635100 | -4.46825400 | -0.34525100 |
| H | -4.59760200 | -2.56333400 | 1.95968000 |
| H | -3.05027300 | -2.54467400 | 2.82551200 |
| H | -3.61775200 | -1.07838300 | 2.00073700 |
| C | 2.91986100 | 2.56620600 | -1.51967300 |
| C | 2.78072800 | 1.70471400 | -2.79433900 |
| C | 2.11454400 | 3.86752600 | -1.67711000 |
| C | 4.39767100 | 2.87423100 | -1.25075500 |
| H | 3.30495800 | 0.74816100 | -2.68431800 |
| H | 1.73059500 | 1.49663200 | -3.01943100 |

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|---|------------|-------------|-------------|
| H | 3.21643000 | 2.23410000 | -3.64972500 |
| H | 2.18429000 | 4.48377400 | -0.77335600 |
| H | 2.51098700 | 4.45145300 | -2.51618100 |
| H | 1.05895000 | 3.65549900 | -1.86257900 |
| H | 4.81560100 | 3.44647900 | -2.08722000 |
| H | 4.51599500 | 3.46458200 | -0.33626000 |
| H | 4.97590500 | 1.95448900 | -1.13032200 |
| N | 1.25953000 | -1.02496500 | 0.05357200 |

int13(sextet)

| | | | |
|----|-------------|-------------|-------------|
| C | -1.38229000 | -1.02814000 | 4.72654400 |
| C | -1.31606700 | -1.77628100 | 3.55744600 |
| C | -0.46755600 | -1.37361400 | 2.51372900 |
| C | 0.31904400 | -0.22297500 | 2.65619300 |
| C | 0.24937200 | 0.52253600 | 3.83023300 |
| C | -0.59947200 | 0.12377300 | 4.86354500 |
| H | -2.04452500 | -1.33557800 | 5.53056400 |
| H | -1.91520300 | -2.67039000 | 3.42514300 |
| H | 0.96330600 | 0.10458900 | 1.85231000 |
| H | 0.85002900 | 1.42137200 | 3.92711100 |
| H | -0.65682400 | 0.71112700 | 5.77581900 |
| C | -0.43788300 | -2.21061200 | 1.29850800 |
| O | -1.03534300 | -3.27395600 | 1.19339200 |
| C | 0.98770100 | -2.50121700 | -0.58237500 |
| C | 1.40537300 | -3.83941200 | -0.30015600 |
| C | 2.20374200 | -2.64386300 | -2.68261500 |
| C | 2.20339200 | -4.52386600 | -1.17303200 |
| H | 1.06809600 | -4.27603100 | 0.62887900 |
| C | 2.61508400 | -3.91361800 | -2.38674600 |
| H | 2.46087100 | -2.08999200 | -3.57454400 |
| H | 2.52795000 | -5.53176100 | -0.93799000 |
| H | 3.25524200 | -4.43600100 | -3.08777000 |
| O | 1.01801800 | -0.77372000 | -2.16100600 |
| N | 1.39583800 | -1.95450400 | -1.82132800 |
| Co | -0.08828300 | 0.25816900 | -0.66937700 |
| O | -1.95666200 | -0.07107100 | 0.15428300 |
| O | -0.68377200 | 1.87973700 | -1.59412200 |
| O | 1.67027900 | 0.80120600 | -0.14511700 |
| C | -0.77377700 | 2.65705400 | -0.55708600 |
| O | -0.50833400 | 2.20577100 | 0.57627900 |
| C | -2.41045500 | -0.70151100 | -0.86318900 |
| O | -1.61958900 | -0.93337800 | -1.81971500 |
| C | 2.91151700 | 0.38917500 | -0.02783600 |
| O | 3.28459400 | -0.76700600 | -0.19733700 |
| C | -1.21173800 | 4.10003600 | -0.79066100 |
| C | -0.20911200 | 4.75100600 | -1.76446600 |
| C | -2.61526100 | 4.06325600 | -1.42992900 |
| C | -1.24592100 | 4.86523600 | 0.53757700 |
| H | 0.79750600 | 4.77742200 | -1.33041000 |
| H | -0.16202000 | 4.19406800 | -2.70404300 |
| H | -0.51270500 | 5.78211200 | -1.97989700 |
| H | -3.33729500 | 3.58187400 | -0.76013800 |
| H | -2.96226900 | 5.08394500 | -1.62857800 |
| H | -2.59837800 | 3.50781400 | -2.37160900 |
| H | -1.56483100 | 5.89955000 | 0.36351200 |
| H | -1.94090400 | 4.39940900 | 1.24230700 |
| H | -0.25786200 | 4.88066500 | 1.00762900 |
| C | 3.85535400 | 1.53549700 | 0.38220000 |
| C | 3.33385200 | 2.13638300 | 1.70410400 |
| C | 5.27839000 | 0.99512200 | 0.55690900 |
| C | 3.81364200 | 2.61127900 | -0.72147900 |
| H | 2.31205300 | 2.50766800 | 1.58325100 |
| H | 3.33737200 | 1.38600700 | 2.50430900 |
| H | 3.97752100 | 2.96620700 | 2.01901700 |

| | | | |
|---|-------------|-------------|-------------|
| H | 5.64829400 | 0.55282100 | -0.37295800 |
| H | 5.95406200 | 1.80755000 | 0.84926500 |
| H | 5.31289500 | 0.21993100 | 1.32833800 |
| H | 4.46938300 | 3.44855000 | -0.45482800 |
| H | 4.15543700 | 2.20608100 | -1.68117500 |
| H | 2.79661100 | 2.99125300 | -0.85387200 |
| C | -3.87452900 | -1.11573100 | -0.88339000 |
| C | -4.19012800 | -1.83695700 | 0.44214700 |
| C | -4.70385300 | 0.18325200 | -0.98771200 |
| C | -4.15444800 | -2.03149200 | -2.08134000 |
| H | -3.58775400 | -2.74510500 | 0.54857400 |
| H | -3.97907500 | -1.18871100 | 1.29689700 |
| H | -5.24943500 | -2.11752000 | 0.46509500 |
| H | -4.47333700 | 0.72419500 | -1.91234600 |
| H | -5.77267000 | -0.05900900 | -0.98879500 |
| H | -4.49444100 | 0.84368500 | -0.14120900 |
| H | -5.21540700 | -2.30595800 | -2.09658800 |
| H | -3.90910600 | -1.53515600 | -3.02448800 |
| H | -3.56252700 | -2.95042600 | -2.02067200 |
| N | 0.29504900 | -1.69597800 | 0.18862300 |

TS14(doublet)

| | | | |
|----|-------------|-------------|-------------|
| C | 0.28173500 | -3.60896900 | 3.00119900 |
| C | 1.33105600 | -2.98056700 | 2.32291900 |
| C | 1.23935500 | -1.60849700 | 2.17559700 |
| C | 0.15079500 | -0.84128500 | 2.53094100 |
| C | -0.87951600 | -1.48706300 | 3.23140400 |
| C | -0.81463300 | -2.86001900 | 3.44726900 |
| H | 0.32526400 | -4.67983500 | 3.18081300 |
| H | 2.19262400 | -3.53871400 | 1.97119600 |
| H | 2.33730900 | -0.97262400 | 1.75714100 |
| H | -1.73730000 | -0.89830100 | 3.53557200 |
| H | -1.63653400 | -3.36103700 | 3.95035700 |
| C | 0.07080700 | 0.63695100 | 2.28653100 |
| O | -0.20304900 | 1.38663200 | 3.21717300 |
| N | 0.39026300 | 1.03048300 | 1.00136000 |
| C | 0.40665200 | 2.35135000 | 0.65758700 |
| C | 0.20791000 | 3.50481900 | 1.44426200 |
| C | 0.26137100 | 4.76161200 | 0.86294600 |
| H | -0.00049000 | 3.35816700 | 2.49231900 |
| C | 0.69514500 | 3.76421000 | -1.26332100 |
| C | 0.50787500 | 4.90318500 | -0.50936900 |
| H | 0.09733000 | 5.63906200 | 1.48019100 |
| H | 0.87748900 | 3.73698100 | -2.32909400 |
| H | 0.54175900 | 5.87292900 | -0.99084200 |
| N | 0.65442000 | 2.54787700 | -0.67927500 |
| O | 0.88087500 | 1.46805100 | -1.44507300 |
| Co | 0.10607400 | -0.04026600 | -0.60159400 |
| C | 3.02340400 | -0.48442400 | -0.08753700 |
| O | 3.27850600 | -0.48777100 | 1.18816000 |
| O | 1.96127200 | -0.88716600 | -0.58479500 |
| C | 4.16573500 | 0.06736900 | -0.95550100 |
| C | 3.84087000 | -0.18041000 | -2.43432800 |
| C | 4.23966000 | 1.58590100 | -0.67805900 |
| C | 5.49072100 | -0.60956800 | -0.56046400 |
| H | 3.75806400 | -1.25031000 | -2.64912200 |
| H | 2.89639700 | 0.29359300 | -2.70992700 |
| H | 4.64392400 | 0.23514600 | -3.05366800 |
| H | 4.44204700 | 1.78743600 | 0.37781100 |
| H | 5.04666700 | 2.02163000 | -1.27758000 |
| H | 3.30129600 | 2.06971600 | -0.96069400 |
| H | 6.30089700 | -0.21321200 | -1.18215400 |
| H | 5.73538400 | -0.42631400 | 0.48902200 |
| H | 5.44418200 | -1.69294300 | -0.71963200 |

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|---|-------------|-------------|-------------|
| C | -2.48174300 | 0.77062500 | 0.08021700 |
| O | -1.54575300 | 0.74400400 | -0.84249000 |
| O | -2.42637000 | 0.27118300 | 1.19637700 |
| C | -3.71412000 | 1.56824000 | -0.40917400 |
| C | -3.25623400 | 3.00383700 | -0.73588000 |
| C | -4.27456400 | 0.89558300 | -1.67614500 |
| C | -4.77461900 | 1.59009300 | 0.69735800 |
| H | -2.79712100 | 3.47737700 | 0.14034900 |
| H | -2.52303500 | 3.00253900 | -1.54675200 |
| H | -4.11490800 | 3.61470900 | -1.03974200 |
| H | -4.60073900 | -0.12911900 | -1.46148000 |
| H | -5.14233700 | 1.45355700 | -2.04852700 |
| H | -3.51695900 | 0.85608800 | -2.46339200 |
| H | -5.65398900 | 2.15237000 | 0.36038300 |
| H | -5.08870500 | 0.57582000 | 0.96026800 |
| H | -4.38544300 | 2.05947700 | 1.60553600 |
| C | -0.75725600 | -2.04791900 | -1.31311500 |
| O | -0.68900500 | -1.72093000 | -0.08010200 |
| O | -0.27392400 | -1.20124700 | -2.13310400 |
| C | -1.43764200 | -3.33109200 | -1.73495400 |
| C | -1.10189100 | -3.65910200 | -3.19500100 |
| C | -0.98498500 | -4.46079200 | -0.79180800 |
| C | -2.95549000 | -3.08357900 | -1.56877700 |
| H | -1.40438500 | -2.84653300 | -3.86118800 |
| H | -0.02646300 | -3.81780300 | -3.32677500 |
| H | -1.62486100 | -4.57313200 | -3.49804600 |
| H | -1.18579900 | -4.20189200 | 0.25086900 |
| H | -1.51870500 | -5.38551100 | -1.03854600 |
| H | 0.09002600 | -4.64867900 | -0.89326900 |
| H | -3.50850600 | -3.99214100 | -1.83246500 |
| H | -3.19192600 | -2.81260400 | -0.53549500 |
| H | -3.29204300 | -2.27221100 | -2.22296000 |

TS14(quartet)

| | | | |
|----|-------------|-------------|-------------|
| C | -1.64811200 | -2.40715300 | 3.29975200 |
| C | -0.41779900 | -2.59866600 | 2.66438600 |
| C | 0.32352000 | -1.46605900 | 2.38197800 |
| C | -0.11449200 | -0.16886800 | 2.56993800 |
| C | -1.33916900 | 0.00082500 | 3.23232800 |
| C | -2.10011900 | -1.11268700 | 3.57726500 |
| H | -2.25301700 | -3.26901300 | 3.56746200 |
| H | -0.05140700 | -3.59186200 | 2.42731000 |
| H | 1.59395100 | -1.64084100 | 2.03177700 |
| H | -1.69213100 | 1.00975800 | 3.41409100 |
| H | -3.06848400 | -0.97208700 | 4.04819300 |
| C | 0.69818400 | 1.02809100 | 2.16897300 |
| O | 1.06128800 | 1.84326300 | 3.00062800 |
| N | 1.00994300 | 1.04534100 | 0.79886300 |
| C | 1.74706900 | 2.02953600 | 0.25510200 |
| C | 2.21536500 | 3.23014200 | 0.84402500 |
| C | 2.94376500 | 4.14100300 | 0.10835800 |
| H | 1.96760300 | 3.38673200 | 1.88280800 |
| C | 2.76327600 | 2.72248900 | -1.81947700 |
| C | 3.22488900 | 3.88473600 | -1.24506400 |
| H | 3.29083100 | 5.05703000 | 0.57463400 |
| H | 2.91356300 | 2.43115500 | -2.84990200 |
| H | 3.79089000 | 4.58261500 | -1.85104700 |
| N | 2.04783700 | 1.82187800 | -1.09619400 |
| O | 1.65608300 | 0.72629400 | -1.69642700 |
| Co | 0.07904200 | -0.14513900 | -0.70043800 |
| C | 2.43791800 | -1.92836500 | 0.21912700 |
| O | 2.66841000 | -1.79815100 | 1.49957200 |
| O | 1.30960500 | -1.88617200 | -0.28058200 |
| C | 3.70897800 | -2.14173400 | -0.62320600 |

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|---|-------------|-------------|-------------|
| C | 3.31259000 | -2.32757100 | -2.09303600 |
| C | 4.59306500 | -0.88700900 | -0.46480700 |
| C | 4.45099600 | -3.38387600 | -0.09288700 |
| H | 2.65470300 | -3.19168300 | -2.22116800 |
| H | 2.78750500 | -1.44639300 | -2.46904500 |
| H | 4.21629000 | -2.48527800 | -2.69295800 |
| H | 4.86432500 | -0.71874300 | 0.58098300 |
| H | 5.51169700 | -1.01604200 | -1.04794700 |
| H | 4.07341300 | -0.00168800 | -0.84287200 |
| H | 5.35662500 | -3.54772200 | -0.68724100 |
| H | 4.73885900 | -3.25883000 | 0.95443500 |
| H | 3.82738100 | -4.28111900 | -0.17613700 |
| C | -1.68647600 | 2.09565500 | -0.14018900 |
| O | -1.10306800 | 1.50046000 | -1.09496800 |
| O | -1.27462500 | 2.18159300 | 1.04280600 |
| C | -3.05146300 | 2.75494900 | -0.47937700 |
| C | -2.84038000 | 3.71045600 | -1.66570700 |
| C | -3.98633000 | 1.59955600 | -0.88888800 |
| C | -3.62353800 | 3.50782400 | 0.72649900 |
| H | -2.17113200 | 4.53560400 | -1.39381600 |
| H | -2.40650700 | 3.17827700 | -2.51573000 |
| H | -3.80083800 | 4.14314000 | -1.97115900 |
| H | -4.09759500 | 0.87800200 | -0.07241500 |
| H | -4.97772300 | 1.99554000 | -1.14054900 |
| H | -3.58280100 | 1.07146700 | -1.75628100 |
| H | -4.58694900 | 3.95876600 | 0.46031900 |
| H | -3.78009100 | 2.83443300 | 1.57434600 |
| H | -2.94874400 | 4.30488100 | 1.05406300 |
| C | -1.81182800 | -1.61561200 | -1.13844700 |
| O | -1.65950700 | -1.10193900 | 0.01511200 |
| O | -0.97502900 | -1.34165400 | -2.05780400 |
| C | -2.95712400 | -2.58861000 | -1.41537400 |
| C | -3.93256200 | -2.62136500 | -0.23180100 |
| C | -3.68047600 | -2.15652000 | -2.70349700 |
| C | -2.32109000 | -3.98035400 | -1.61896500 |
| H | -3.41827900 | -2.90146400 | 0.69176800 |
| H | -4.38661000 | -1.63852600 | -0.07038100 |
| H | -4.73435300 | -3.34463300 | -0.42459700 |
| H | -2.97698600 | -2.09246400 | -3.53749800 |
| H | -4.46622100 | -2.87866400 | -2.95597500 |
| H | -4.15022100 | -1.17426100 | -2.57795400 |
| H | -3.09687300 | -4.72136800 | -1.84599500 |
| H | -1.60290700 | -3.95797600 | -2.44363200 |
| H | -1.79357000 | -4.30294800 | -0.71348400 |

TS14(sextet)

| | | | |
|---|-------------|-------------|------------|
| C | -1.66174000 | -2.39058500 | 3.30455500 |
| C | -0.44109000 | -2.58912900 | 2.65380500 |
| C | 0.31044900 | -1.46208700 | 2.37406900 |
| C | -0.11477500 | -0.16216000 | 2.57401200 |
| C | -1.33010800 | 0.01502200 | 3.25162200 |
| C | -2.09805100 | -1.09349500 | 3.59663400 |
| H | -2.27179500 | -3.24827900 | 3.57394900 |
| H | -0.08686800 | -3.58407500 | 2.40575400 |
| H | 1.58577400 | -1.64601200 | 2.02958600 |
| H | -1.67145600 | 1.02609600 | 3.44364200 |
| H | -3.06009900 | -0.94706600 | 4.07861900 |
| C | 0.70069900 | 1.03148000 | 2.17005400 |
| O | 1.06160500 | 1.85067100 | 2.99870900 |
| N | 1.01517300 | 1.04207500 | 0.80047300 |
| C | 1.75597900 | 2.02231700 | 0.25426400 |
| C | 2.22858300 | 3.22267700 | 0.84012000 |
| C | 2.96058900 | 4.12888000 | 0.10222700 |
| H | 1.98095500 | 3.38309900 | 1.87835300 |

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|----|-------------|-------------|-------------|
| C | 2.77523400 | 2.70596400 | -1.82185600 |
| C | 3.24104900 | 3.86800000 | -1.25041200 |
| H | 3.31102100 | 5.04478200 | 0.56622000 |
| H | 2.92462100 | 2.41131700 | -2.85146600 |
| H | 3.80985200 | 4.56211400 | -1.85809200 |
| N | 2.05634000 | 1.80990100 | -1.09631500 |
| O | 1.66025500 | 0.71455100 | -1.69371800 |
| Co | 0.08191600 | -0.15148300 | -0.69407600 |
| C | 2.42807600 | -1.93834600 | 0.22290100 |
| O | 2.65937200 | -1.80766600 | 1.50206000 |
| O | 1.29744600 | -1.89729500 | -0.27425100 |
| C | 3.69595800 | -2.15398700 | -0.62301900 |
| C | 3.29751000 | -2.33122800 | -2.09333900 |
| C | 4.58929200 | -0.90668800 | -0.45927500 |
| C | 4.42993900 | -3.40377200 | -0.09882000 |
| H | 2.63368100 | -3.19031500 | -2.22446200 |
| H | 2.77825000 | -1.44504600 | -2.46560800 |
| H | 4.19973000 | -2.49272600 | -2.69447600 |
| H | 4.86248600 | -0.74569000 | 0.58713100 |
| H | 5.50650900 | -1.03962500 | -1.04375100 |
| H | 4.07611900 | -0.01554400 | -0.83238800 |
| H | 5.33408000 | -3.57095900 | -0.69451300 |
| H | 4.71917600 | -3.28535200 | 0.94890600 |
| H | 3.80017600 | -4.29634800 | -0.18586400 |
| C | -1.67624200 | 2.09918900 | -0.14509600 |
| O | -1.09402500 | 1.49794000 | -1.09669300 |
| O | -1.26635200 | 2.18661100 | 1.03849400 |
| C | -3.03669200 | 2.76526500 | -0.48930900 |
| C | -2.81710800 | 3.71666900 | -1.67739800 |
| C | -3.97719700 | 1.61439700 | -0.89853200 |
| C | -3.60747400 | 3.52434500 | 0.71330600 |
| H | -2.14367100 | 4.53851600 | -1.40585400 |
| H | -2.38432800 | 3.17990300 | -2.52509600 |
| H | -3.77427200 | 4.15424000 | -1.98621800 |
| H | -4.09513500 | 0.89559900 | -0.08056500 |
| H | -4.96554200 | 2.01554900 | -1.15399600 |
| H | -3.57437400 | 1.08176800 | -1.76346300 |
| H | -4.56788900 | 3.97966700 | 0.44376600 |
| H | -3.76936000 | 2.85402400 | 1.56257300 |
| H | -2.92919300 | 4.31869600 | 1.04024600 |
| C | -1.81740400 | -1.61082800 | -1.13625000 |
| O | -1.66429900 | -1.09753900 | 0.01751800 |
| O | -0.97734600 | -1.34256000 | -2.05401500 |
| C | -2.96768900 | -2.57765200 | -1.41439700 |
| C | -3.94591900 | -2.60344500 | -0.23297000 |
| C | -3.68568300 | -2.14356500 | -2.70481800 |
| C | -2.33882500 | -3.97317900 | -1.61447600 |
| H | -3.43520300 | -2.88520500 | 0.69208200 |
| H | -4.39487400 | -1.61791700 | -0.07377300 |
| H | -4.75125200 | -3.32254600 | -0.42657700 |
| H | -2.97977000 | -2.08414400 | -3.53711300 |
| H | -4.47442600 | -2.86205000 | -2.95840300 |
| H | -4.15077900 | -1.15880000 | -2.58170700 |
| H | -3.11817100 | -4.71038600 | -1.84168800 |
| H | -1.61895900 | -3.95606000 | -2.43779600 |
| H | -1.81475100 | -4.29707900 | -0.70745200 |

int15(doublet)

| | | | |
|---|------------|-------------|------------|
| C | 2.66360400 | -1.91577600 | 3.22613300 |
| C | 2.97433200 | -0.82523300 | 2.39925900 |
| C | 1.93978400 | 0.02861400 | 2.09735700 |
| C | 0.63734400 | -0.09086800 | 2.52628300 |
| C | 0.35482400 | -1.17948300 | 3.37078000 |
| C | 1.35942500 | -2.08430400 | 3.70411600 |

| | | | |
|----|-------------|-------------|-------------|
| H | 3.44121100 | -2.62681900 | 3.49449000 |
| H | 3.98290600 | -0.67741800 | 2.02319300 |
| H | 0.97109200 | 2.21457200 | 0.52684800 |
| H | -0.66524700 | -1.31004900 | 3.71461300 |
| H | 1.12530200 | -2.93382500 | 4.33883300 |
| C | -0.46218400 | 0.86172900 | 2.18563000 |
| O | -1.24189000 | 1.24880900 | 3.04259200 |
| N | -0.47180100 | 1.30091700 | 0.84780200 |
| C | -1.46330700 | 2.15428700 | 0.40691400 |
| C | -2.45516300 | 2.84993800 | 1.11772700 |
| C | -3.34283800 | 3.67680900 | 0.44212900 |
| H | -2.49994000 | 2.69655800 | 2.18418300 |
| C | -2.28438600 | 3.12438400 | -1.62699200 |
| C | -3.26058600 | 3.82377500 | -0.94670100 |
| H | -4.11011400 | 4.20157500 | 1.00204700 |
| H | -2.13195700 | 3.13465600 | -2.69763400 |
| H | -3.94766200 | 4.45263500 | -1.49984300 |
| N | -1.42266500 | 2.33522900 | -0.95385900 |
| O | -0.47822800 | 1.68359800 | -1.64876600 |
| Co | -0.02266300 | 0.11511100 | -0.67743000 |
| C | 2.46583300 | 1.65275500 | -0.45619900 |
| O | 1.87270000 | 2.57725100 | 0.26497600 |
| O | 1.90101900 | 0.61548500 | -0.82765700 |
| C | 3.91087600 | 1.94176100 | -0.82521100 |
| C | 4.54931200 | 0.68152400 | -1.42497200 |
| C | 3.89347500 | 3.08335000 | -1.86731400 |
| C | 4.67523200 | 2.38953100 | 0.43621800 |
| H | 4.53779600 | -0.14487400 | -0.70711100 |
| H | 4.01371200 | 0.35375400 | -2.31960100 |
| H | 5.58945500 | 0.89233200 | -1.69500300 |
| H | 3.43158200 | 3.98579400 | -1.45647000 |
| H | 4.92141700 | 3.32196300 | -2.16075800 |
| H | 3.34061000 | 2.78643100 | -2.76513400 |
| H | 5.72032900 | 2.58869500 | 0.17609900 |
| H | 4.24274900 | 3.29779600 | 0.86272600 |
| H | 4.65735300 | 1.61126500 | 1.20671500 |
| C | -2.46096000 | -0.96142900 | 0.18733100 |
| O | -1.78937700 | -0.42100400 | -0.80435100 |
| O | -2.04891100 | -1.16197000 | 1.32239700 |
| C | -3.90236300 | -1.31848500 | -0.24483200 |
| C | -4.58720600 | -0.04214900 | -0.77097600 |
| C | -3.82708300 | -2.37273400 | -1.36549500 |
| C | -4.66984000 | -1.87278400 | 0.96064900 |
| H | -4.60424900 | 0.73826900 | -0.00083600 |
| H | -4.05883300 | 0.35117500 | -1.64332700 |
| H | -5.62386200 | -0.25865500 | -1.05625400 |
| H | -3.33642000 | -3.28584400 | -1.00740200 |
| H | -4.83524500 | -2.64293700 | -1.70260700 |
| H | -3.26045300 | -1.99128900 | -2.21941000 |
| H | -5.69415700 | -2.13179500 | 0.66616400 |
| H | -4.18307300 | -2.76800800 | 1.35775400 |
| H | -4.71348800 | -1.13730400 | 1.76947000 |
| C | 0.67355500 | -2.01425800 | -1.18282500 |
| O | 0.53390100 | -1.59146300 | 0.01429900 |
| O | 0.40740200 | -1.16574700 | -2.09603300 |
| C | 1.09991600 | -3.43984600 | -1.44917100 |
| C | 1.34479000 | -3.65594800 | -2.94713500 |
| C | 2.38037900 | -3.70932800 | -0.63302600 |
| C | -0.04568600 | -4.34592900 | -0.94510800 |
| H | 0.44344300 | -3.44355800 | -3.52928800 |
| H | 2.14287100 | -3.00364700 | -3.31577100 |
| H | 1.63806500 | -4.69642300 | -3.12639300 |
| H | 2.21339800 | -3.51554100 | 0.42983600 |
| H | 2.68727400 | -4.75345500 | -0.76113100 |

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|---|-------------|-------------|-------------|
| H | 3.20175500 | -3.06725200 | -0.97168600 |
| H | 0.23121800 | -5.39814900 | -1.07544700 |
| H | -0.24868800 | -4.16015300 | 0.11334500 |
| H | -0.96637800 | -4.16055600 | -1.50927700 |

int15(quartet)

| | | | |
|----|-------------|-------------|-------------|
| C | -2.87259000 | -0.48443300 | 3.65212300 |
| C | -2.49223100 | 0.05694900 | 2.41317300 |
| C | -1.40937100 | -0.52450100 | 1.80040500 |
| C | -0.65525200 | -1.56632400 | 2.29343600 |
| C | -1.04471300 | -2.07908000 | 3.54416700 |
| C | -2.14661600 | -1.54420000 | 4.20888200 |
| H | -3.72604700 | -0.06990900 | 4.18317400 |
| H | -3.01880300 | 0.89694700 | 1.97057000 |
| H | -0.84439400 | -2.15275200 | -0.50928800 |
| H | -0.46197300 | -2.89194000 | 3.96690000 |
| H | -2.44181700 | -1.95002600 | 5.17196500 |
| C | 0.52119900 | -2.14905200 | 1.58417900 |
| O | 1.27848600 | -2.92634100 | 2.15627900 |
| N | 0.60416300 | -1.77794900 | 0.23881900 |
| C | 1.67189200 | -2.14169500 | -0.51228200 |
| C | 2.80934700 | -2.91699100 | -0.18879400 |
| C | 3.80880000 | -3.11988500 | -1.12299200 |
| H | 2.85117400 | -3.32965900 | 0.80723800 |
| C | 2.61459400 | -1.79372300 | -2.70825900 |
| C | 3.72032800 | -2.55422900 | -2.40521600 |
| H | 4.67281800 | -3.71941200 | -0.85368000 |
| H | 2.43422400 | -1.29175700 | -3.64910200 |
| H | 4.49626700 | -2.69037500 | -3.14852000 |
| N | 1.63277400 | -1.62607900 | -1.79530900 |
| O | 0.57242300 | -0.87970600 | -2.14299600 |
| Co | 0.05436500 | 0.28998000 | -0.73455800 |
| C | -2.41201700 | -1.22455500 | -1.09117000 |
| O | -1.79534300 | -2.34412500 | -0.83095300 |
| O | -1.85670200 | -0.10980900 | -1.08054200 |
| C | -3.89541300 | -1.35072900 | -1.39678600 |
| C | -4.50090900 | 0.04076800 | -1.62335500 |
| C | -4.05069300 | -2.22112200 | -2.66214400 |
| C | -4.56869600 | -2.04162800 | -0.19062700 |
| H | -4.39384800 | 0.66667200 | -0.73226500 |
| H | -4.01304600 | 0.55730600 | -2.45466900 |
| H | -5.56753800 | -0.05896900 | -1.85069100 |
| H | -3.61286200 | -3.21221000 | -2.51601500 |
| H | -5.11499800 | -2.34083000 | -2.89122100 |
| H | -3.56736500 | -1.75060600 | -3.52555700 |
| H | -5.64484100 | -2.12485700 | -0.37677400 |
| H | -4.16195700 | -3.04359700 | -0.03230500 |
| H | -4.42029700 | -1.46354300 | 0.72751200 |
| C | 2.32436300 | 0.85699400 | 0.74782200 |
| O | 1.81867400 | 0.79087500 | -0.47194200 |
| O | 1.76744300 | 0.50066400 | 1.77139000 |
| C | 3.75221700 | 1.45445300 | 0.72399700 |
| C | 4.62377000 | 0.64164500 | -0.25129000 |
| C | 3.64729600 | 2.91575400 | 0.24614600 |
| C | 4.33828100 | 1.39321900 | 2.13923200 |
| H | 4.66597800 | -0.41211500 | 0.04636400 |
| H | 4.22764000 | 0.69258300 | -1.26880100 |
| H | 5.64753000 | 1.03446500 | -0.25441300 |
| H | 3.01034800 | 3.50168100 | 0.91860200 |
| H | 4.64166200 | 3.37806500 | 0.23272300 |
| H | 3.22255700 | 2.96718800 | -0.76025400 |
| H | 5.34871400 | 1.81927500 | 2.14013900 |
| H | 3.71949700 | 1.95380300 | 2.84485400 |
| H | 4.39409900 | 0.36101900 | 2.49781000 |

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|---|-------------|------------|-------------|
| C | -0.70205200 | 2.60363200 | -0.62862000 |
| O | -0.47844100 | 1.78544400 | 0.35388700 |
| O | -0.48157800 | 2.21617900 | -1.79614900 |
| C | -1.20967500 | 3.99614800 | -0.27218900 |
| C | -1.50119900 | 4.79212800 | -1.54977000 |
| C | -2.48855200 | 3.83732100 | 0.57432600 |
| C | -0.11345400 | 4.69132400 | 0.56310700 |
| H | -0.60326900 | 4.88945000 | -2.16648000 |
| H | -2.26816800 | 4.29935000 | -2.15510100 |
| H | -1.85585400 | 5.79564300 | -1.28791700 |
| H | -2.28174400 | 3.27086200 | 1.48642100 |
| H | -2.87591200 | 4.82372600 | 0.85381700 |
| H | -3.26918700 | 3.31303000 | 0.01016700 |
| H | -0.44752100 | 5.69384500 | 0.85406600 |
| H | 0.10896900 | 4.11751700 | 1.46711600 |
| H | 0.81189700 | 4.79428200 | -0.01468500 |

int15(sextet)

| | | | |
|----|-------------|-------------|-------------|
| C | -0.32876900 | 2.09980400 | 3.83425200 |
| C | 0.36181000 | 1.75414800 | 2.66237400 |
| C | -0.17932500 | 0.73922100 | 1.91145700 |
| C | -1.33302500 | 0.04421900 | 2.21251400 |
| C | -2.00936800 | 0.40587100 | 3.39320800 |
| C | -1.50598800 | 1.42841900 | 4.19290800 |
| H | 0.05145300 | 2.89952900 | 4.46525500 |
| H | 1.26607900 | 2.25958500 | 2.34327800 |
| H | -1.98581200 | 0.16707600 | -2.23859600 |
| H | -2.91886000 | -0.12786700 | 3.65244100 |
| H | -2.02986200 | 1.70876300 | 5.10186800 |
| C | -1.86986100 | -1.02741900 | 1.34599400 |
| O | -2.90029100 | -1.63928200 | 1.60877900 |
| N | -1.14148000 | -1.21341300 | 0.15729200 |
| C | -1.42928700 | -2.26910000 | -0.64207600 |
| C | -1.91035000 | -3.53904700 | -0.26368700 |
| C | -2.05019600 | -4.54509200 | -1.20082200 |
| H | -2.15001200 | -3.68783500 | 0.77830600 |
| C | -1.24304300 | -3.05590300 | -2.89895100 |
| C | -1.70930800 | -4.30332200 | -2.54024600 |
| H | -2.41093100 | -5.52179700 | -0.89599800 |
| H | -0.95020000 | -2.76013200 | -3.89707500 |
| H | -1.79895300 | -5.07155900 | -3.29914200 |
| N | -1.11979300 | -2.07532100 | -1.97469500 |
| O | -0.68988500 | -0.88130600 | -2.38473500 |
| Co | 0.31722200 | 0.13974400 | -0.82386300 |
| C | -2.32393600 | 1.60282700 | -1.03630400 |
| O | -2.76035100 | 0.72809800 | -1.92781800 |
| O | -1.13232700 | 1.70095800 | -0.72868100 |
| C | -3.40828800 | 2.46889900 | -0.41422100 |
| C | -2.79315700 | 3.35490800 | 0.67730200 |
| C | -4.03382100 | 3.33511100 | -1.52877000 |
| C | -4.48291400 | 1.54055400 | 0.19347600 |
| H | -2.35444600 | 2.75240400 | 1.47674800 |
| H | -2.00543200 | 3.99522700 | 0.27091000 |
| H | -3.57294800 | 3.99150200 | 1.10954600 |
| H | -4.46131500 | 2.71401400 | -2.32096300 |
| H | -4.83171200 | 3.95322700 | -1.10327400 |
| H | -3.28824800 | 4.00284400 | -1.97486900 |
| H | -5.26362300 | 2.15219700 | 0.65865000 |
| H | -4.94414600 | 0.91241600 | -0.57300000 |
| H | -4.05932100 | 0.88782500 | 0.96303300 |
| C | 1.62515800 | -1.94387200 | 0.74100700 |
| O | 1.65719000 | -1.36005300 | -0.37400900 |
| O | 0.58174600 | -2.25320300 | 1.38890300 |
| C | 2.97630400 | -2.23223400 | 1.44451300 |

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|---|------------|-------------|-------------|
| C | 4.05571300 | -2.49399700 | 0.38576300 |
| C | 3.28769100 | -0.92635500 | 2.21176100 |
| C | 2.86368600 | -3.41319500 | 2.41653100 |
| H | 3.83643000 | -3.40017000 | -0.19036900 |
| H | 4.12696400 | -1.65764400 | -0.31243900 |
| H | 5.02533100 | -2.63159200 | 0.87896100 |
| H | 2.53668500 | -0.74234800 | 2.98704500 |
| H | 4.27013200 | -1.01037900 | 2.69187000 |
| H | 3.28777500 | -0.06803700 | 1.53375400 |
| H | 3.82117900 | -3.56434300 | 2.92828000 |
| H | 2.09196200 | -3.23354700 | 3.16955500 |
| H | 2.61242300 | -4.33982300 | 1.88797800 |
| C | 2.25186500 | 1.67929400 | -1.05452300 |
| O | 1.86729700 | 1.45829900 | 0.13064500 |
| O | 1.60635100 | 1.17582600 | -2.03397800 |
| C | 3.52254600 | 2.48537500 | -1.32965600 |
| C | 3.29302100 | 3.40703300 | -2.53904500 |
| C | 3.91830900 | 3.30510200 | -0.09443200 |
| C | 4.62834300 | 1.45782000 | -1.65842200 |
| H | 2.98156600 | 2.82912800 | -3.41238400 |
| H | 2.51174800 | 4.14589700 | -2.32557700 |
| H | 4.21537400 | 3.94843100 | -2.78141600 |
| H | 4.08556500 | 2.65786700 | 0.77074500 |
| H | 4.83899900 | 3.86603100 | -0.29490400 |
| H | 3.13217100 | 4.02048400 | 0.17046100 |
| H | 5.56972500 | 1.97471200 | -1.87991100 |
| H | 4.79935600 | 0.78414600 | -0.81091500 |
| H | 4.34811400 | 0.85271900 | -2.52599900 |

int16(doublet)

| | | | |
|----|-------------|-------------|-------------|
| C | -0.94067300 | 1.41512400 | 3.61717300 |
| C | -1.54730000 | 0.27248500 | 4.15705400 |
| C | -1.63963000 | -0.88566300 | 3.39304800 |
| C | -1.13272100 | -0.87767800 | 2.08698000 |
| C | -0.54674700 | 0.27451000 | 1.53555000 |
| C | -0.43538300 | 1.42473700 | 2.31191400 |
| H | -0.85376200 | 2.31217600 | 4.22544000 |
| H | -1.93264300 | 0.28943100 | 5.17233300 |
| H | -2.08548200 | -1.79608800 | 3.78260100 |
| H | 0.07120200 | 2.29810500 | 1.92025700 |
| C | -1.18414300 | -2.07162200 | 1.23334800 |
| O | -1.69876000 | -3.14576000 | 1.49365300 |
| N | -0.56202200 | -1.76943100 | -0.01866700 |
| C | -0.48220900 | -2.60685100 | -1.05865800 |
| C | -0.78828900 | -3.98787100 | -1.10322200 |
| C | 0.17634200 | -2.70209600 | -3.36829600 |
| C | -0.61112100 | -4.69733300 | -2.27149200 |
| H | -1.15656100 | -4.43435600 | -0.19119000 |
| C | -0.12060500 | -4.04536900 | -3.41961400 |
| H | 0.55710900 | -2.11171600 | -4.19044000 |
| H | -0.84316600 | -5.75631900 | -2.30277700 |
| H | 0.03228200 | -4.57955700 | -4.35024200 |
| O | 0.28040600 | -0.72248600 | -2.20652400 |
| N | -0.00019500 | -1.99503600 | -2.21858200 |
| Co | -0.06186400 | 0.02565700 | -0.28660200 |
| O | 0.37209300 | 1.81992600 | -0.80047000 |
| C | 1.49412800 | 2.48253400 | -0.49652100 |
| O | 1.86522000 | 2.72005300 | 0.64054800 |
| C | 2.26261900 | 2.95998100 | -1.73911800 |
| C | 2.68882900 | 1.72324700 | -2.55621100 |
| C | 1.32188600 | 3.83763900 | -2.58873900 |
| C | 3.49570700 | 3.76390000 | -1.31043000 |
| H | 3.33954500 | 1.06924600 | -1.96735500 |
| H | 1.81997000 | 1.13910300 | -2.86707100 |

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|---|-------------|-------------|-------------|
| H | 3.23995900 | 2.04461300 | -3.44865800 |
| H | 0.99741000 | 4.72498500 | -2.03163800 |
| H | 1.84219200 | 4.17946300 | -3.49124400 |
| H | 0.43445300 | 3.27494900 | -2.89165900 |
| H | 4.03580100 | 4.12120200 | -2.19534000 |
| H | 3.21313500 | 4.62845400 | -0.70231900 |
| H | 4.17722500 | 3.15021200 | -0.71379000 |
| O | 1.72480200 | -0.22013600 | 0.18265400 |
| C | 2.15457800 | -1.18211000 | 0.92429600 |
| O | 1.54736100 | -2.23842000 | 1.16623600 |
| C | 3.50771100 | -0.89152200 | 1.60776000 |
| C | 4.44699500 | -0.15136500 | 0.64319700 |
| C | 3.15597700 | 0.03218700 | 2.79705500 |
| C | 4.14495200 | -2.19517600 | 2.10145000 |
| H | 4.65302400 | -0.74961800 | -0.25223000 |
| H | 4.01120000 | 0.80042100 | 0.33469700 |
| H | 5.40194800 | 0.04742200 | 1.14396100 |
| H | 2.46182800 | -0.46242000 | 3.48551800 |
| H | 4.07018300 | 0.27994500 | 3.34955900 |
| H | 2.69599500 | 0.95773400 | 2.44028400 |
| H | 5.07867600 | -1.97371900 | 2.63109100 |
| H | 3.47474300 | -2.72853500 | 2.78042500 |
| H | 4.37763900 | -2.86397800 | 1.26524500 |
| O | -1.96459700 | 0.34928500 | -0.74083900 |
| C | -4.07946500 | 1.40999800 | -0.30943400 |
| C | -4.74311100 | 2.63341800 | -0.96258300 |
| C | -4.69254600 | 0.10667200 | -0.84026300 |
| C | -4.23481300 | 1.47531700 | 1.23189800 |
| H | -4.31377400 | 3.56560000 | -0.58807100 |
| H | -4.62232900 | 2.61413600 | -2.05157600 |
| H | -5.81565900 | 2.62924800 | -0.74055400 |
| H | -4.23571800 | -0.76639700 | -0.36754200 |
| H | -5.76685300 | 0.09627700 | -0.62831800 |
| H | -4.55625000 | 0.01677100 | -1.92335400 |
| H | -5.29999200 | 1.45608200 | 1.48737000 |
| H | -3.74646000 | 0.62285600 | 1.71484400 |
| H | -3.79497400 | 2.39299400 | 1.63256700 |
| O | -1.99238100 | 2.57738000 | -0.46942500 |
| H | -0.97407800 | 2.42735600 | -0.58203900 |
| C | -2.58015900 | 1.42019000 | -0.55221600 |

int16(quartet)

| | | | |
|---|-------------|-------------|-------------|
| C | -1.63003300 | 1.39979200 | 3.38871700 |
| C | -1.91401500 | 0.18280200 | 4.02090000 |
| C | -1.62184600 | -1.02159700 | 3.38723600 |
| C | -1.05005200 | -1.00086000 | 2.10883200 |
| C | -0.80157600 | 0.22909100 | 1.50421500 |
| C | -1.06399000 | 1.44378400 | 2.10512500 |
| H | -1.83860200 | 2.33599700 | 3.89963500 |
| H | -2.35699600 | 0.18026600 | 5.01223300 |
| H | -1.82453200 | -1.98305400 | 3.85007500 |
| H | -0.79878200 | 2.38305100 | 1.62886300 |
| C | -0.71198100 | -2.23251000 | 1.36785000 |
| O | -0.88002300 | -3.37506900 | 1.76822300 |
| N | -0.16820900 | -1.87766600 | 0.12193300 |
| C | 0.17725900 | -2.74610800 | -0.83648500 |
| C | 0.19898600 | -4.15886300 | -0.81020700 |
| C | 1.00532600 | -2.79588200 | -3.09416200 |
| C | 0.63599700 | -4.85792000 | -1.91529300 |
| H | -0.11640100 | -4.63954300 | 0.10414800 |
| C | 1.05082400 | -4.16997500 | -3.07262600 |

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|----|-------------|-------------|-------------|
| H | 1.29509100 | -2.16819300 | -3.92559000 |
| H | 0.66760800 | -5.94199700 | -1.88867100 |
| H | 1.40567300 | -4.69941900 | -3.94876900 |
| O | 0.51554900 | -0.80113900 | -2.06113000 |
| N | 0.57107400 | -2.11177400 | -2.00620300 |
| Co | 0.00975900 | 0.02688800 | -0.31624100 |
| O | -0.10640900 | 1.87708700 | -0.97072900 |
| C | 0.67334000 | 2.89459400 | -0.59606500 |
| O | 0.50761200 | 3.51576400 | 0.44353900 |
| C | 1.72154700 | 3.30469200 | -1.64375900 |
| C | 2.51357800 | 2.08573100 | -2.14612500 |
| C | 0.93547900 | 3.92326900 | -2.82205700 |
| C | 2.67320600 | 4.34526100 | -1.04070500 |
| H | 3.08935800 | 1.63127700 | -1.33666800 |
| H | 1.85145200 | 1.32065400 | -2.55769500 |
| H | 3.21140500 | 2.40319100 | -2.93076400 |
| H | 0.35539100 | 4.79430400 | -2.49555900 |
| H | 1.63175900 | 4.25228200 | -3.60241800 |
| H | 0.24804600 | 3.19092100 | -3.25631200 |
| H | 3.39317200 | 4.67673000 | -1.79825900 |
| H | 2.12404700 | 5.21592000 | -0.67265300 |
| H | 3.22961600 | 3.92232700 | -0.19839100 |
| O | 1.71139100 | 0.37107000 | 0.50163100 |
| C | 2.65705300 | -0.53086700 | 0.62312300 |
| O | 2.71286600 | -1.57740500 | -0.01805800 |
| C | 3.69491700 | -0.16508000 | 1.70364700 |
| C | 4.19601100 | 1.27195100 | 1.47434500 |
| C | 2.96324300 | -0.24611500 | 3.06087500 |
| C | 4.86204300 | -1.15731000 | 1.66662300 |
| H | 4.71793900 | 1.35796500 | 0.51388800 |
| H | 3.36374400 | 1.98024600 | 1.47713900 |
| H | 4.90176500 | 1.55349300 | 2.26513000 |
| H | 2.56989500 | -1.25487600 | 3.23539900 |
| H | 3.65729000 | -0.00795500 | 3.87577900 |
| H | 2.12866800 | 0.45996700 | 3.09561400 |
| H | 5.58949200 | -0.91091800 | 2.44917300 |
| H | 4.51224800 | -2.18152800 | 1.82356600 |
| H | 5.37274000 | -1.12644800 | 0.69876000 |
| O | -2.13524100 | -0.13208700 | -0.91356200 |
| C | -4.44167000 | 0.46302700 | -0.50094100 |
| C | -5.34216300 | 1.48719200 | -1.21158000 |
| C | -4.76574800 | -0.96303100 | -0.96620700 |
| C | -4.62473700 | 0.57023800 | 1.03332200 |
| H | -5.11941500 | 2.50548800 | -0.88440000 |
| H | -5.21124000 | 1.44126700 | -2.29852800 |
| H | -6.39237700 | 1.26998900 | -0.98755100 |
| H | -4.13520500 | -1.69687100 | -0.45768100 |
| H | -5.81438900 | -1.19187300 | -0.74764900 |
| H | -4.60814300 | -1.07295400 | -2.04441000 |
| H | -5.66681700 | 0.35076400 | 1.29087500 |
| H | -3.98226800 | -0.14421700 | 1.55835400 |
| H | -4.38160300 | 1.57537600 | 1.38920800 |
| O | -2.65384800 | 2.04092100 | -0.72128300 |
| H | -1.63699200 | 2.11330600 | -0.82023400 |
| C | -2.97289300 | 0.77003600 | -0.75797500 |

int16(sextet)

| | | | |
|---|-------------|-------------|------------|
| C | -1.27618700 | 1.74715600 | 3.43662500 |
| C | -1.94858600 | 0.63028400 | 3.95190700 |
| C | -1.98209600 | -0.56799600 | 3.24290100 |
| C | -1.33822000 | -0.65332900 | 1.99508100 |
| C | -0.70400100 | 0.48260000 | 1.52610700 |
| C | -0.62651300 | 1.68456200 | 2.19321100 |
| H | -1.25136100 | 2.67378500 | 4.00462200 |

| | | | |
|----|-------------|-------------|-------------|
| H | -2.44285600 | 0.69836800 | 4.91651400 |
| H | -2.49009300 | -1.44737200 | 3.62726700 |
| H | -0.08052200 | 2.52562200 | 1.77385600 |
| C | -1.35274900 | -1.91723200 | 1.22278400 |
| O | -1.97053800 | -2.91091400 | 1.58130900 |
| N | -0.62043600 | -1.82342700 | 0.01830800 |
| C | -0.45279300 | -2.86801000 | -0.80416000 |
| C | -0.72423200 | -4.23951900 | -0.58509100 |
| C | 0.39801500 | -3.43415000 | -2.98314600 |
| C | -0.43792100 | -5.17746200 | -1.55664900 |
| H | -1.16437700 | -4.50190400 | 0.36497900 |
| C | 0.13126300 | -4.77076800 | -2.77442600 |
| H | 0.83581300 | -3.01769400 | -3.88002200 |
| H | -0.64861100 | -6.22591300 | -1.37469500 |
| H | 0.36946200 | -5.48177200 | -3.55689100 |
| O | 0.38833800 | -1.25508200 | -2.28633300 |
| N | 0.11427600 | -2.51261300 | -2.03017200 |
| Co | 0.06828200 | 0.03618500 | -0.76650200 |
| O | 0.43827600 | 1.91569300 | -1.22806100 |
| C | 1.48647800 | 2.60499500 | -0.77636200 |
| O | 1.46536200 | 3.21430600 | 0.28389800 |
| C | 2.67899100 | 2.68018300 | -1.74305900 |
| C | 2.95093300 | 1.32280900 | -2.41342500 |
| C | 2.28480300 | 3.71305700 | -2.82352500 |
| C | 3.92302400 | 3.16340100 | -0.98690300 |
| H | 3.17673200 | 0.55431500 | -1.66957500 |
| H | 2.08789200 | 0.98682300 | -2.99487100 |
| H | 3.80746200 | 1.41335900 | -3.09249500 |
| H | 2.09065200 | 4.69422100 | -2.37596700 |
| H | 3.09804100 | 3.82338100 | -3.55066700 |
| H | 1.38488700 | 3.39091100 | -3.35746200 |
| H | 4.76474500 | 3.27857900 | -1.67997100 |
| H | 3.73486700 | 4.12163500 | -0.49659800 |
| H | 4.21227700 | 2.44651800 | -0.21150800 |
| O | 1.79338200 | -0.10827900 | 0.27197700 |
| C | 2.05410200 | -0.98783900 | 1.15996800 |
| O | 1.40035900 | -2.03557900 | 1.36404700 |
| C | 3.26643300 | -0.67571200 | 2.06992600 |
| C | 4.51036700 | -0.53874300 | 1.17394700 |
| C | 2.96159600 | 0.66903600 | 2.76201500 |
| C | 3.47316600 | -1.78264400 | 3.10958100 |
| H | 4.73168300 | -1.47921600 | 0.65537500 |
| H | 4.36829300 | 0.24371900 | 0.42503800 |
| H | 5.38081600 | -0.27900800 | 1.78782400 |
| H | 2.07229800 | 0.58943400 | 3.39723600 |
| H | 3.80907800 | 0.95364800 | 3.39717800 |
| H | 2.78296500 | 1.45925700 | 2.02877900 |
| H | 4.32754300 | -1.53401100 | 3.74982200 |
| H | 2.58874600 | -1.89871100 | 3.74278200 |
| H | 3.67031200 | -2.74686700 | 2.63074900 |
| O | -2.01176000 | 0.41294200 | -1.10151600 |
| C | -4.08495200 | 1.53338600 | -0.55387800 |
| C | -4.74355500 | 2.63617100 | -1.40409500 |
| C | -4.72161900 | 0.16863400 | -0.84593800 |
| C | -4.22738100 | 1.86997900 | 0.94935700 |
| H | -4.29102600 | 3.61079500 | -1.20531600 |
| H | -4.64455400 | 2.42223700 | -2.47447000 |
| H | -5.81182400 | 2.69194100 | -1.16772000 |
| H | -4.26476200 | -0.61794100 | -0.23905900 |
| H | -5.79198400 | 0.20728400 | -0.61633900 |
| H | -4.60439600 | -0.10785000 | -1.89860800 |
| H | -5.29094000 | 1.92070900 | 1.20794900 |
| H | -3.75902800 | 1.10216400 | 1.57286300 |
| H | -3.76345000 | 2.83172400 | 1.18307300 |

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|---|-------------|------------|-------------|
| O | -1.97360600 | 2.63315800 | -0.77034500 |
| H | -0.96712900 | 2.47874900 | -0.91858900 |
| C | -2.59280900 | 1.48454900 | -0.85047000 |

int17(doublet)

| | | | |
|----|-------------|-------------|-------------|
| C | -1.19406000 | 3.52428500 | 1.69321000 |
| C | -0.42814100 | 3.36018300 | 2.85697600 |
| C | 0.29551300 | 2.18880800 | 3.05105000 |
| C | 0.24130800 | 1.18945600 | 2.07094300 |
| C | -0.53395600 | 1.34698500 | 0.91142700 |
| C | -1.25073900 | 2.52379600 | 0.71733200 |
| H | -1.75050900 | 4.44699000 | 1.54620500 |
| H | -0.39807300 | 4.15021900 | 3.60152800 |
| H | 0.90484500 | 2.03266700 | 3.93634800 |
| H | -1.83934000 | 2.66365100 | -0.18327000 |
| C | 0.99272900 | -0.06781900 | 2.18997700 |
| O | 1.67137700 | -0.44416600 | 3.12898000 |
| N | 0.77487500 | -0.84192200 | 1.00255700 |
| C | 1.25230300 | -2.07314900 | 0.77983300 |
| C | 2.12865100 | -2.84106300 | 1.58112500 |
| C | 1.20327600 | -3.84972900 | -0.83598300 |
| C | 2.52128500 | -4.09557900 | 1.16529000 |
| H | 2.46020600 | -2.39301000 | 2.50656700 |
| C | 2.05187300 | -4.60690400 | -0.05986500 |
| H | 0.79171200 | -4.14802900 | -1.79048500 |
| H | 3.19362900 | -4.68408200 | 1.78004900 |
| H | 2.34584200 | -5.58899600 | -0.41172400 |
| O | 0.01288800 | -1.91526900 | -1.19294100 |
| N | 0.81195100 | -2.61183700 | -0.42967600 |
| Co | -0.41371000 | -0.13959000 | -0.24827300 |
| O | -1.97677400 | 0.34219800 | -1.32730500 |
| C | -2.70043200 | -0.33862000 | -0.52606000 |
| O | -2.08577400 | -0.89366900 | 0.44760900 |
| C | -4.20372800 | -0.42866700 | -0.69770300 |
| C | -4.77016800 | 0.96974900 | -0.36140300 |
| C | -4.51455500 | -0.77905100 | -2.16457500 |
| C | -4.78694400 | -1.48231400 | 0.25302500 |
| H | -4.51521400 | 1.26191000 | 0.66328900 |
| H | -4.37106100 | 1.72511900 | -1.04483400 |
| H | -5.86187000 | 0.95680400 | -0.45437500 |
| H | -4.12334700 | -1.76941600 | -2.42308400 |
| H | -5.59903300 | -0.78831900 | -2.32149700 |
| H | -4.06692100 | -0.04797700 | -2.84275300 |
| H | -5.87515300 | -1.52544500 | 0.13213700 |
| H | -4.37700400 | -2.47509500 | 0.04151400 |
| H | -4.56170100 | -1.24217800 | 1.29580400 |
| O | 0.82896600 | 0.79128000 | -1.28121300 |
| C | 2.05879900 | 0.98729700 | -0.94516800 |
| O | 2.63602400 | 0.48276300 | 0.03038800 |
| C | 2.80213300 | 1.98681000 | -1.86081200 |
| C | 2.61909600 | 1.55798700 | -3.32682900 |
| C | 2.14483100 | 3.36257600 | -1.62536300 |
| C | 4.29011900 | 2.03696900 | -1.49536900 |
| H | 3.07072400 | 0.57556700 | -3.50858100 |
| H | 1.55982800 | 1.50114900 | -3.58783100 |
| H | 3.10887700 | 2.28197500 | -3.98904300 |
| H | 2.23324000 | 3.66511400 | -0.57576700 |
| H | 2.64045400 | 4.12128300 | -2.24272000 |
| H | 1.08324500 | 3.33414100 | -1.88478100 |
| H | 4.80562700 | 2.75900100 | -2.13942500 |
| H | 4.43093100 | 2.33622500 | -0.45312300 |
| H | 4.76363700 | 1.05883500 | -1.62744800 |

int17(quartet)

| | | | |
|----|-------------|-------------|-------------|
| C | -2.01171500 | 3.05419400 | 2.07231600 |
| C | -1.37669400 | 2.84789000 | 3.30395000 |
| C | -0.47558600 | 1.79807100 | 3.46535900 |
| C | -0.21191100 | 0.95374700 | 2.38225300 |
| C | -0.85876900 | 1.18454900 | 1.17019300 |
| C | -1.76515000 | 2.21129000 | 0.98015700 |
| H | -2.70595500 | 3.88209200 | 1.95501700 |
| H | -1.59051100 | 3.51102500 | 4.13670200 |
| H | 0.02806100 | 1.60931800 | 4.40894800 |
| H | -2.24841500 | 2.36321100 | 0.02309800 |
| C | 0.71904800 | -0.19580600 | 2.45432200 |
| O | 1.35036900 | -0.54822500 | 3.43896900 |
| N | 0.75582100 | -0.81423600 | 1.19726400 |
| C | 1.41822600 | -1.95089700 | 0.90209000 |
| C | 2.27168300 | -2.72626600 | 1.71188900 |
| C | 1.77437800 | -3.47649800 | -0.91292500 |
| C | 2.87124600 | -3.85521200 | 1.18806700 |
| H | 2.43689100 | -2.38671200 | 2.72405800 |
| C | 2.62465200 | -4.23655500 | -0.14267700 |
| H | 1.51107200 | -3.67382500 | -1.94293500 |
| H | 3.53917400 | -4.44482600 | 1.80722100 |
| H | 3.08857800 | -5.11395000 | -0.57697000 |
| O | 0.36149400 | -1.67151200 | -1.15187300 |
| N | 1.18903400 | -2.37164600 | -0.39180200 |
| Co | -0.24711000 | -0.03375900 | -0.25081400 |
| O | -1.93031800 | 0.33116800 | -1.33402800 |
| C | -2.67064100 | -0.52915200 | -0.72964900 |
| O | -2.19754600 | -1.17363900 | 0.24080500 |
| C | -4.11083800 | -0.71011200 | -1.20870800 |
| C | -4.82999900 | 0.64400200 | -1.03768000 |
| C | -4.07864500 | -1.09790300 | -2.69989400 |
| C | -4.81407400 | -1.79547000 | -0.38442000 |
| H | -4.82579600 | 0.96184600 | 0.01161900 |
| H | -4.34424100 | 1.42015400 | -1.63595400 |
| H | -5.87346300 | 0.55560300 | -1.36096600 |
| H | -3.56219600 | -2.05363500 | -2.84478100 |
| H | -5.10132200 | -1.20266600 | -3.08056700 |
| H | -3.55992300 | -0.33629900 | -3.28813600 |
| H | -5.84699800 | -1.91429700 | -0.73184600 |
| H | -4.30236900 | -2.75755500 | -0.48213600 |
| H | -4.83177900 | -1.53550800 | 0.67796800 |
| O | 0.86417600 | 1.23133000 | -1.07358400 |
| C | 2.17750600 | 1.07671500 | -1.17542000 |
| O | 2.77527200 | 0.05124200 | -0.87671700 |
| C | 2.88488100 | 2.34032800 | -1.69522200 |
| C | 2.27785900 | 2.72711400 | -3.05744900 |
| C | 2.63593700 | 3.46921000 | -0.67386000 |
| C | 4.38709400 | 2.06999500 | -1.83573800 |
| H | 2.43354700 | 1.93245300 | -3.79637900 |
| H | 1.20307600 | 2.90590500 | -2.96975500 |
| H | 2.75694800 | 3.63838200 | -3.43499000 |
| H | 3.05388300 | 3.21027800 | 0.30630100 |
| H | 3.11693700 | 4.39436800 | -1.01279200 |
| H | 1.56526700 | 3.65505900 | -0.55198700 |
| H | 4.89633600 | 2.97034300 | -2.19929100 |
| H | 4.82727300 | 1.78391100 | -0.87605200 |
| H | 4.57541900 | 1.25566700 | -2.54196500 |

int17(sextet)

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|---|-------------|-------------|------------|
| C | 1.01012000 | -3.43285200 | 1.96710100 |
| C | -0.00701000 | -3.27613200 | 2.91954700 |
| C | -0.77688100 | -2.11749200 | 2.94513300 |
| C | -0.53185800 | -1.10584400 | 2.00094500 |
| C | 0.48071700 | -1.29528300 | 1.07458500 |

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|----|-------------|-------------|-------------|
| C | 1.26787200 | -2.42954000 | 1.02310000 |
| H | 1.60277200 | -4.34436600 | 1.95531100 |
| H | -0.19410400 | -4.06542100 | 3.64156500 |
| H | -1.56842600 | -1.97163900 | 3.67408000 |
| H | 2.04236000 | -2.54285300 | 0.27197900 |
| C | -1.33211000 | 0.13770700 | 1.98758800 |
| O | -2.16553100 | 0.42178300 | 2.83554900 |
| N | -0.98881000 | 0.95186800 | 0.88170000 |
| C | -1.55048400 | 2.14380100 | 0.65420700 |
| C | -2.52147600 | 2.84853000 | 1.40622600 |
| C | -1.51574800 | 3.96340300 | -0.92260600 |
| C | -2.96162200 | 4.08975900 | 0.99382900 |
| H | -2.88573600 | 2.36504400 | 2.30028900 |
| C | -2.45120800 | 4.65789700 | -0.18567400 |
| H | -1.06833200 | 4.30548500 | -1.84576100 |
| H | -3.70215200 | 4.62284100 | 1.58052400 |
| H | -2.77696400 | 5.63069400 | -0.53507000 |
| O | -0.21512100 | 2.11106600 | -1.26548400 |
| N | -1.08306000 | 2.74365100 | -0.51831800 |
| Co | 0.51706800 | 0.36476400 | -0.52110100 |
| O | 2.34820600 | -0.30162600 | -1.22804400 |
| C | 2.94847300 | 0.47754400 | -0.40665200 |
| O | 2.25315000 | 1.23055300 | 0.34542500 |
| C | 4.47145900 | 0.46354400 | -0.33772700 |
| C | 4.90364900 | -0.96899000 | 0.04067500 |
| C | 5.01698600 | 0.81556800 | -1.73659700 |
| C | 4.97782600 | 1.46712400 | 0.70550900 |
| H | 4.50006100 | -1.25562500 | 1.01872300 |
| H | 4.55123000 | -1.68891800 | -0.70323200 |
| H | 5.99693200 | -1.02548800 | 0.09329300 |
| H | 4.72327800 | 1.83050800 | -2.02854200 |
| H | 6.11203200 | 0.76757400 | -1.73183100 |
| H | 4.63668300 | 0.11847800 | -2.48801200 |
| H | 6.07333000 | 1.44473000 | 0.74054600 |
| H | 4.65935200 | 2.48481800 | 0.46081600 |
| H | 4.59297800 | 1.22949500 | 1.70154700 |
| O | -0.63215200 | -0.90772200 | -1.52327400 |
| C | -1.85554500 | -1.12734200 | -1.21219800 |
| O | -2.54531500 | -0.42996400 | -0.43779000 |
| C | -2.47212400 | -2.42296900 | -1.78775100 |
| C | -2.13015200 | -2.52591300 | -3.28226800 |
| C | -1.80011900 | -3.57468600 | -1.00779800 |
| C | -3.98992700 | -2.45065200 | -1.57332000 |
| H | -2.59937300 | -1.71454500 | -3.85076500 |
| H | -1.05033900 | -2.47355900 | -3.43801900 |
| H | -2.50098800 | -3.47707600 | -3.68266400 |
| H | -1.98795500 | -3.48505800 | 0.06806900 |
| H | -2.20419400 | -4.53550500 | -1.34837300 |
| H | -0.71846500 | -3.57050300 | -1.16581600 |
| H | -4.40353900 | -3.38680900 | -1.96635400 |
| H | -4.24128200 | -2.37753800 | -0.51179000 |
| H | -4.47781700 | -1.61782700 | -2.09061800 |

int18(doublet)

| | | | |
|---|-------------|------------|------------|
| C | -0.62792800 | 3.21326200 | 2.55201100 |
| C | 0.67886600 | 3.36179400 | 3.04153900 |
| C | 1.65446100 | 2.42820200 | 2.70980500 |
| C | 1.30702300 | 1.35021400 | 1.88454700 |
| C | -0.00365400 | 1.19353600 | 1.40300800 |
| C | -0.97443800 | 2.13463200 | 1.73227200 |
| H | -1.38214300 | 3.95202700 | 2.81279900 |
| H | 0.92680800 | 4.20828800 | 3.67514100 |
| H | 2.67631100 | 2.51663800 | 3.06692100 |
| H | -1.98370900 | 2.02624200 | 1.34990600 |

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|----|-------------|-------------|-------------|
| C | 2.28165700 | 0.32310700 | 1.48200500 |
| O | 3.43498500 | 0.20725800 | 1.85877300 |
| N | 1.63668900 | -0.58394200 | 0.58335500 |
| C | 2.17122500 | -1.70887800 | 0.09147300 |
| C | 3.48198700 | -2.20996600 | 0.26071400 |
| C | 1.64964100 | -3.59536800 | -1.29890600 |
| C | 3.85191100 | -3.39319500 | -0.34357600 |
| H | 4.15189800 | -1.62291500 | 0.87230400 |
| C | 2.92240600 | -4.09555400 | -1.13339100 |
| H | 0.86586500 | -4.05588700 | -1.88463100 |
| H | 4.85704800 | -3.77848500 | -0.21101400 |
| H | 3.18477000 | -5.02805600 | -1.61952500 |
| O | 0.07041500 | -1.97595400 | -0.90114500 |
| N | 1.27995700 | -2.42922300 | -0.70551200 |
| Co | -0.19317600 | -0.31241600 | 0.27785700 |
| O | -2.06295200 | -0.05563400 | -0.04302700 |
| C | -2.96397000 | -0.95735000 | 0.10231200 |
| O | -2.80751500 | -2.04422900 | 0.71302100 |
| C | -4.31371600 | -0.62554300 | -0.55292700 |
| C | -4.08214400 | -0.56263000 | -2.07701500 |
| C | -5.35380700 | -1.70032400 | -0.21596100 |
| C | -4.78333500 | 0.75173700 | -0.04698100 |
| H | -3.32594600 | 0.18832700 | -2.32198600 |
| H | -3.74109000 | -1.53096300 | -2.46127300 |
| H | -5.01730200 | -0.30445200 | -2.58798900 |
| H | -5.51893100 | -1.76662800 | 0.86394400 |
| H | -6.30840500 | -1.45810900 | -0.69809500 |
| H | -5.02851800 | -2.68543800 | -0.56151400 |
| H | -5.73892600 | 1.01645900 | -0.51443300 |
| H | -4.93128600 | 0.74399500 | 1.03975900 |
| H | -4.04934800 | 1.52434800 | -0.29027800 |
| C | -0.79267500 | -1.21458700 | 3.06118700 |
| H | 0.13084000 | -0.78859600 | 3.45515700 |
| H | -1.58602200 | -0.46236600 | 3.11699200 |
| H | -1.07087200 | -2.09484100 | 3.65005900 |
| O | 2.27879700 | 0.99354500 | -1.14888100 |
| C | 1.15484900 | 1.33475200 | -1.56129000 |
| O | 0.02740500 | 0.85273400 | -1.18148500 |
| C | 1.03278900 | 2.50177100 | -2.56767200 |
| C | -0.04322700 | 2.17672300 | -3.61577500 |
| C | 0.60113800 | 3.72066000 | -1.72305600 |
| C | 2.38320800 | 2.77090800 | -3.24187300 |
| H | 0.23643300 | 1.29798100 | -4.20830500 |
| H | -1.00479800 | 1.97333600 | -3.13940100 |
| H | -0.15889200 | 3.02436200 | -4.30185000 |
| H | 1.34939900 | 3.94986400 | -0.95618600 |
| H | 0.49033000 | 4.59952600 | -2.36921200 |
| H | -0.35218800 | 3.52718800 | -1.22300000 |
| H | 2.29281400 | 3.62218400 | -3.92661300 |
| H | 3.15535100 | 2.99709500 | -2.50208600 |
| H | 2.71670400 | 1.90200500 | -3.81930000 |
| O | -0.56100500 | -1.62624200 | 1.71070500 |
| H | -1.47160100 | -1.96499100 | 1.32828000 |

int18(quartet)

| | | | |
|---|-------------|------------|------------|
| C | -1.41285600 | 3.33706000 | 1.89256000 |
| C | -0.62770900 | 3.13630800 | 3.03354300 |
| C | 0.22088800 | 2.03284400 | 3.11970500 |
| C | 0.27497300 | 1.13642700 | 2.05203300 |
| C | -0.51140400 | 1.35727900 | 0.92429100 |
| C | -1.37122900 | 2.43669600 | 0.81787700 |
| H | -2.06795100 | 4.20204500 | 1.83288000 |
| H | -0.68366200 | 3.84230700 | 3.85658500 |
| H | 0.83573000 | 1.84461800 | 3.99493800 |

| | | | |
|----|-------------|-------------|-------------|
| H | -1.97594600 | 2.59004500 | -0.06712000 |
| C | 1.11733400 | -0.07812500 | 2.04194100 |
| O | 1.87427700 | -0.44254500 | 2.92372200 |
| N | 0.93073700 | -0.72725500 | 0.80711000 |
| C | 1.33841500 | -1.98523200 | 0.53311800 |
| C | 2.17064200 | -2.84038500 | 1.27948600 |
| C | 1.12547500 | -3.66845500 | -1.15678200 |
| C | 2.47706100 | -4.09215300 | 0.78143600 |
| H | 2.54978900 | -2.46955900 | 2.22030100 |
| C | 1.95675400 | -4.51237900 | -0.45533200 |
| H | 0.66043600 | -3.88646700 | -2.10829200 |
| H | 3.12763700 | -4.75001400 | 1.34794100 |
| H | 2.19192000 | -5.48580600 | -0.86846700 |
| O | -0.01449300 | -1.66394000 | -1.32136400 |
| N | 0.82565800 | -2.44825000 | -0.65459600 |
| Co | -0.12123200 | 0.10717400 | -0.52793800 |
| O | -1.82370700 | 0.44435100 | -1.28414400 |
| C | -2.83436900 | -0.20265200 | -0.77451200 |
| O | -2.76686000 | -0.89695500 | 0.24439900 |
| C | -4.14784700 | -0.02170200 | -1.55358100 |
| C | -3.93271100 | -0.53622800 | -2.99062800 |
| C | -5.27041600 | -0.80818100 | -0.86653000 |
| C | -4.48977700 | 1.48117300 | -1.58419800 |
| H | -3.12908600 | 0.01446200 | -3.48669100 |
| H | -3.66926200 | -1.60010700 | -2.98968600 |
| H | -4.85424100 | -0.41504300 | -3.57187900 |
| H | -5.42418700 | -0.46257300 | 0.15995600 |
| H | -6.20685000 | -0.67966700 | -1.42189700 |
| H | -5.03431900 | -1.87526500 | -0.82403300 |
| H | -5.43048900 | 1.63988800 | -2.12384700 |
| H | -4.61407600 | 1.87753900 | -0.56908500 |
| H | -3.70232700 | 2.05116200 | -2.08554200 |
| C | -1.96865500 | -0.98126900 | 3.50377300 |
| H | -1.37872900 | -1.08549600 | 4.41980400 |
| H | -2.12796100 | 0.09200900 | 3.31899200 |
| H | -2.95002200 | -1.45209300 | 3.66860900 |
| O | 2.81270900 | -0.36404600 | -1.56330100 |
| C | 2.40231000 | 0.78458700 | -1.52769700 |
| O | 1.10735200 | 1.10357200 | -1.49248200 |
| C | 3.32000400 | 2.01587100 | -1.46718200 |
| C | 2.92150000 | 3.01465900 | -2.56900600 |
| C | 3.11527300 | 2.66123200 | -0.07844500 |
| C | 4.77831400 | 1.57592000 | -1.63879700 |
| H | 3.05098700 | 2.57481100 | -3.56453200 |
| H | 1.87709200 | 3.31916400 | -2.46274700 |
| H | 3.55493800 | 3.90748400 | -2.50879600 |
| H | 3.35652700 | 1.95433200 | 0.72438600 |
| H | 3.77465200 | 3.53049100 | 0.02769200 |
| H | 2.08105900 | 2.99129000 | 0.05432400 |
| H | 5.44023600 | 2.44784400 | -1.58117500 |
| H | 5.06879700 | 0.86473500 | -0.86042600 |
| H | 4.93055900 | 1.08853300 | -2.60674500 |
| O | -1.24592900 | -1.60254900 | 2.45935900 |
| H | -1.73138700 | -1.41868900 | 1.62934200 |

int18(sextet)

| | | | |
|---|------------|-------------|-------------|
| C | 1.01120600 | -4.59549600 | -0.29249300 |
| C | 2.36213700 | -4.49610400 | -0.65587300 |
| C | 2.98219000 | -3.25399400 | -0.74127100 |
| C | 2.24961600 | -2.08133500 | -0.46524500 |
| C | 0.92724100 | -2.23995100 | -0.10210600 |
| C | 0.26691400 | -3.44292800 | -0.00319800 |
| H | 0.53612500 | -5.57177300 | -0.23525600 |
| H | 2.92815200 | -5.39659800 | -0.87480000 |

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|----|-------------|-------------|-------------|
| H | 4.02572200 | -3.15494700 | -1.02395400 |
| H | -0.77947100 | -3.48299400 | 0.27807500 |
| C | 2.91408500 | -0.76296800 | -0.58059800 |
| O | 4.10755500 | -0.66766500 | -0.85200800 |
| N | 2.07130700 | 0.35056000 | -0.39459300 |
| C | 2.62318700 | 1.53425700 | -0.09523100 |
| C | 3.93106000 | 1.82947700 | 0.38127200 |
| C | 2.09676000 | 3.89150400 | 0.12211300 |
| C | 4.28321900 | 3.11447900 | 0.72003000 |
| H | 4.62827500 | 1.00999800 | 0.45933900 |
| C | 3.35435800 | 4.16969000 | 0.58964800 |
| H | 1.30027600 | 4.60943900 | -0.01769000 |
| H | 5.28149500 | 3.31533900 | 1.09485500 |
| H | 3.61087200 | 5.18887600 | 0.85274200 |
| O | 0.54759100 | 2.41261700 | -0.69046600 |
| N | 1.75318100 | 2.61754700 | -0.21846900 |
| Co | -0.05358400 | 0.52236800 | -0.50436700 |
| O | -1.86540500 | 1.18150400 | -0.91585900 |
| C | -2.81385200 | 0.46852200 | -1.41981500 |
| O | -2.63312900 | -0.44855500 | -2.25283100 |
| C | -4.22971200 | 0.82132400 | -0.94360900 |
| C | -4.51532100 | 2.28610500 | -1.33002700 |
| C | -5.26194400 | -0.11246300 | -1.58531700 |
| C | -4.25750200 | 0.67600900 | 0.59097400 |
| H | -3.76727200 | 2.95345900 | -0.89340600 |
| H | -4.49905800 | 2.41577100 | -2.41861700 |
| H | -5.50716100 | 2.58327800 | -0.96888600 |
| H | -5.06612800 | -1.15564600 | -1.31993100 |
| H | -6.26930200 | 0.15133100 | -1.24119400 |
| H | -5.23645000 | -0.03846800 | -2.67638300 |
| H | -5.25293500 | 0.92920200 | 0.97488100 |
| H | -4.02130400 | -0.35126200 | 0.88654600 |
| H | -3.52098400 | 1.33957400 | 1.05266200 |
| C | 0.70033300 | -1.15212800 | -3.20120100 |
| H | 1.72086200 | -0.76703000 | -3.13954900 |
| H | 0.70239000 | -2.21249800 | -2.92437500 |
| H | 0.34123900 | -1.04153500 | -4.23068100 |
| O | -1.25080300 | -1.01574100 | 0.74777000 |
| C | -0.84127600 | -0.34623200 | 1.73132400 |
| O | -0.07183700 | 0.66284700 | 1.53531500 |
| C | -1.18820700 | -0.72550200 | 3.17044700 |
| C | 0.12997700 | -1.16668800 | 3.84329500 |
| C | -1.75544300 | 0.51326800 | 3.88775200 |
| C | -2.20237900 | -1.87541200 | 3.19603800 |
| H | 0.56573600 | -2.02664300 | 3.32146400 |
| H | 0.86109300 | -0.35330400 | 3.83400500 |
| H | -0.06064000 | -1.45713600 | 4.88285600 |
| H | -2.68842700 | 0.84391200 | 3.41809400 |
| H | -1.96804900 | 0.27423700 | 4.93633200 |
| H | -1.04296200 | 1.34155700 | 3.85273300 |
| H | -2.42578800 | -2.14928600 | 4.23377300 |
| H | -3.13799300 | -1.59007700 | 2.70616200 |
| H | -1.81126200 | -2.75788000 | 2.68168600 |
| O | -0.11462200 | -0.38868200 | -2.32771900 |
| H | -1.12640600 | -0.54080800 | -2.44720700 |

TS19(doublet)

| | | | |
|---|-------------|-------------|------------|
| C | -1.54690500 | -3.13007600 | 2.12444400 |
| C | -0.41928500 | -3.41275400 | 2.91086000 |
| C | 0.83932400 | -2.95404800 | 2.52443100 |
| C | 0.97664000 | -2.20996300 | 1.35154700 |
| C | -0.17098900 | -1.90585500 | 0.59926900 |
| C | -1.42735000 | -2.41456900 | 0.93650400 |
| H | -2.52543700 | -3.48789700 | 2.43129100 |

| | | | |
|----|-------------|-------------|-------------|
| H | -0.52865600 | -3.99559800 | 3.82026700 |
| H | 1.72727200 | -3.13314700 | 3.12348100 |
| H | -2.29298400 | -2.24010900 | 0.31195100 |
| C | 2.26588400 | -1.58436700 | 0.95879400 |
| O | 3.35918700 | -1.85588600 | 1.44971700 |
| N | 2.01310600 | -0.67100700 | -0.03696800 |
| C | 2.92923000 | 0.12328100 | -0.63736100 |
| C | 4.29910200 | 0.27208600 | -0.35481000 |
| C | 3.13256400 | 1.71856500 | -2.40578800 |
| C | 5.06484600 | 1.14911600 | -1.10579300 |
| H | 4.70099400 | -0.31790600 | 0.45668600 |
| C | 4.47743500 | 1.88567900 | -2.14472500 |
| H | 2.57550900 | 2.23364500 | -3.17671800 |
| H | 6.11988200 | 1.26782400 | -0.88140200 |
| H | 5.04896500 | 2.58550400 | -2.74263600 |
| O | 1.10218300 | 0.68873700 | -1.97424000 |
| N | 2.39297800 | 0.85433300 | -1.67379700 |
| Co | 0.21803100 | -0.26549700 | -0.47826800 |
| O | -1.54412100 | 0.35372100 | -1.02861300 |
| C | -2.52895800 | -0.21652300 | -1.51453400 |
| O | -2.48121600 | -1.43143200 | -2.01861500 |
| C | -3.89529000 | 0.44054000 | -1.45214800 |
| C | -3.72476700 | 1.96570900 | -1.37728200 |
| C | -4.76589900 | 0.03644400 | -2.65086300 |
| C | -4.51648600 | -0.07048900 | -0.12572000 |
| H | -3.13014900 | 2.24479700 | -0.50490800 |
| H | -3.22479900 | 2.35432300 | -2.27094900 |
| H | -4.70982600 | 2.43823500 | -1.30090100 |
| H | -4.88874700 | -1.04804700 | -2.70870400 |
| H | -5.75658900 | 0.49262400 | -2.55066000 |
| H | -4.32771300 | 0.38182900 | -3.59395000 |
| H | -5.48534300 | 0.41776300 | 0.02714000 |
| H | -4.68347300 | -1.15277000 | -0.16042400 |
| H | -3.86261800 | 0.16545000 | 0.72003500 |
| O | -0.06993200 | -2.00082100 | -1.36813200 |
| H | -1.53281800 | -1.78275000 | -1.90176300 |
| C | 1.00260700 | -2.71979400 | -1.95011200 |
| H | 1.62881300 | -2.05005300 | -2.54934200 |
| H | 1.62384000 | -3.19149400 | -1.18017300 |
| H | 0.58319600 | -3.50549300 | -2.58904400 |
| O | -1.58395500 | 0.68054800 | 1.73810800 |
| C | -0.64225600 | 1.43741400 | 1.50541000 |
| O | 0.33321200 | 1.20828300 | 0.66265100 |
| C | -0.49659900 | 2.80569400 | 2.20875800 |
| C | 0.85634500 | 2.84491700 | 2.94413000 |
| C | -0.53456500 | 3.90717600 | 1.13164600 |
| C | -1.64736200 | 2.99820800 | 3.20277800 |
| H | 0.91053200 | 2.05832000 | 3.70614400 |
| H | 1.68309900 | 2.69798900 | 2.24404400 |
| H | 0.98763200 | 3.81134200 | 3.44635100 |
| H | -1.48499000 | 3.88839900 | 0.58461600 |
| H | -0.43229400 | 4.89606100 | 1.59547800 |
| H | 0.27416700 | 3.77116500 | 0.40859300 |
| H | -1.55137700 | 3.96833400 | 3.70554700 |
| H | -2.61507300 | 2.96323400 | 2.69356600 |
| H | -1.64688100 | 2.21001000 | 3.96134300 |

TS19(quartet)

| | | | |
|---|-------------|------------|------------|
| C | -1.69527400 | 2.22577900 | 2.36039100 |
| C | -0.56999300 | 2.88978000 | 2.90127400 |
| C | 0.71912800 | 2.39916600 | 2.68211200 |
| C | 0.88401100 | 1.25621200 | 1.91735000 |
| C | -0.24705000 | 0.55793600 | 1.38622600 |
| C | -1.55391100 | 1.05026400 | 1.64698800 |

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|----|-------------|-------------|-------------|
| H | -2.68707100 | 2.63883600 | 2.52226300 |
| H | -0.71426800 | 3.79212900 | 3.48753900 |
| H | 1.59908800 | 2.90915400 | 3.06108100 |
| H | -2.42132100 | 0.51375200 | 1.28387100 |
| C | 2.21789500 | 0.72640200 | 1.53487700 |
| O | 3.27604700 | 1.07069100 | 2.04876300 |
| N | 2.05095900 | -0.17851400 | 0.49938500 |
| C | 3.06609000 | -0.77622600 | -0.17810800 |
| C | 4.45246600 | -0.70972100 | 0.05144300 |
| C | 3.46006300 | -2.21179900 | -2.04935800 |
| C | 5.32258200 | -1.39682000 | -0.77915000 |
| H | 4.78751800 | -0.10437300 | 0.88132700 |
| C | 4.82297000 | -2.16018200 | -1.84401900 |
| H | 2.96433200 | -2.76383400 | -2.83633300 |
| H | 6.39155200 | -1.33993900 | -0.60182400 |
| H | 5.47842800 | -2.70819900 | -2.51040600 |
| O | 1.30501600 | -1.61799700 | -1.46058300 |
| N | 2.61522700 | -1.53516700 | -1.23521600 |
| Co | 0.28937500 | -0.46677700 | -0.20263400 |
| O | -1.19482200 | -1.68935400 | -0.26515200 |
| C | -2.24600700 | -2.03266700 | 0.37715500 |
| O | -2.34300700 | -2.03325600 | 1.63022800 |
| C | -3.43907000 | -2.44857500 | -0.49354000 |
| C | -2.98677000 | -3.58233100 | -1.43420700 |
| C | -4.61395400 | -2.90830100 | 0.37671800 |
| C | -3.83668300 | -1.21377300 | -1.33029600 |
| H | -2.13845700 | -3.26306300 | -2.04485400 |
| H | -2.68681400 | -4.46974100 | -0.86471400 |
| H | -3.81249000 | -3.86826900 | -2.09600100 |
| H | -4.94068300 | -2.11270500 | 1.05287300 |
| H | -5.45976600 | -3.19236400 | -0.26011100 |
| H | -4.33784800 | -3.77128900 | 0.99024900 |
| H | -4.66128000 | -1.46942100 | -2.00565900 |
| H | -4.17377900 | -0.39173800 | -0.68667100 |
| H | -2.98897600 | -0.85909800 | -1.92266100 |
| O | -0.16562300 | -1.14216000 | 2.49981200 |
| H | -1.06965100 | -1.56193900 | 2.17495000 |
| C | -0.25266100 | -0.86044200 | 3.89556600 |
| H | 0.70727800 | -0.45761800 | 4.22278900 |
| H | -1.04833500 | -0.13655000 | 4.10807700 |
| H | -0.46006600 | -1.79417500 | 4.42984700 |
| O | 0.42104800 | 2.68719000 | -0.36559000 |
| C | -0.26157200 | 2.14707300 | -1.24127000 |
| O | -0.35641600 | 0.86485900 | -1.43106400 |
| C | -1.12669000 | 2.98932000 | -2.20589800 |
| C | -0.82084800 | 2.57542100 | -3.65573800 |
| C | -2.60082400 | 2.67932800 | -1.87351800 |
| C | -0.84216600 | 4.48136000 | -2.00041900 |
| H | 0.22429000 | 2.78630400 | -3.91112600 |
| H | -0.99808400 | 1.50687600 | -3.80025100 |
| H | -1.45772700 | 3.13743000 | -4.34978400 |
| H | -2.82748200 | 2.93544900 | -0.83154400 |
| H | -3.26446600 | 3.26666600 | -2.51950900 |
| H | -2.81775600 | 1.61810500 | -2.02095700 |
| H | -1.46938300 | 5.07915400 | -2.67275600 |
| H | -1.04844500 | 4.78193100 | -0.96927000 |
| H | 0.20692200 | 4.71427300 | -2.20728200 |

TS19(sextet)

| | | | |
|---|-------------|-------------|------------|
| C | -0.87994100 | -2.06407000 | 3.51500600 |
| C | -1.99161600 | -1.27704100 | 3.91247700 |
| C | -2.28819100 | -0.06733800 | 3.25590500 |
| C | -1.47443800 | 0.36763000 | 2.22996200 |
| C | -0.27271200 | -0.36067200 | 1.87606300 |

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|----|-------------|-------------|-------------|
| C | -0.04421300 | -1.63973900 | 2.50892900 |
| H | -0.71095300 | -3.02333200 | 3.99737200 |
| H | -2.63991800 | -1.63024900 | 4.70868000 |
| H | -3.17160900 | 0.51006800 | 3.51297600 |
| H | 0.79301400 | -2.24362600 | 2.17430900 |
| C | -1.77780300 | 1.58134600 | 1.42462200 |
| O | -2.59413800 | 2.43626400 | 1.76428600 |
| N | -0.98860700 | 1.58848300 | 0.29040700 |
| C | -0.76135700 | 2.68023300 | -0.46702400 |
| C | -1.41300200 | 3.93038900 | -0.46061900 |
| C | 0.67967700 | 3.47955600 | -2.21182800 |
| C | -1.01120100 | 4.92964900 | -1.32974900 |
| H | -2.22708800 | 4.05265600 | 0.23987200 |
| C | 0.04628300 | 4.70395100 | -2.22441600 |
| H | 1.50758200 | 3.19725000 | -2.84798600 |
| H | -1.52464600 | 5.88587000 | -1.32294500 |
| H | 0.37550000 | 5.46333000 | -2.92359900 |
| O | 0.96501000 | 1.36158200 | -1.33791300 |
| N | 0.29092100 | 2.50995200 | -1.35078100 |
| Co | 0.00417200 | -0.07874200 | -0.32575900 |
| O | 1.63492500 | -1.20004600 | -0.20006300 |
| C | 2.78930100 | -0.81236800 | 0.17033100 |
| O | 3.00586900 | -0.09489700 | 1.19149100 |
| C | 3.99047200 | -1.19879700 | -0.69917300 |
| C | 5.18816200 | -1.56948200 | 0.18987000 |
| C | 3.63362900 | -2.35828100 | -1.63892800 |
| C | 4.32018300 | 0.06505000 | -1.52848800 |
| H | 5.42830300 | -0.75709800 | 0.87984300 |
| H | 4.97727500 | -2.46846500 | 0.78116300 |
| H | 6.06633100 | -1.77456500 | -0.43323600 |
| H | 2.79632800 | -2.09428400 | -2.28971300 |
| H | 4.49924400 | -2.60805400 | -2.26354000 |
| H | 3.34927100 | -3.25299600 | -1.07477500 |
| H | 5.14592900 | -0.14944600 | -2.21691300 |
| H | 3.44985600 | 0.38491400 | -2.11092600 |
| H | 4.61562700 | 0.89021200 | -0.87318800 |
| O | 1.06165800 | 0.72040900 | 2.44333600 |
| H | 1.92662400 | 0.34268000 | 1.87062700 |
| C | 1.32487100 | 0.68364000 | 3.84952100 |
| H | 0.40146300 | 0.93873900 | 4.37453200 |
| H | 1.67212100 | -0.30330300 | 4.17152600 |
| H | 2.08952900 | 1.43593700 | 4.06511800 |
| C | -1.67879400 | -1.67905600 | -1.29176000 |
| O | -1.51437400 | -1.85222300 | -0.05991000 |
| O | -1.00516300 | -0.75774700 | -1.89165200 |
| C | -2.65473500 | -2.51686900 | -2.11204800 |
| C | -3.70600500 | -1.56002800 | -2.71183900 |
| C | -1.86226600 | -3.19551200 | -3.24764300 |
| C | -3.33135200 | -3.56872500 | -1.22458400 |
| H | -4.27421300 | -1.05564500 | -1.92162800 |
| H | -3.22767300 | -0.79673800 | -3.33164500 |
| H | -4.41278400 | -2.12402700 | -3.33136700 |
| H | -1.10343000 | -3.87588900 | -2.84451700 |
| H | -2.54239500 | -3.77915700 | -3.87902100 |
| H | -1.35823300 | -2.45006700 | -3.86851500 |
| H | -4.03453100 | -4.16199700 | -1.82072900 |
| H | -2.59340700 | -4.24523500 | -0.78308500 |
| H | -3.88195300 | -3.09801900 | -0.40467700 |

int20(doublet)

| | | | |
|---|------------|-------------|-------------|
| C | 3.38865400 | -2.59216500 | -2.03185700 |
| C | 4.34776100 | -1.68836700 | -1.58053400 |
| C | 3.95911100 | -0.39851100 | -1.22954300 |
| C | 2.62321600 | 0.01907000 | -1.29878300 |

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|----|-------------|-------------|-------------|
| C | 2.05274000 | -2.20311500 | -2.12963400 |
| H | 3.66964900 | -3.60364000 | -2.31010100 |
| H | 5.38994700 | -1.98219300 | -1.50564500 |
| H | 4.68543600 | 0.33315800 | -0.89537900 |
| H | 1.31099900 | -2.91076500 | -2.47863400 |
| C | 2.36829000 | 1.44505100 | -0.87284000 |
| O | 3.31319300 | 2.23800600 | -0.90161400 |
| N | 1.10853200 | 1.74555500 | -0.40951100 |
| C | 0.85040800 | 2.93703900 | 0.20933000 |
| C | 1.62694300 | 4.11308800 | 0.28030200 |
| C | -0.83346100 | 4.03205800 | 1.52558000 |
| C | 1.16221200 | 5.22106600 | 0.96962500 |
| H | 2.58291700 | 4.10059700 | -0.21848900 |
| C | -0.08732300 | 5.18801400 | 1.60322900 |
| H | -1.80867500 | 3.88308200 | 1.96910100 |
| H | 1.77179900 | 6.11810400 | 1.00969600 |
| H | -0.48109400 | 6.03987000 | 2.14468600 |
| O | -1.13631200 | 1.85521400 | 0.83643700 |
| N | -0.36624300 | 2.95336600 | 0.85620400 |
| Co | -0.39036600 | 0.54892500 | -0.30861300 |
| C | 1.67716900 | -0.91088800 | -1.76416400 |
| O | 0.35889900 | -0.49984700 | -1.86583400 |
| C | -0.53588600 | -1.22997800 | -2.72705100 |
| H | -0.03772200 | -1.41000100 | -3.68283800 |
| H | -0.83295200 | -2.17218600 | -2.25881700 |
| H | -1.40108800 | -0.58239200 | -2.85193000 |
| C | 0.25193000 | -1.85964500 | 1.58472800 |
| O | 0.65302500 | -0.80730600 | 1.08120000 |
| C | 1.18757700 | -2.71987000 | 2.43016300 |
| C | 2.42463700 | -3.03733600 | 1.56450100 |
| C | 1.61420200 | -1.86546600 | 3.64294800 |
| C | 0.51472800 | -4.01533100 | 2.90119700 |
| H | 2.15380800 | -3.64493500 | 0.69429300 |
| H | 2.89381300 | -2.12008500 | 1.20100500 |
| H | 3.15525700 | -3.59861900 | 2.15762700 |
| H | 0.75306900 | -1.61610200 | 4.27339500 |
| H | 2.33216100 | -2.42431200 | 4.25329700 |
| H | 2.08226100 | -0.93401800 | 3.31326600 |
| H | 1.22207600 | -4.59627400 | 3.50374200 |
| H | -0.36867900 | -3.80833800 | 3.51218900 |
| H | 0.19878100 | -4.63208800 | 2.05422000 |
| O | -0.97863700 | -2.31511200 | 1.43940500 |
| H | -1.50293000 | -1.66942900 | 0.85976000 |
| C | -2.99091500 | -0.12339500 | -0.83654300 |
| O | -1.95230300 | -0.55738000 | -0.16176700 |
| O | -2.88782600 | 0.75174600 | -1.69674200 |
| C | -4.31907000 | -0.81234800 | -0.49240800 |
| C | -4.58284900 | -0.65368300 | 1.01777200 |
| C | -5.45703800 | -0.17784500 | -1.30034700 |
| C | -4.19118600 | -2.30938600 | -0.84354000 |
| H | -3.78902700 | -1.11566100 | 1.61146900 |
| H | -4.63949400 | 0.40492000 | 1.29492200 |
| H | -5.53469900 | -1.12794700 | 1.28459400 |
| H | -5.27211900 | -0.26436600 | -2.37484600 |
| H | -6.40624400 | -0.67429000 | -1.06659200 |
| H | -5.55464500 | 0.88694700 | -1.06900900 |
| H | -5.12732100 | -2.83121800 | -0.61342900 |
| H | -3.98588300 | -2.44582000 | -1.91227000 |
| H | -3.38696300 | -2.78633700 | -0.27504200 |

int20(quartet)

| | | | |
|---|-------------|------------|-------------|
| C | 0.85793600 | 4.05717000 | -1.41843100 |
| C | -0.16957000 | 4.51751400 | -0.59494600 |
| C | -1.22392200 | 3.66365100 | -0.28125000 |

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|----|-------------|-------------|-------------|
| C | -1.26998300 | 2.34163800 | -0.75224700 |
| C | 0.82953700 | 2.75837500 | -1.92311800 |
| H | 1.69470800 | 4.70300200 | -1.66643200 |
| H | -0.15071200 | 5.52895300 | -0.20211900 |
| H | -2.05402000 | 3.99420300 | 0.33308100 |
| H | 1.64480900 | 2.40579500 | -2.53987700 |
| C | -2.48248300 | 1.53171300 | -0.35083300 |
| O | -3.52379800 | 2.14368600 | -0.09012600 |
| N | -2.28560100 | 0.18190800 | -0.27676400 |
| C | -3.29983000 | -0.66386500 | 0.03689400 |
| C | -4.66174900 | -0.39064400 | 0.29784700 |
| C | -3.77535300 | -2.99692000 | 0.37204600 |
| C | -5.54945500 | -1.41399200 | 0.58375300 |
| H | -4.96376100 | 0.64468800 | 0.26514400 |
| C | -5.10664800 | -2.74238100 | 0.62374700 |
| H | -3.31589500 | -3.97611500 | 0.37625300 |
| H | -6.59088400 | -1.17823500 | 0.77952400 |
| H | -5.77339400 | -3.56664900 | 0.84751900 |
| O | -1.64191100 | -2.32363700 | -0.14930000 |
| N | -2.91344800 | -1.99293000 | 0.08987500 |
| Co | -0.41763800 | -0.78102700 | -0.35311600 |
| C | -0.22623900 | 1.90571500 | -1.59552900 |
| O | -0.28933300 | 0.60943900 | -2.06926700 |
| C | 0.54782700 | 0.24658400 | -3.17842800 |
| H | 0.34739700 | 0.91750700 | -4.01907100 |
| H | 1.59884500 | 0.28136300 | -2.89051900 |
| H | 0.26656400 | -0.77525200 | -3.42943600 |
| C | 0.94568900 | 0.82629800 | 1.95325100 |
| O | 0.06768800 | 0.07860700 | 1.52130400 |
| C | 1.99966200 | 0.39499000 | 2.95854200 |
| C | 2.01352700 | -1.13723800 | 3.04007700 |
| C | 3.37635800 | 0.93165000 | 2.51848500 |
| C | 1.60883100 | 0.99861300 | 4.32734700 |
| H | 1.04543200 | -1.52649100 | 3.36728000 |
| H | 2.23586300 | -1.58190700 | 2.06703700 |
| H | 2.77877000 | -1.45872300 | 3.75467800 |
| H | 3.39739500 | 2.02454600 | 2.53583200 |
| H | 4.14487000 | 0.55779200 | 3.20403500 |
| H | 3.60649500 | 0.60358400 | 1.50217800 |
| H | 2.35169900 | 0.70461000 | 5.07677900 |
| H | 1.57675700 | 2.09131000 | 4.28279800 |
| H | 0.62987700 | 0.63332200 | 4.65746100 |
| O | 1.00412900 | 2.11123800 | 1.62982800 |
| H | 0.29868600 | 2.30987300 | 0.97792500 |
| C | 2.28096000 | -1.10333200 | -0.74998100 |
| O | 1.20294400 | -1.81476100 | -0.74976000 |
| O | 2.28894400 | 0.12285000 | -0.52208800 |
| C | 3.57236100 | -1.86700200 | -1.10303100 |
| C | 3.42580300 | -2.37253600 | -2.55335000 |
| C | 4.79425900 | -0.94877700 | -0.98883700 |
| C | 3.71987300 | -3.07363000 | -0.15777500 |
| H | 2.53871200 | -3.00396900 | -2.65373900 |
| H | 3.33665300 | -1.53501100 | -3.25672700 |
| H | 4.30786000 | -2.95598600 | -2.84272700 |
| H | 4.93665100 | -0.60567400 | 0.04064500 |
| H | 5.69939500 | -1.48558600 | -1.29755900 |
| H | 4.68166500 | -0.06165800 | -1.61853900 |
| H | 4.60055800 | -3.66617200 | -0.43405300 |
| H | 3.85020000 | -2.74625000 | 0.88025900 |
| H | 2.83473700 | -3.71293000 | -0.20541400 |

int20(sextet)

| | | | |
|---|------------|------------|------------|
| C | 1.85814800 | 4.09812400 | 1.84075400 |
| C | 1.00703200 | 3.71071900 | 2.87477400 |

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|----|-------------|-------------|-------------|
| C | -0.04046500 | 2.83997400 | 2.60581600 |
| C | -0.28109100 | 2.33295500 | 1.31408000 |
| C | 1.65964200 | 3.60470500 | 0.54857000 |
| H | 2.68434000 | 4.77747800 | 2.02816800 |
| H | 1.15910200 | 4.08428400 | 3.88271300 |
| H | -0.71992300 | 2.51986800 | 3.38712500 |
| H | 2.34233800 | 3.90075400 | -0.23748300 |
| C | -1.44506100 | 1.44094300 | 1.17302600 |
| O | -2.09331600 | 1.04050900 | 2.18448900 |
| N | -1.75324100 | 1.02115200 | -0.09796100 |
| C | -2.91169700 | 0.48914500 | -0.45706400 |
| C | -4.16117300 | 0.41526300 | 0.19351200 |
| C | -3.97880900 | -0.51986100 | -2.47403900 |
| C | -5.27669600 | -0.06448400 | -0.45136300 |
| H | -4.18978900 | 0.77019400 | 1.21568500 |
| C | -5.17067900 | -0.51638600 | -1.82900700 |
| H | -3.80696000 | -0.85966500 | -3.48665000 |
| H | -6.23352100 | -0.10828500 | 0.05461500 |
| H | -6.05122900 | -0.86160900 | -2.35993500 |
| O | -1.66796100 | -0.27865100 | -2.35639900 |
| N | -2.84068000 | -0.07480000 | -1.82010100 |
| Co | -0.15697600 | 0.04915400 | -0.98921900 |
| C | 0.60869800 | 2.73184500 | 0.28038800 |
| O | 0.41457700 | 2.21179800 | -0.99041600 |
| C | 1.29285200 | 2.62109200 | -2.04172300 |
| H | 1.21372300 | 3.70112300 | -2.19876000 |
| H | 2.32696400 | 2.34415100 | -1.81713700 |
| H | 0.95841900 | 2.08438100 | -2.92896800 |
| C | -0.58334600 | -1.99203100 | 1.40816700 |
| O | -0.77228700 | -1.56873600 | 0.26219400 |
| C | 0.26843500 | -3.22331800 | 1.68837800 |
| C | 0.58338200 | -3.93478400 | 0.36590800 |
| C | 1.57353000 | -2.70909000 | 2.34272400 |
| C | -0.46713200 | -4.17206500 | 2.65265400 |
| H | -0.33058500 | -4.29794700 | -0.11536800 |
| H | 1.08312400 | -3.26519300 | -0.33775000 |
| H | 1.23558200 | -4.79384400 | 0.55768100 |
| H | 1.36780300 | -2.24868800 | 3.31333600 |
| H | 2.25921000 | -3.55054800 | 2.49294500 |
| H | 2.05811000 | -1.96296600 | 1.70639000 |
| H | 0.16917900 | -5.03712900 | 2.86965800 |
| H | -0.70724200 | -3.67189500 | 3.59401100 |
| H | -1.39964900 | -4.54114900 | 2.21049400 |
| O | -1.07316100 | -1.42143700 | 2.48715000 |
| H | -1.56368800 | -0.55950100 | 2.30054300 |
| C | 2.25383300 | -0.48073300 | -0.99018000 |
| O | 1.47158500 | -0.62764300 | -1.99994100 |
| O | 1.77859300 | -0.05952700 | 0.10143200 |
| C | 3.73559200 | -0.82278500 | -1.14499900 |
| C | 4.51798100 | -0.40278900 | 0.10604500 |
| C | 3.84754500 | -2.34698500 | -1.35953000 |
| C | 4.27877900 | -0.09152100 | -2.38790300 |
| H | 4.41297100 | 0.66992400 | 0.29621600 |
| H | 4.15946300 | -0.93020200 | 0.99427600 |
| H | 5.58214300 | -0.63100800 | -0.02611100 |
| H | 3.27162500 | -2.66011300 | -2.23519900 |
| H | 4.89678400 | -2.62530800 | -1.51156300 |
| H | 3.47515400 | -2.89531800 | -0.48748800 |
| H | 5.32458900 | -0.37087600 | -2.55957400 |
| H | 3.69454900 | -0.34715000 | -3.27543600 |
| H | 4.24317000 | 0.99651900 | -2.25310700 |

TS-S1(singlet)

| | | | |
|---|-------------|------------|-------------|
| C | -1.32986700 | 4.25755500 | -0.49661000 |
|---|-------------|------------|-------------|

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|----|-------------|-------------|-------------|
| C | -2.71013100 | 4.08620100 | -0.34249100 |
| C | -3.23982600 | 2.80529600 | -0.18930900 |
| C | -2.37129300 | 1.71188000 | -0.18337200 |
| C | -0.98293800 | 1.87730400 | -0.32456300 |
| C | -0.46088200 | 3.15734900 | -0.48801600 |
| H | -0.92481500 | 5.25911000 | -0.62058900 |
| H | -3.36784000 | 4.95060400 | -0.34941300 |
| H | -4.30794300 | 2.63714400 | -0.08431400 |
| H | 0.60948100 | 3.30311100 | -0.59952000 |
| C | -2.84601500 | 0.31131500 | -0.06294900 |
| O | -4.00483400 | -0.05639800 | 0.08112700 |
| N | -1.73985400 | -0.54475500 | -0.16717000 |
| C | -1.76948400 | -1.89734100 | -0.09693400 |
| C | -2.86099600 | -2.76173200 | 0.11555000 |
| C | -0.31547300 | -3.79379300 | -0.25351000 |
| C | -2.65572700 | -4.13025300 | 0.14245100 |
| H | -3.83253500 | -2.30772900 | 0.24879900 |
| C | -1.36765400 | -4.65862700 | -0.04196400 |
| H | 0.71431800 | -4.08369600 | -0.41292300 |
| H | -3.49724400 | -4.79452900 | 0.31026300 |
| H | -1.18080700 | -5.72557000 | -0.02220100 |
| O | 0.50756200 | -1.64137000 | -0.52803700 |
| N | -0.52379900 | -2.45635100 | -0.28172300 |
| Co | -0.05562800 | 0.21464800 | -0.22474100 |
| O | 2.77610000 | 0.15080300 | -1.98463600 |
| C | 2.80965100 | 0.37841500 | -0.79819000 |
| O | 1.76108000 | 0.99113400 | -0.18278300 |
| C | 3.97981000 | 0.02316300 | 0.12562300 |
| C | 3.52940900 | -1.14971000 | 1.02640600 |
| C | 5.17351700 | -0.41006500 | -0.73561400 |
| C | 4.36636100 | 1.23613400 | 0.99393900 |
| H | 2.68869400 | -0.87469900 | 1.67007800 |
| H | 3.21654300 | -2.00540400 | 0.42033400 |
| H | 4.36456400 | -1.45899400 | 1.66522200 |
| H | 5.49912100 | 0.40141700 | -1.39385000 |
| H | 6.01366000 | -0.69336500 | -0.09163400 |
| H | 4.91048900 | -1.26269700 | -1.36669400 |
| H | 5.22543800 | 0.97798600 | 1.62327800 |
| H | 4.64694900 | 2.09457300 | 0.37372000 |
| H | 3.54970600 | 1.54622300 | 1.65309600 |
| O | 0.46339900 | 0.36744400 | 1.57022400 |
| H | 1.46242300 | 0.80615500 | 0.94784900 |
| C | -0.18447700 | 1.22891800 | 2.49870400 |
| H | -1.23991800 | 0.95503000 | 2.58119200 |
| H | 0.29997700 | 1.08198400 | 3.47144000 |
| H | -0.11309700 | 2.28062200 | 2.20404400 |

TS-S1(triplet)

| | | | |
|---|-------------|-------------|-------------|
| C | 2.09944100 | 3.29881800 | 0.28159400 |
| C | 1.16437600 | 4.19827100 | -0.24263600 |
| C | -0.14614100 | 3.78620500 | -0.47906100 |
| C | -0.50673000 | 2.47242400 | -0.17726500 |
| C | 0.42408200 | 1.57361600 | 0.36114800 |
| C | 1.73575900 | 1.98092200 | 0.57990100 |
| H | 3.12249800 | 3.62342200 | 0.45311700 |
| H | 1.46457300 | 5.21604300 | -0.47397700 |
| H | -0.89096200 | 4.45454300 | -0.90115500 |
| H | 2.47658600 | 1.29474100 | 0.97096000 |
| C | -1.86359500 | 1.93573500 | -0.44337100 |
| O | -2.80359400 | 2.55451100 | -0.92127300 |
| N | -1.89107500 | 0.58877400 | -0.06337900 |
| C | -2.94571900 | -0.25024100 | -0.24142000 |
| C | -4.22168300 | 0.00818100 | -0.77503000 |
| C | -3.56349700 | -2.53624300 | 0.10310400 |

| | | | |
|----|-------------|-------------|-------------|
| C | -5.14870800 | -1.01795300 | -0.85806000 |
| H | -4.42799200 | 1.01636000 | -1.10373400 |
| C | -4.82129800 | -2.30812500 | -0.41420000 |
| H | -3.19571600 | -3.48476400 | 0.47059500 |
| H | -6.13219900 | -0.81744500 | -1.27039700 |
| H | -5.52813700 | -3.12724200 | -0.46929000 |
| O | -1.44869800 | -1.77801000 | 0.67917200 |
| N | -2.66567600 | -1.52715600 | 0.18000700 |
| Co | -0.33989200 | -0.17451900 | 0.70213000 |
| O | 1.90149200 | -0.36092600 | -2.07908000 |
| C | 2.23306500 | -0.95678000 | -1.07467700 |
| O | 1.35421900 | -1.25327400 | -0.10877700 |
| C | 3.65939200 | -1.48806300 | -0.83382000 |
| C | 3.58636300 | -3.01364200 | -0.62147500 |
| C | 4.52746500 | -1.16292600 | -2.05566000 |
| C | 4.25991100 | -0.82114600 | 0.41944100 |
| H | 2.97566400 | -3.26721500 | 0.24976200 |
| H | 3.15029000 | -3.50890300 | -1.49600500 |
| H | 4.59397800 | -3.41824600 | -0.46946900 |
| H | 4.56981800 | -0.08405500 | -2.23058500 |
| H | 5.54733500 | -1.53425300 | -1.90171000 |
| H | 4.11950800 | -1.62564000 | -2.95855100 |
| H | 5.26680500 | -1.21346600 | 0.60170000 |
| H | 4.34400300 | 0.26315000 | 0.28647100 |
| H | 3.66381900 | -1.01647800 | 1.31731500 |
| O | 0.87505900 | -0.83296100 | 2.06125500 |
| H | 1.52868900 | -1.18720500 | 1.03440500 |
| C | 1.35367700 | -0.18178000 | 3.21328100 |
| H | 1.86794200 | 0.76274400 | 2.98630200 |
| H | 0.51790900 | 0.03878500 | 3.88938100 |
| H | 2.05515600 | -0.84253600 | 3.73979000 |

TS-S1(quinet)

| | | | |
|----|-------------|-------------|-------------|
| C | 1.75071200 | 3.35932100 | -0.96187300 |
| C | 0.80578300 | 4.23199700 | -0.41051300 |
| C | -0.43330800 | 3.75138700 | 0.01092200 |
| C | -0.71099900 | 2.38577900 | -0.10231500 |
| C | 0.25522700 | 1.51244300 | -0.61802200 |
| C | 1.47467600 | 1.99016700 | -1.08721200 |
| H | 2.70623400 | 3.74645900 | -1.30727900 |
| H | 1.03211000 | 5.29137100 | -0.32978900 |
| H | -1.19699000 | 4.41182400 | 0.41164700 |
| H | 2.20125400 | 1.32435000 | -1.54185500 |
| C | -2.04681000 | 1.82614700 | 0.25932700 |
| O | -3.02564800 | 2.49882900 | 0.56297400 |
| N | -2.01140000 | 0.44211200 | 0.14435200 |
| C | -3.08244800 | -0.35362900 | -0.00800800 |
| C | -4.45571700 | -0.06254700 | 0.13189500 |
| C | -3.65058900 | -2.61257600 | -0.59303800 |
| C | -5.39818600 | -1.04977700 | -0.08936300 |
| H | -4.71415500 | 0.94697400 | 0.42041800 |
| C | -4.99503200 | -2.34580600 | -0.45302400 |
| H | -3.22763800 | -3.56744900 | -0.87468900 |
| H | -6.45287100 | -0.82061400 | 0.02470100 |
| H | -5.71236400 | -3.13917400 | -0.62503800 |
| O | -1.44032000 | -1.93431900 | -0.55574400 |
| N | -2.73253300 | -1.64046800 | -0.37944100 |
| Co | -0.22304900 | -0.47424500 | -0.05487700 |
| O | 2.87360300 | -0.97472600 | -1.96521100 |
| C | 2.86265500 | -1.16923500 | -0.76720000 |
| O | 1.70924300 | -1.39668700 | -0.11342900 |
| C | 4.12142200 | -1.17069100 | 0.11193300 |
| C | 4.19065000 | -2.48290500 | 0.91759000 |
| C | 5.35546100 | -1.03497000 | -0.78905400 |

| | | | |
|---|-------------|-------------|-------------|
| C | 4.04666900 | 0.03223300 | 1.07749700 |
| H | 3.32269700 | -2.60359900 | 1.57295700 |
| H | 4.23624600 | -3.35129200 | 0.25137900 |
| H | 5.09172800 | -2.48610200 | 1.54137000 |
| H | 5.32230700 | -0.10538800 | -1.36395700 |
| H | 6.26500900 | -1.03721700 | -0.17794100 |
| H | 5.41250000 | -1.86187000 | -1.50266000 |
| H | 4.97667500 | 0.09886100 | 1.65278400 |
| H | 3.91476500 | 0.97360700 | 0.53300700 |
| H | 3.22371100 | -0.06447500 | 1.79139200 |
| O | 0.53341100 | -0.72624700 | 1.73251700 |
| H | 1.51942800 | -1.13228200 | 0.98741300 |
| C | 0.61343300 | 0.34812200 | 2.64822800 |
| H | -0.39575300 | 0.69290700 | 2.90280200 |
| H | 1.10719300 | 0.00893400 | 3.56814200 |
| H | 1.17387800 | 1.19971400 | 2.23702900 |

int-S2(singlet)

| | | | |
|----|-------------|-------------|-------------|
| C | -3.37969400 | -2.94371200 | 0.23278200 |
| C | -2.71113500 | -3.91030300 | -0.52733100 |
| C | -1.37800200 | -3.71210300 | -0.88165100 |
| C | -0.73549800 | -2.53984000 | -0.47489200 |
| C | -1.40099700 | -1.55906000 | 0.27739800 |
| C | -2.72801500 | -1.77226200 | 0.64020900 |
| H | -4.41610500 | -3.10885600 | 0.51902700 |
| H | -3.22961600 | -4.81487000 | -0.83264600 |
| H | -0.82582400 | -4.44600300 | -1.46198100 |
| H | -3.26167800 | -1.05099500 | 1.25562900 |
| C | 0.68319300 | -2.26007200 | -0.79749200 |
| O | 1.43967200 | -2.98413200 | -1.43849400 |
| N | 1.03972500 | -1.01928900 | -0.26532600 |
| C | 2.25530600 | -0.43440800 | -0.33935500 |
| C | 3.44316100 | -0.94061900 | -0.90892600 |
| C | 3.43631000 | 1.55341700 | 0.27876800 |
| C | 4.60416500 | -0.18874400 | -0.87386600 |
| H | 3.38767000 | -1.92120500 | -1.35920500 |
| C | 4.60863000 | 1.07801400 | -0.26976100 |
| H | 3.32084600 | 2.50947200 | 0.77155500 |
| H | 5.51308800 | -0.58749700 | -1.31297400 |
| H | 5.50350900 | 1.68678700 | -0.22031300 |
| O | 1.18203600 | 1.33368100 | 0.76538300 |
| N | 2.29833800 | 0.82121500 | 0.23260600 |
| Co | -0.25799900 | -0.08808600 | 0.66311800 |
| O | -0.10654400 | -0.68801200 | 2.33386800 |
| C | 1.07640600 | -0.46721600 | 3.05394100 |
| H | 1.36471900 | 0.59346700 | 3.10636200 |
| H | 0.91921200 | -0.84076400 | 4.07599800 |
| H | 1.92191800 | -1.03255900 | 2.62783400 |
| C | -1.33591000 | 1.94703800 | -1.24971100 |
| O | -0.84483800 | 0.83490200 | -1.08239200 |
| O | -1.41003000 | 2.44820300 | -2.48806100 |
| H | -1.01299600 | 1.78397600 | -3.08506600 |
| C | -1.86725100 | 2.88011800 | -0.17525300 |
| C | -0.78777500 | 3.96803700 | 0.04254000 |
| C | -3.18810000 | 3.51863400 | -0.64850200 |
| C | -2.09842000 | 2.10260000 | 1.12906000 |
| H | 0.15630600 | 3.50682200 | 0.34699300 |
| H | -0.62915000 | 4.55246900 | -0.86889000 |
| H | -1.12174900 | 4.64679800 | 0.83481400 |
| H | -3.95948200 | 2.75856300 | -0.81533600 |
| H | -3.55016900 | 4.20500800 | 0.12373000 |
| H | -3.05266900 | 4.08092700 | -1.57526000 |
| H | -2.61223000 | 2.74497800 | 1.85155900 |
| H | -2.72177900 | 1.21725600 | 0.96954300 |

H -1.15492100 1.80683900 1.60328800

int-S2(triplet)

C 2.23460900 3.74606800 -0.00405600
C 1.28120000 4.45009400 -0.74080600
C 0.01130300 3.90274000 -0.91538700
C -0.28442900 2.65884900 -0.35605000
C 0.66074800 1.93787300 0.39794800
C 1.92851400 2.49968800 0.56583600
H 3.22666200 4.16732500 0.14007700
H 1.52773100 5.41494100 -1.17426100
H -0.75853100 4.41206100 -1.48805000
H 2.69112200 2.00248300 1.15272500
C -1.60968100 2.02488900 -0.57068900
O -2.53798100 2.52247000 -1.19842700
N -1.61935800 0.77434500 0.04193300
C -2.64706300 -0.11024400 -0.03340400
C -3.91082400 0.03213600 -0.63868200
C -3.23222800 -2.33811200 0.61594800
C -4.81339700 -1.01772700 -0.60639000
H -4.12452900 0.97690000 -1.11679900
C -4.47442900 -2.22172400 0.02861700
H -2.86156200 -3.21328900 1.13232000
H -5.78509900 -0.90331700 -1.07587000
H -5.16054600 -3.05931500 0.06974500
O -1.16409700 -1.45314600 1.16501400
N -2.35473500 -1.30795400 0.57898900
Co -0.03339800 0.16928300 0.89188700
O 1.11769300 -0.37671800 2.12802000
C 2.37480700 0.02587500 2.57670200
H 2.72390600 -0.69632000 3.32931700
H 3.12782300 0.05478600 1.77391200
H 2.33957600 1.01531000 3.05703500
C 1.98042200 -1.06406000 -0.99260900
O 0.82355900 -0.66483700 -1.06372500
O 3.00984700 -0.21023200 -0.90368900
H 2.63130000 0.69435800 -0.84196200
C 2.37614600 -2.53066900 -0.95130500
C 1.11686200 -3.38331000 -1.16149100
C 3.43027800 -2.82037500 -2.03686700
C 2.96487800 -2.80642800 0.45226300
H 0.36510600 -3.15634200 -0.40025900
H 0.67120000 -3.19608200 -2.14364300
H 1.38054100 -4.44459300 -1.09825500
H 4.32485000 -2.20737800 -1.89662400
H 3.72204600 -3.87500100 -1.98746000
H 3.03167100 -2.62664900 -3.03913400
H 3.20505800 -3.87197600 0.53563500
H 3.88051800 -2.23128300 0.61703100
H 2.24306400 -2.54568400 1.23212100

int-S2(quinet)

C -1.66725100 -3.70570100 -0.63565600
C -0.54485000 -4.48676500 -0.34248300
C 0.67738800 -3.87066600 -0.08092000
C 0.76073100 -2.47460500 -0.10687300
C -0.36149300 -1.67386800 -0.38360300
C -1.57343700 -2.30816200 -0.65977300
H -2.61979400 -4.18804300 -0.84477000
H -0.62475500 -5.57026700 -0.32738700
H 1.57203700 -4.44852600 0.13300800
H -2.46724300 -1.73143400 -0.88670100
C 2.07176100 -1.79449400 0.10850500
O 3.14112000 -2.37695400 0.27016400

| | | | |
|----|-------------|-------------|-------------|
| N | 1.90631100 | -0.41564000 | 0.05503300 |
| C | 2.89726600 | 0.48046900 | -0.09956600 |
| C | 4.29345700 | 0.31515300 | 0.00444700 |
| C | 3.24104600 | 2.79818300 | -0.61463700 |
| C | 5.13787400 | 1.39245300 | -0.20061400 |
| H | 4.64918800 | -0.67655600 | 0.24654000 |
| C | 4.60891300 | 2.65526900 | -0.50953100 |
| H | 2.72640500 | 3.71872800 | -0.85502500 |
| H | 6.21154100 | 1.25739600 | -0.11579900 |
| H | 5.24484800 | 3.51818400 | -0.66745800 |
| O | 1.10510800 | 1.90981100 | -0.57421900 |
| N | 2.41946500 | 1.73994400 | -0.42323600 |
| Co | 0.04924000 | 0.32953900 | 0.07605700 |
| O | -0.51747200 | 0.54110400 | 1.78259500 |
| C | -0.06621400 | -0.25168400 | 2.85132900 |
| H | -0.69963700 | -0.06438600 | 3.72966600 |
| H | -0.11135900 | -1.32329300 | 2.60908200 |
| H | 0.97192200 | -0.00315900 | 3.11770000 |
| C | -2.87862900 | 0.99389800 | -0.96138200 |
| O | -1.65429100 | 1.05944400 | -1.01155400 |
| O | -3.55908500 | 0.49232100 | -2.00143500 |
| H | -2.89222300 | 0.19934600 | -2.65387300 |
| C | -3.73830400 | 1.40750100 | 0.21929000 |
| C | -3.03883300 | 2.55116800 | 0.97484500 |
| C | -5.14063800 | 1.83839000 | -0.24342400 |
| C | -3.83882600 | 0.16180600 | 1.13663500 |
| H | -2.07633800 | 2.22763700 | 1.37552400 |
| H | -2.88157700 | 3.41807400 | 0.32373100 |
| H | -3.67515000 | 2.86426000 | 1.80965500 |
| H | -5.66460600 | 1.02946200 | -0.75885100 |
| H | -5.73034700 | 2.12794300 | 0.63248100 |
| H | -5.09184700 | 2.69988700 | -0.91832500 |
| H | -4.43826200 | 0.42347200 | 2.01542700 |
| H | -4.32915700 | -0.67236600 | 0.62413200 |
| H | -2.84635500 | -0.14990900 | 1.47118200 |

TS-S3(singlet)

| | | | |
|----|-------------|-------------|-------------|
| C | 0.80322300 | 4.40269200 | -0.98922100 |
| C | 2.09968200 | 4.09002500 | -1.40021200 |
| C | 2.71352100 | 2.93911200 | -0.90667300 |
| C | 2.05893900 | 2.08686500 | -0.01317300 |
| C | 0.76422000 | 2.44097400 | 0.42259300 |
| C | 0.14175000 | 3.59430100 | -0.06559300 |
| H | 0.30769100 | 5.29258700 | -1.36752400 |
| H | 2.62402900 | 4.72923200 | -2.10357300 |
| H | 3.71371600 | 2.65931400 | -1.22179100 |
| H | -0.84783000 | 3.84390800 | 0.30206200 |
| C | 2.71664900 | 0.77251900 | 0.29173600 |
| O | 3.93566700 | 0.67294200 | 0.42473200 |
| N | 1.81157600 | -0.27158400 | 0.24578100 |
| C | 2.20110100 | -1.55548500 | 0.08450300 |
| C | 3.46754600 | -2.15699300 | 0.26335800 |
| C | 1.33005700 | -3.70878200 | -0.55588300 |
| C | 3.63713200 | -3.51238600 | 0.04914300 |
| H | 4.27358100 | -1.50690500 | 0.57070700 |
| C | 2.55300900 | -4.30998400 | -0.35924400 |
| H | 0.43533500 | -4.21574000 | -0.89270300 |
| H | 4.61373300 | -3.96047500 | 0.20291900 |
| H | 2.65518500 | -5.37545900 | -0.52655500 |
| O | -0.01423800 | -1.80949100 | -0.63801500 |
| N | 1.17509600 | -2.38169600 | -0.34394600 |
| Co | -0.05975800 | -0.04477400 | 0.06723900 |
| O | 0.16206800 | 1.76726900 | 1.43870500 |
| C | -0.46524900 | 1.06558000 | 2.49707600 |

| | | | |
|---|-------------|-------------|-------------|
| H | 0.04768400 | 0.11535400 | 2.66067900 |
| H | -0.40087500 | 1.69029300 | 3.39852700 |
| H | -1.51334000 | 0.89001900 | 2.24700100 |
| C | -2.84632900 | -0.65069400 | -0.17226800 |
| O | -1.95553400 | 0.20466800 | -0.05162600 |
| O | -2.59137300 | -1.94085900 | -0.31547100 |
| H | -1.59859400 | -2.08561100 | -0.33979800 |
| C | -4.32254300 | -0.28979400 | -0.17140800 |
| C | -4.48716200 | 1.21878600 | 0.05386800 |
| C | -4.91825600 | -0.69289400 | -1.53834400 |
| C | -5.02416000 | -1.07900800 | 0.95417400 |
| H | -5.55140700 | 1.47753400 | 0.04064600 |
| H | -4.07046200 | 1.52400700 | 1.01879600 |
| H | -3.97889700 | 1.79355300 | -0.72535800 |
| H | -4.80327400 | -1.76532600 | -1.71722500 |
| H | -5.98591300 | -0.44796400 | -1.55943700 |
| H | -4.42858500 | -0.15148900 | -2.35529300 |
| H | -6.09383700 | -0.84244400 | 0.95603900 |
| H | -4.90614200 | -2.15665700 | 0.81454400 |
| H | -4.61653800 | -0.81112100 | 1.93585900 |

TS-S3(triplet)

| | | | |
|----|-------------|-------------|-------------|
| C | 1.25427200 | 4.32621300 | -0.78725900 |
| C | 2.64290400 | 4.17185600 | -0.72825000 |
| C | 3.18504900 | 2.93857400 | -0.35567300 |
| C | 2.35448000 | 1.86767500 | -0.03246300 |
| C | 0.94984200 | 2.04529600 | -0.06103100 |
| C | 0.40020100 | 3.27882300 | -0.42812500 |
| H | 0.82663800 | 5.27438500 | -1.10420900 |
| H | 3.29578000 | 5.00031600 | -0.98545400 |
| H | 4.25840400 | 2.77126700 | -0.34168300 |
| H | -0.67600700 | 3.42167000 | -0.44554100 |
| C | 2.92206100 | 0.50642100 | 0.17833000 |
| O | 4.11027600 | 0.28635800 | 0.40748900 |
| N | 1.92979000 | -0.44766300 | 0.00152600 |
| C | 2.12508300 | -1.76852300 | 0.00977300 |
| C | 3.30437000 | -2.51135500 | 0.26895700 |
| C | 0.96330700 | -3.85394500 | -0.32984200 |
| C | 3.28696300 | -3.89096900 | 0.23544600 |
| H | 4.19237700 | -1.93676800 | 0.49184200 |
| C | 2.09998400 | -4.58395800 | -0.06431700 |
| H | 0.00285800 | -4.27942600 | -0.58939900 |
| H | 4.19845400 | -4.44264000 | 0.44433900 |
| H | 2.05834500 | -5.66587900 | -0.09614200 |
| O | -0.14239700 | -1.82637000 | -0.61544100 |
| N | 0.98308700 | -2.50244500 | -0.28885000 |
| Co | 0.01052600 | 0.17695100 | -0.17202300 |
| O | 0.17302800 | 1.30207700 | 1.43880400 |
| C | -0.85802700 | 2.11507200 | 1.95669300 |
| H | -1.10211900 | 1.72862500 | 2.95457300 |
| H | -0.52036400 | 3.15565600 | 2.05546100 |
| H | -1.76872300 | 2.09601900 | 1.34307800 |
| C | -2.92381300 | -0.48100400 | -0.19791200 |
| O | -2.05903200 | 0.37180600 | -0.44053100 |
| O | -2.65185700 | -1.75475100 | 0.00612600 |
| H | -1.66535100 | -1.93553800 | -0.12827900 |
| C | -4.40175000 | -0.13117400 | -0.08327700 |
| C | -4.61373300 | 1.35093900 | -0.41694200 |
| C | -5.20355200 | -1.02149500 | -1.05491200 |
| C | -4.83789400 | -0.41795600 | 1.37111800 |
| H | -5.67864500 | 1.59432500 | -0.33819100 |
| H | -4.06102500 | 1.99692300 | 0.27134400 |
| H | -4.27987100 | 1.58118800 | -1.43295300 |
| H | -5.06052900 | -2.08145100 | -0.83022300 |

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|---|-------------|-------------|-------------|
| H | -6.26996000 | -0.78698600 | -0.96808000 |
| H | -4.90188300 | -0.84395800 | -2.09327900 |
| H | -5.89810600 | -0.16913800 | 1.48854000 |
| H | -4.69709000 | -1.47179200 | 1.62560800 |
| H | -4.26614800 | 0.19039100 | 2.08106000 |

TS-S3(quinet)

| | | | |
|----|-------------|-------------|-------------|
| C | 1.88786100 | 4.33940300 | -0.60684500 |
| C | 3.23036200 | 3.95318700 | -0.40320800 |
| C | 3.52587300 | 2.62854300 | -0.09248500 |
| C | 2.51228400 | 1.67166500 | 0.01258600 |
| C | 1.13629900 | 2.05482000 | -0.18838600 |
| C | 0.86095100 | 3.42437400 | -0.46545100 |
| H | 1.65964300 | 5.36679200 | -0.88163100 |
| H | 4.02686400 | 4.68608900 | -0.48995400 |
| H | 4.55118100 | 2.29973500 | 0.04953300 |
| H | -0.16759300 | 3.74924300 | -0.59888900 |
| C | 2.90210800 | 0.25518300 | 0.20383200 |
| O | 4.04457400 | -0.10360500 | 0.49978700 |
| N | 1.83640100 | -0.61595200 | -0.03902300 |
| C | 1.90903700 | -1.94699600 | 0.02375200 |
| C | 2.99545100 | -2.78259500 | 0.39643600 |
| C | 0.59182200 | -3.94143400 | -0.33274800 |
| C | 2.85834200 | -4.15389500 | 0.39997700 |
| H | 3.91315200 | -2.27798100 | 0.66321900 |
| C | 1.63835200 | -4.75471200 | 0.03019400 |
| H | -0.38350200 | -4.28970400 | -0.64636800 |
| H | 3.70138900 | -4.77458500 | 0.68761900 |
| H | 1.50707200 | -5.82985300 | 0.02039900 |
| O | -0.32916300 | -1.84125800 | -0.71714000 |
| N | 0.72812500 | -2.59393600 | -0.32313600 |
| Co | 0.02082000 | 0.14318000 | -0.42408700 |
| O | 0.19057700 | 1.43307000 | 1.14339500 |
| C | -0.82987800 | 2.29012800 | 1.61927900 |
| H | -1.32235200 | 1.77414800 | 2.45308400 |
| H | -0.39942800 | 3.22972200 | 1.98563700 |
| H | -1.58430000 | 2.51293000 | 0.85409500 |
| C | -2.96374300 | -0.30438200 | -0.19017800 |
| O | -2.06096400 | 0.44568000 | -0.58892600 |
| O | -2.76838000 | -1.57195500 | 0.10921900 |
| H | -1.81264400 | -1.82917900 | -0.10334000 |
| C | -4.38693900 | 0.18652900 | 0.03621100 |
| C | -4.61695600 | 0.20700900 | 1.56557600 |
| C | -4.54979400 | 1.59893000 | -0.54046800 |
| C | -5.38025000 | -0.78596500 | -0.62937200 |
| H | -5.62848000 | 0.57135300 | 1.77472700 |
| H | -4.51156700 | -0.79335600 | 1.99466700 |
| H | -3.90535700 | 0.87603100 | 2.06211600 |
| H | -4.35557200 | 1.61344500 | -1.61729400 |
| H | -5.57434900 | 1.94585600 | -0.36989600 |
| H | -3.86212800 | 2.30452200 | -0.06679800 |
| H | -6.40358700 | -0.43789800 | -0.45279400 |
| H | -5.22160300 | -0.83275600 | -1.71255800 |
| H | -5.28091200 | -1.79540200 | -0.22300100 |

int-S4(singlet)

| | | | |
|---|-------------|------------|------------|
| C | -2.58673000 | 2.32545900 | 3.59580700 |
| C | -2.81681300 | 1.08112500 | 3.00635800 |
| C | -1.74286200 | 0.27498000 | 2.63456100 |
| C | -0.43228400 | 0.70763400 | 2.86060000 |
| C | -0.20396800 | 1.94174400 | 3.48118600 |
| C | -1.27759500 | 2.75443000 | 3.83396900 |
| H | -3.42471900 | 2.95823300 | 3.87584200 |
| H | -3.83384900 | 0.73957600 | 2.83258400 |

| | | | |
|----|-------------|-------------|-------------|
| H | -1.90982800 | -0.67985200 | 2.15372200 |
| H | 0.81916000 | 2.24950900 | 3.66928400 |
| H | -1.09720800 | 3.71997200 | 4.29815000 |
| C | 0.74752300 | -0.12945700 | 2.50400100 |
| O | 1.76670200 | -0.10374900 | 3.19155100 |
| C | 1.56384900 | -1.84071600 | 1.05605400 |
| C | 2.56692800 | -2.41984400 | 1.86050000 |
| C | 3.45375000 | -3.33269500 | 1.31449900 |
| H | 2.63801400 | -2.09695500 | 2.88684400 |
| C | 2.38758500 | -3.11391900 | -0.81252500 |
| C | 3.37889200 | -3.68203700 | -0.04243800 |
| H | 4.22754400 | -3.76106000 | 1.94352900 |
| H | 2.23178800 | -3.27420900 | -1.87015400 |
| H | 4.08353700 | -4.36630600 | -0.49894900 |
| N | 1.50701800 | -2.26043100 | -0.24817800 |
| O | 0.51915400 | -1.77443100 | -1.01749900 |
| N | 0.59911100 | -0.92696100 | 1.36693900 |
| H | -1.73710400 | -0.41660100 | -2.35576300 |
| Co | -0.05417700 | -0.16023700 | -0.30331700 |
| O | 1.57192900 | 0.70818100 | -0.36252000 |
| O | -0.85028700 | 1.61044100 | 0.08069000 |
| O | -1.86270100 | -1.04437400 | -0.11696700 |
| C | 2.49103100 | 0.55160300 | -1.29407100 |
| O | 2.39552500 | -0.10523700 | -2.31928900 |
| C | -2.54359800 | -1.51428300 | -1.04154500 |
| O | -2.42017400 | -1.14696200 | -2.29604800 |
| C | -1.01871100 | 1.78923800 | -1.15676200 |
| O | -0.68505700 | 0.79477300 | -1.91700900 |
| C | -3.57115400 | -2.59673000 | -0.74909400 |
| C | -4.39539000 | -2.95535900 | -1.99258600 |
| C | -2.77055900 | -3.82516400 | -0.25898100 |
| C | -4.49192800 | -2.08948100 | 0.37947800 |
| H | -4.95147100 | -2.09052100 | -2.36730100 |
| H | -3.75947000 | -3.32414400 | -2.80199400 |
| H | -5.11500200 | -3.73963000 | -1.73445200 |
| H | -2.17703100 | -3.57351800 | 0.62415500 |
| H | -3.46342000 | -4.63376300 | -0.00319100 |
| H | -2.09118200 | -4.18738000 | -1.03814600 |
| H | -5.20890700 | -2.87360800 | 0.64408100 |
| H | -3.91617400 | -1.82819700 | 1.27084800 |
| H | -5.05715600 | -1.20594000 | 0.06178700 |
| C | -1.49186500 | 3.10061000 | -1.73861800 |
| C | -0.21391300 | 3.83911400 | -2.20584700 |
| C | -2.41344700 | 2.82949100 | -2.94012300 |
| C | -2.21562400 | 3.91470600 | -0.65589600 |
| H | 0.46252400 | 4.01641400 | -1.36371200 |
| H | 0.32118800 | 3.25382900 | -2.95976800 |
| H | -0.49043600 | 4.80568000 | -2.64138400 |
| H | -3.30897000 | 2.27480300 | -2.63598600 |
| H | -2.73755700 | 3.77964700 | -3.37777800 |
| H | -1.89655900 | 2.25237500 | -3.71169100 |
| H | -2.51347700 | 4.88684000 | -1.06359900 |
| H | -3.11529900 | 3.39644000 | -0.30727400 |
| H | -1.57049800 | 4.07719500 | 0.21103700 |
| C | 3.79214700 | 1.28890700 | -0.88881100 |
| C | 3.47397800 | 2.74792200 | -0.51677200 |
| C | 4.37241100 | 0.55241900 | 0.33695300 |
| C | 4.78430900 | 1.23972300 | -2.05612600 |
| H | 3.04056600 | 3.28387600 | -1.37003200 |
| H | 2.76353700 | 2.79168400 | 0.31234600 |
| H | 4.39172000 | 3.27165300 | -0.22224500 |
| H | 4.57934500 | -0.49797000 | 0.09779600 |
| H | 5.31670500 | 1.01901100 | 0.64339000 |
| H | 3.67881400 | 0.57945200 | 1.18191600 |

| | | | |
|---|------------|------------|-------------|
| H | 5.72042000 | 1.73603100 | -1.77287900 |
| H | 5.00541500 | 0.20702700 | -2.33907300 |
| H | 4.37843600 | 1.74289000 | -2.93955700 |

int-S4(triplet)

| | | | |
|----|-------------|-------------|-------------|
| C | -1.65155300 | -2.54047300 | 3.81456500 |
| C | -0.43984400 | -1.95812100 | 3.44611300 |
| C | -0.42571900 | -0.77532600 | 2.70787800 |
| C | -1.63166900 | -0.16773600 | 2.34231300 |
| C | -2.84907700 | -0.73902100 | 2.74155400 |
| C | -2.85910800 | -1.92835100 | 3.46138600 |
| H | -1.65937600 | -3.46855300 | 4.37962500 |
| H | 0.49898800 | -2.42876900 | 3.72210700 |
| H | 0.51623000 | -0.32489500 | 2.42008800 |
| H | -3.77334700 | -0.23723900 | 2.47662400 |
| H | -3.80403100 | -2.37845900 | 3.75187400 |
| C | -1.67580500 | 1.12344700 | 1.60517300 |
| O | -2.59056300 | 1.92294200 | 1.78404100 |
| C | -0.43840200 | 2.59640500 | 0.17556700 |
| C | -0.90419800 | 3.84251700 | 0.64754100 |
| C | -0.52382100 | 5.01350500 | 0.01895900 |
| H | -1.56869900 | 3.84075000 | 1.49666600 |
| C | 0.74469700 | 3.75402600 | -1.56224900 |
| C | 0.31686200 | 4.97889600 | -1.10424400 |
| H | -0.88588100 | 5.96316000 | 0.39953800 |
| H | 1.37085800 | 3.58883900 | -2.42830400 |
| H | 0.62256800 | 5.87995800 | -1.62186100 |
| N | 0.37021600 | 2.61770200 | -0.93059200 |
| O | 0.77459400 | 1.45259800 | -1.45430800 |
| N | -0.60724600 | 1.36081400 | 0.72973800 |
| H | 2.48572900 | -0.62159000 | -1.45386500 |
| Co | 0.11780600 | -0.03932200 | -0.41915700 |
| O | -1.59704100 | -0.58045100 | -0.87169200 |
| O | 0.34189900 | -2.27193500 | 0.29475900 |
| O | 1.96701600 | 0.14755400 | 0.67945400 |
| C | -2.47697000 | 0.26897300 | -1.36626700 |
| O | -2.23519600 | 1.41473100 | -1.72046500 |
| C | 3.06722600 | 0.25966300 | 0.12425000 |
| O | 3.31756600 | -0.19416000 | -1.08776500 |
| C | 0.87080200 | -2.39856300 | -0.81759800 |
| O | 0.97848200 | -1.33889600 | -1.58758200 |
| C | 4.21922400 | 1.00850900 | 0.77498500 |
| C | 5.55240400 | 0.28891200 | 0.50765100 |
| C | 4.22980200 | 2.41004900 | 0.11581000 |
| C | 3.96367100 | 1.14031900 | 2.28253900 |
| H | 5.55095600 | -0.71686800 | 0.94224300 |
| H | 5.74908000 | 0.19860200 | -0.56325600 |
| H | 6.37096000 | 0.85412500 | 0.96602700 |
| H | 3.27854900 | 2.92827900 | 0.27978100 |
| H | 5.02957900 | 3.01317600 | 0.55896900 |
| H | 4.40419300 | 2.33693800 | -0.96165900 |
| H | 4.77354100 | 1.71633600 | 2.74248900 |
| H | 3.01616300 | 1.64776300 | 2.48026400 |
| H | 3.92549300 | 0.15774600 | 2.76432900 |
| C | 1.47102900 | -3.71369700 | -1.30526800 |
| C | 1.52964700 | -3.75647500 | -2.83947200 |
| C | 2.90000900 | -3.78237800 | -0.71608200 |
| C | 0.62710500 | -4.87702400 | -0.76005500 |
| H | 0.52886800 | -3.66862200 | -3.27471200 |
| H | 2.14008700 | -2.94249700 | -3.23988100 |
| H | 1.96408200 | -4.70827900 | -3.16580400 |
| H | 2.86882800 | -3.75248600 | 0.37806000 |
| H | 3.38156100 | -4.71730800 | -1.02347300 |
| H | 3.51881500 | -2.94939200 | -1.06765700 |

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|---|-------------|-------------|-------------|
| H | 1.08442500 | -5.83246100 | -1.04108200 |
| H | 0.55089100 | -4.82598200 | 0.32863700 |
| H | -0.38827800 | -4.84872000 | -1.17000100 |
| C | -3.90197400 | -0.32147700 | -1.48094600 |
| C | -4.00902300 | -1.72097100 | -0.86183700 |
| C | -4.84584400 | 0.65889900 | -0.75837800 |
| C | -4.24951000 | -0.37058300 | -2.98117200 |
| H | -3.35098500 | -2.43199300 | -1.36977800 |
| H | -3.72951600 | -1.71111700 | 0.19541100 |
| H | -5.04124700 | -2.08271800 | -0.94607600 |
| H | -4.77802900 | 1.65401200 | -1.20495300 |
| H | -5.88031800 | 0.30291500 | -0.83330000 |
| H | -4.58771500 | 0.75231800 | 0.30178500 |
| H | -5.28279400 | -0.71245500 | -3.11548700 |
| H | -4.14552200 | 0.61995900 | -3.43294800 |
| H | -3.59008700 | -1.06500200 | -3.51502300 |

int-S4(quintet)

| | | | |
|----|-------------|-------------|-------------|
| C | 1.63113200 | -2.40378700 | 3.81840500 |
| C | 1.89428500 | -1.20244200 | 3.15849700 |
| C | 0.85799900 | -0.49852700 | 2.54997000 |
| C | -0.45159200 | -0.99101300 | 2.61210000 |
| C | -0.71712900 | -2.18487100 | 3.29685600 |
| C | 0.32341600 | -2.89473900 | 3.88715800 |
| H | 2.44291600 | -2.95868100 | 4.28082300 |
| H | 2.90965100 | -0.81863700 | 3.10789600 |
| H | 1.06276700 | 0.42187900 | 2.01642100 |
| H | -1.74057900 | -2.54105400 | 3.34483700 |
| H | 0.11939200 | -3.82946700 | 4.40123400 |
| C | -1.59028200 | -0.25839000 | 2.00110100 |
| O | -2.75077000 | -0.43304100 | 2.36338200 |
| C | -1.94740000 | 1.70956300 | 0.71721400 |
| C | -2.87706200 | 2.36510700 | 1.57532100 |
| C | -3.45729900 | 3.55148600 | 1.20578100 |
| H | -3.11667600 | 1.87799500 | 2.50939100 |
| C | -2.28110200 | 3.50219300 | -0.88358700 |
| C | -3.15568400 | 4.13872900 | -0.04709300 |
| H | -4.15951800 | 4.03828600 | 1.87483700 |
| H | -1.99889600 | 3.83423700 | -1.87299000 |
| H | -3.61397100 | 5.06837500 | -0.36196300 |
| N | -1.68754300 | 2.33137300 | -0.50886600 |
| O | -0.92790000 | 1.72681000 | -1.38090200 |
| N | -1.24394000 | 0.60861300 | 0.94895600 |
| H | 2.43502000 | 0.52694900 | -2.02546200 |
| Co | -0.06012100 | -0.04216900 | -0.67022300 |
| O | -1.47842000 | -1.20618400 | -1.40084600 |
| O | 1.12716000 | -1.69899100 | -0.13656100 |
| O | 1.53541700 | 1.35122300 | -0.04028500 |
| C | -2.66870800 | -0.75857600 | -1.54905500 |
| O | -2.94677700 | 0.39835500 | -1.92825000 |
| C | 2.56690800 | 1.76517000 | -0.58297500 |
| O | 3.01212400 | 1.31500500 | -1.73511200 |
| C | 1.79696500 | -1.63367600 | -1.19981000 |
| O | 1.49426200 | -0.73735300 | -2.07816500 |
| C | 3.45134700 | 2.80226100 | 0.09991100 |
| C | 4.39621900 | 2.00093600 | 1.02790000 |
| C | 4.27280100 | 3.59987900 | -0.92425500 |
| C | 2.57136600 | 3.74294400 | 0.93842900 |
| H | 3.82588500 | 1.41720800 | 1.75821800 |
| H | 5.02716200 | 1.31495500 | 0.45319400 |
| H | 5.04827300 | 2.69248300 | 1.57230900 |
| H | 3.62144100 | 4.15317400 | -1.60918600 |
| H | 4.90748800 | 4.32237100 | -0.39945500 |
| H | 4.91158000 | 2.94486100 | -1.52104500 |

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|---|-------------|-------------|-------------|
| H | 3.20288400 | 4.45982800 | 1.47378600 |
| H | 1.88075200 | 4.30626600 | 0.30098900 |
| H | 1.97878800 | 3.18480300 | 1.66725200 |
| C | 3.00815200 | -2.54299000 | -1.39265400 |
| C | 3.39724100 | -2.63625500 | -2.87375000 |
| C | 4.15575800 | -1.89784900 | -0.57914000 |
| C | 2.69164900 | -3.93514400 | -0.82056500 |
| H | 2.58012700 | -3.05635400 | -3.46914200 |
| H | 3.63765900 | -1.65232900 | -3.28572200 |
| H | 4.27441700 | -3.28373300 | -2.98791300 |
| H | 3.87173800 | -1.80066100 | 0.47387800 |
| H | 5.05464400 | -2.52145400 | -0.64320400 |
| H | 4.40290900 | -0.90329600 | -0.96712300 |
| H | 3.57448900 | -4.58052200 | -0.89669200 |
| H | 2.39181100 | -3.86353700 | 0.22770700 |
| H | 1.87349500 | -4.40854400 | -1.37448100 |
| C | -3.84352700 | -1.72156100 | -1.24305200 |
| C | -3.34614600 | -2.92641100 | -0.43458000 |
| C | -4.91090100 | -0.95160500 | -0.44525100 |
| C | -4.41514600 | -2.17964900 | -2.59925400 |
| H | -2.56177300 | -3.46815500 | -0.96842500 |
| H | -2.94091800 | -2.60905200 | 0.53097600 |
| H | -4.18287200 | -3.61037800 | -0.24544200 |
| H | -5.26620700 | -0.08366900 | -1.00736800 |
| H | -5.76380600 | -1.60815000 | -0.23576700 |
| H | -4.50353000 | -0.60502600 | 0.51067200 |
| H | -5.26883200 | -2.84849300 | -2.43678400 |
| H | -4.75288400 | -1.32157100 | -3.18866700 |
| H | -3.66150500 | -2.72352900 | -3.18002800 |

int-S5(singlet)

| | | | |
|----|-------------|-------------|-------------|
| C | -5.04141300 | 1.15647000 | -0.45552500 |
| C | -4.20176000 | 1.29843800 | 0.65076600 |
| C | -2.83062200 | 1.48656400 | 0.47078700 |
| C | -2.29948700 | 1.55670200 | -0.82293700 |
| C | -3.14779400 | 1.43077900 | -1.93106400 |
| C | -4.51025200 | 1.21446300 | -1.74836200 |
| H | -6.10776500 | 1.00489900 | -0.31251300 |
| H | -4.61421600 | 1.26978900 | 1.65517800 |
| H | -2.16967700 | 1.58766000 | 1.32308000 |
| H | -2.72130600 | 1.51580900 | -2.92476700 |
| H | -5.16222700 | 1.10275700 | -2.60992500 |
| C | -0.87769500 | 1.94603400 | -1.05244700 |
| O | -0.56429400 | 2.60810500 | -2.03649400 |
| N | 0.02525600 | 1.59165900 | -0.04369000 |
| C | 1.09774400 | 2.38190700 | 0.21549400 |
| C | 1.39573700 | 3.68325900 | -0.24819400 |
| C | 2.50885200 | 4.35217000 | 0.22484900 |
| H | 0.74324200 | 4.11317600 | -0.99316100 |
| C | 3.06810000 | 2.47209200 | 1.58874900 |
| C | 3.36485600 | 3.74625400 | 1.16016900 |
| H | 2.72594200 | 5.34980300 | -0.14342200 |
| H | 3.64784600 | 1.89375900 | 2.29557600 |
| H | 4.24993200 | 4.24467600 | 1.53602600 |
| N | 1.96934000 | 1.83679300 | 1.12414100 |
| O | 1.69438900 | 0.60548200 | 1.60398800 |
| Co | 0.50674200 | -0.23308600 | 0.42005800 |
| C | -1.48358900 | -1.36262600 | 0.59555800 |
| O | -0.88287900 | -1.18721100 | -0.52272100 |
| O | -0.98926700 | -0.72323800 | 1.58435100 |
| C | -2.60746000 | -2.36382800 | 0.73953200 |
| C | -1.91096100 | -3.74081300 | 0.87612000 |
| C | -3.43398500 | -2.06716000 | 1.99787800 |
| C | -3.48625600 | -2.34469600 | -0.52162800 |

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|---|-------------|-------------|-------------|
| H | -1.30412100 | -3.95933900 | -0.00767600 |
| H | -1.25998700 | -3.76585400 | 1.75603300 |
| H | -2.67109500 | -4.52273500 | 0.98229800 |
| H | -3.93407200 | -1.09850300 | 1.91658200 |
| H | -4.20015100 | -2.84039000 | 2.12299600 |
| H | -2.80290400 | -2.05283400 | 2.89049300 |
| H | -4.25242000 | -3.12428900 | -0.44289100 |
| H | -3.98620500 | -1.38023700 | -0.64045300 |
| H | -2.88863400 | -2.53228500 | -1.41747300 |
| C | 2.20778500 | -1.54672000 | -0.38248000 |
| O | 1.47578700 | -1.92090900 | 0.59134700 |
| O | 1.92548100 | -0.39777400 | -0.87678600 |
| C | 3.33735700 | -2.38408900 | -0.94077000 |
| C | 3.00761000 | -2.68664900 | -2.41808100 |
| C | 4.63014000 | -1.54626700 | -0.85320100 |
| C | 3.47755900 | -3.68487600 | -0.13957700 |
| H | 2.08453300 | -3.27071200 | -2.50232500 |
| H | 2.88160600 | -1.76228600 | -2.98836700 |
| H | 3.82267000 | -3.26744400 | -2.86395100 |
| H | 4.87390900 | -1.30850600 | 0.18839000 |
| H | 5.46540500 | -2.11324700 | -1.27879800 |
| H | 4.52577500 | -0.60852600 | -1.40589200 |
| H | 4.29495600 | -4.28492100 | -0.55450800 |
| H | 3.69629200 | -3.48035900 | 0.91272000 |
| H | 2.55793400 | -4.27577700 | -0.18127600 |

int-S5(triplet)

| | | | |
|----|-------------|-------------|-------------|
| C | 5.09450400 | 0.54333200 | -0.09698200 |
| C | 4.11619400 | 0.72268900 | -1.07653200 |
| C | 2.83365300 | 1.13581500 | -0.71710700 |
| C | 2.52910000 | 1.37704700 | 0.62842100 |
| C | 3.51892200 | 1.21068100 | 1.60814800 |
| C | 4.79321600 | 0.78552300 | 1.24768300 |
| H | 6.09133500 | 0.21623100 | -0.37922400 |
| H | 4.34840700 | 0.54115800 | -2.12151300 |
| H | 2.06965000 | 1.26356900 | -1.47334500 |
| H | 3.26764900 | 1.42083400 | 2.64200200 |
| H | 5.55383800 | 0.64451200 | 2.00995900 |
| C | 1.21630600 | 1.93330400 | 1.04695400 |
| O | 1.08713300 | 2.57506300 | 2.07960600 |
| N | 0.13867400 | 1.73670700 | 0.15032700 |
| C | -0.76837200 | 2.72744100 | -0.03691800 |
| C | -0.77017900 | 4.05874800 | 0.44010400 |
| C | -1.76731700 | 4.92926000 | 0.04901200 |
| H | 0.00668200 | 4.35042500 | 1.13115500 |
| C | -2.78159900 | 3.20695900 | -1.26572000 |
| C | -2.79254300 | 4.50629800 | -0.81840700 |
| H | -1.76367200 | 5.94653500 | 0.42676700 |
| H | -3.51105300 | 2.75714500 | -1.92576100 |
| H | -3.58938000 | 5.17105000 | -1.12829600 |
| N | -1.79293400 | 2.36802100 | -0.87395600 |
| O | -1.79394000 | 1.11060800 | -1.35702500 |
| Co | -0.59380100 | 0.04403900 | -0.40439000 |
| C | 1.23252700 | -1.54606300 | -0.56082500 |
| O | 0.68084200 | -1.06131600 | 0.50584700 |
| O | 0.91633000 | -1.04254000 | -1.66655000 |
| C | 2.14986700 | -2.75043400 | -0.42007000 |
| C | 1.21085100 | -3.97602600 | -0.31746400 |
| C | 3.04798100 | -2.87396100 | -1.65814200 |
| C | 2.99324800 | -2.62754500 | 0.85955600 |
| H | 0.55414800 | -3.89014100 | 0.55340100 |
| H | 0.58487900 | -4.06387300 | -1.21157600 |
| H | 1.80817100 | -4.88951700 | -0.21820400 |
| H | 3.71483000 | -2.01043400 | -1.74295000 |

| | | | |
|---|-------------|-------------|-------------|
| H | 3.66308800 | -3.77759200 | -1.57943000 |
| H | 2.45142000 | -2.93295700 | -2.57206400 |
| H | 3.61509600 | -3.52260300 | 0.97744000 |
| H | 3.65101100 | -1.75512000 | 0.81576800 |
| H | 2.35490800 | -2.52701500 | 1.74105600 |
| C | -2.40553000 | -1.39960900 | 0.38347000 |
| O | -1.70296600 | -1.51469300 | -0.69725100 |
| O | -2.17306200 | -0.44129100 | 1.15883000 |
| C | -3.46498800 | -2.46141400 | 0.65996300 |
| C | -2.73325000 | -3.80912400 | 0.83627600 |
| C | -4.24529500 | -2.10616400 | 1.93158800 |
| C | -4.41076500 | -2.53731500 | -0.55457300 |
| H | -2.16735400 | -4.06623900 | -0.06324100 |
| H | -2.03673500 | -3.76897500 | 1.68150700 |
| H | -3.46190000 | -4.60392400 | 1.03299300 |
| H | -4.75725000 | -1.14489500 | 1.82438700 |
| H | -4.99636100 | -2.87890300 | 2.13228400 |
| H | -3.57921700 | -2.03277900 | 2.79576000 |
| H | -5.16504600 | -3.31567900 | -0.39102500 |
| H | -4.93280200 | -1.58532300 | -0.70523900 |
| H | -3.85578800 | -2.77091400 | -1.46693100 |

int-S5(quintet)

| | | | |
|----|-------------|-------------|-------------|
| C | -3.73966800 | 2.99589100 | -1.11821300 |
| C | -3.02977300 | 2.82957500 | 0.07303500 |
| C | -1.67753800 | 2.49489600 | 0.04010100 |
| C | -1.02525400 | 2.34919500 | -1.19102200 |
| C | -1.73497800 | 2.53861200 | -2.38468800 |
| C | -3.09169700 | 2.84394800 | -2.34780000 |
| H | -4.79656600 | 3.24600800 | -1.08914900 |
| H | -3.52992000 | 2.95804100 | 1.02803100 |
| H | -1.13230800 | 2.33208600 | 0.96214300 |
| H | -1.20609000 | 2.43709000 | -3.32614000 |
| H | -3.64461400 | 2.97055000 | -3.27386400 |
| C | 0.43569700 | 2.09355800 | -1.27254100 |
| O | 1.10078500 | 2.39012400 | -2.25507600 |
| N | 1.00347000 | 1.48749400 | -0.12576500 |
| C | 2.24619400 | 1.81642100 | 0.25853600 |
| C | 3.05882600 | 2.89577700 | -0.17129600 |
| C | 4.28272900 | 3.12571600 | 0.41656200 |
| H | 2.68933400 | 3.50848600 | -0.98073900 |
| C | 3.96606000 | 1.22804700 | 1.84639000 |
| C | 4.74873100 | 2.28274600 | 1.44592700 |
| H | 4.89215500 | 3.95784600 | 0.07958200 |
| H | 4.21957100 | 0.51078200 | 2.61512700 |
| H | 5.70923500 | 2.44199300 | 1.92080700 |
| N | 2.75909200 | 1.00688600 | 1.26151900 |
| O | 2.04754300 | -0.03391100 | 1.66471200 |
| Co | 0.44993200 | -0.33920800 | 0.55848300 |
| C | -1.95582100 | -0.57383900 | 0.89369200 |
| O | -1.54320700 | -0.73631900 | -0.28301000 |
| O | -1.11657800 | -0.14304000 | 1.78116400 |
| C | -3.36720700 | -0.95617800 | 1.31070500 |
| C | -3.27833100 | -2.43540100 | 1.75804500 |
| C | -3.84106600 | -0.08538800 | 2.48398100 |
| C | -4.31785800 | -0.82556100 | 0.11125500 |
| H | -2.90747000 | -3.06475800 | 0.94282300 |
| H | -2.59969400 | -2.54515800 | 2.60978600 |
| H | -4.27196300 | -2.79195000 | 2.05285000 |
| H | -3.91154500 | 0.96663000 | 2.18899700 |
| H | -4.83435300 | -0.41296200 | 2.81166300 |
| H | -3.15160600 | -0.15538200 | 3.32895200 |
| H | -5.32628600 | -1.14250900 | 0.40151800 |
| H | -4.36647300 | 0.20993300 | -0.24028200 |

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|---|-------------|-------------|-------------|
| H | -3.98004900 | -1.44586600 | -0.72254800 |
| C | 1.01361600 | -2.49751200 | -0.44539500 |
| O | 0.51784400 | -2.51124300 | 0.71202100 |
| O | 1.28760900 | -1.35583500 | -0.98123100 |
| C | 1.25009300 | -3.76427700 | -1.25544100 |
| C | 0.22389200 | -3.74541800 | -2.41065900 |
| C | 2.67989900 | -3.73562300 | -1.82715600 |
| C | 1.04041600 | -5.00361700 | -0.37646700 |
| H | -0.80015600 | -3.72358300 | -2.02230600 |
| H | 0.36762000 | -2.86488800 | -3.04282100 |
| H | 0.34271800 | -4.64563500 | -3.02453800 |
| H | 3.42546500 | -3.74427100 | -1.02347500 |
| H | 2.84746000 | -4.61882800 | -2.45412600 |
| H | 2.83889200 | -2.83963700 | -2.43283600 |
| H | 1.19108200 | -5.91039500 | -0.97367300 |
| H | 1.74589400 | -5.01989000 | 0.46041800 |
| H | 0.02983300 | -5.02337300 | 0.04052800 |

int-S6(singlet)

| | | | |
|----|-------------|-------------|-------------|
| C | 2.32069300 | 2.71945300 | 2.39776300 |
| C | 1.80435500 | 2.33587300 | 3.64115600 |
| C | 0.89040600 | 1.28725700 | 3.72002100 |
| C | 0.50647100 | 0.62864200 | 2.54786300 |
| C | 1.03029600 | 1.00741600 | 1.30395000 |
| C | 1.93600200 | 2.05900500 | 1.22368700 |
| H | 3.02960200 | 3.54253200 | 2.34197500 |
| H | 2.11427100 | 2.85840800 | 4.54174700 |
| H | 0.46642200 | 0.96762900 | 4.66773500 |
| H | 2.33675900 | 2.36893400 | 0.26327300 |
| C | -0.46502800 | -0.49145000 | 2.54892700 |
| O | -1.00763800 | -0.96872000 | 3.54132100 |
| N | -0.66588900 | -0.92239800 | 1.23553200 |
| C | -1.38094700 | -1.99548000 | 0.86583500 |
| C | -2.12679200 | -2.88610300 | 1.67817900 |
| C | -2.00713000 | -3.30301100 | -1.05144300 |
| C | -2.78763200 | -3.95628100 | 1.11096100 |
| H | -2.13929600 | -2.67799200 | 2.73837700 |
| C | -2.73240400 | -4.17881500 | -0.27740700 |
| H | -1.88558700 | -3.37186600 | -2.12426600 |
| H | -3.35177100 | -4.63188000 | 1.74633700 |
| H | -3.23861900 | -5.01373900 | -0.74614900 |
| O | -0.66940000 | -1.41942500 | -1.31342500 |
| N | -1.36676000 | -2.25113900 | -0.49017800 |
| Co | 0.32879800 | -0.04456900 | -0.11159100 |
| O | 1.63066300 | 0.53480900 | -1.45896400 |
| C | 2.37516900 | -0.42788700 | -1.07245000 |
| O | 1.90703000 | -1.14736800 | -0.12357700 |
| C | 3.75702800 | -0.68008600 | -1.63815400 |
| C | 3.91778700 | -2.18673600 | -1.91129100 |
| C | 3.96060400 | 0.13438800 | -2.92233700 |
| C | 4.76251400 | -0.23323700 | -0.55158100 |
| H | 3.74288900 | -2.76923700 | -1.00304500 |
| H | 3.21009900 | -2.52499800 | -2.67650000 |
| H | 4.93271700 | -2.39152800 | -2.26994100 |
| H | 3.83703100 | 1.20461800 | -2.73532100 |
| H | 4.97030500 | -0.03756300 | -3.31156600 |
| H | 3.23962800 | -0.15599600 | -3.69328200 |
| H | 5.78577500 | -0.39196800 | -0.91001100 |
| H | 4.64061200 | 0.82948900 | -0.31587800 |
| H | 4.61946900 | -0.80494700 | 0.36977100 |
| C | -1.94849200 | 1.40017000 | -1.20470800 |
| O | -1.03115200 | 1.34370200 | -0.36691800 |
| O | -2.24905500 | 0.42441200 | -2.02227800 |
| H | -1.62456000 | -0.37702300 | -1.83232300 |

| | | | |
|---|-------------|------------|-------------|
| C | -2.80398700 | 2.65170000 | -1.33606600 |
| C | -2.61787800 | 3.20220000 | -2.76680900 |
| C | -4.27907000 | 2.25603300 | -1.11425400 |
| C | -2.36669400 | 3.69546200 | -0.30043200 |
| H | -1.57256800 | 3.47446100 | -2.95038300 |
| H | -2.92088900 | 2.46635700 | -3.51651600 |
| H | -3.23066200 | 4.10144900 | -2.89188400 |
| H | -4.43066700 | 1.84921500 | -0.10798500 |
| H | -4.91316600 | 3.14296600 | -1.21923200 |
| H | -4.60249100 | 1.50850200 | -1.84344200 |
| H | -2.98033200 | 4.59620300 | -0.40933500 |
| H | -2.48267300 | 3.31615200 | 0.71891500 |
| H | -1.31650200 | 3.96957100 | -0.43332800 |

int-S6(triplet)

| | | | |
|----|-------------|-------------|-------------|
| C | 1.56961400 | -3.11151900 | 2.41713700 |
| C | 0.42726500 | -3.79921800 | 2.84548700 |
| C | -0.82829400 | -3.44008600 | 2.36061200 |
| C | -0.92657000 | -2.39182700 | 1.44106600 |
| C | 0.22047000 | -1.71766600 | 1.01088300 |
| C | 1.47522000 | -2.06333600 | 1.49327700 |
| H | 2.54477000 | -3.39481500 | 2.80578800 |
| H | 0.52230700 | -4.61115000 | 3.56063300 |
| H | -1.73396900 | -3.94725100 | 2.68080400 |
| H | 2.36152600 | -1.52947800 | 1.16743900 |
| C | -2.21938000 | -1.91446400 | 0.89768400 |
| O | -3.32611900 | -2.36304800 | 1.16653500 |
| N | -1.96668000 | -0.84209300 | 0.02962900 |
| C | -2.90883800 | -0.10096400 | -0.58993100 |
| C | -4.31580100 | -0.22713600 | -0.54031100 |
| C | -3.16744100 | 1.75976100 | -2.08503300 |
| C | -5.11454300 | 0.64317300 | -1.25644400 |
| H | -4.71268900 | -1.02325600 | 0.07294400 |
| C | -4.53910600 | 1.65564400 | -2.04392000 |
| H | -2.61287500 | 2.48799300 | -2.66170600 |
| H | -6.19380700 | 0.53890000 | -1.20979400 |
| H | -5.14279400 | 2.34760800 | -2.61838700 |
| O | -1.04808500 | 1.04004500 | -1.46181200 |
| N | -2.39185300 | 0.90939700 | -1.37207400 |
| Co | -0.16298900 | -0.30598800 | -0.24326800 |
| O | 1.70125800 | 0.21422000 | -0.65452600 |
| C | 1.85390100 | -0.67212800 | -1.57715400 |
| O | 0.90873300 | -1.46674400 | -1.81868900 |
| C | 3.17909800 | -0.77019300 | -2.32883400 |
| C | 2.87949400 | -0.81180400 | -3.83883500 |
| C | 4.09110900 | 0.41692500 | -1.99238500 |
| C | 3.84332500 | -2.09475400 | -1.89451900 |
| H | 2.20684400 | -1.63977400 | -4.07634700 |
| H | 2.40539700 | 0.11937500 | -4.16996100 |
| H | 3.81115800 | -0.93839600 | -4.40219400 |
| H | 4.31425600 | 0.45417400 | -0.92221300 |
| H | 5.03595100 | 0.32712000 | -2.54107300 |
| H | 3.62120700 | 1.36656300 | -2.26709500 |
| H | 4.79136100 | -2.22913600 | -2.42806700 |
| H | 4.05646400 | -2.09501200 | -0.81913100 |
| H | 3.19130000 | -2.94469500 | -2.11419000 |
| C | 0.39546400 | 2.32876000 | 1.10892300 |
| O | -0.08541300 | 1.22438700 | 1.37801900 |
| O | 0.16108100 | 2.95231700 | -0.03613500 |
| H | -0.36389800 | 2.33817200 | -0.62836000 |
| C | 1.36100500 | 3.05265900 | 2.03383700 |
| C | 2.76186500 | 2.87354100 | 1.39782700 |
| C | 1.00965500 | 4.54802100 | 2.12465400 |
| C | 1.32756100 | 2.39881000 | 3.42150700 |

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|---|------------|------------|------------|
| H | 2.99039600 | 1.81352100 | 1.25148700 |
| H | 2.81572400 | 3.36781400 | 0.42395600 |
| H | 3.51786000 | 3.31225000 | 2.05852800 |
| H | 0.01533900 | 4.69589400 | 2.56141800 |
| H | 1.73826600 | 5.05634000 | 2.76573500 |
| H | 1.02585500 | 5.02064100 | 1.13934700 |
| H | 2.05362200 | 2.89192300 | 4.07696200 |
| H | 0.33617700 | 2.48715900 | 3.87787600 |
| H | 1.57260600 | 1.33544300 | 3.36065000 |

int-S6(quintet)

| | | | |
|----|-------------|-------------|-------------|
| C | 1.07558900 | 3.72542100 | 1.79114300 |
| C | 0.19668200 | 3.51278300 | 2.86015600 |
| C | -0.50333500 | 2.31302100 | 2.97699300 |
| C | -0.32888600 | 1.30963200 | 2.01068600 |
| C | 0.55087500 | 1.56465600 | 0.97705900 |
| C | 1.26641000 | 2.73200200 | 0.81675400 |
| H | 1.61685200 | 4.66503400 | 1.71121100 |
| H | 0.06032600 | 4.29076400 | 3.60576700 |
| H | -1.18918900 | 2.12396900 | 3.79774000 |
| H | 1.94076900 | 2.87375200 | -0.02146400 |
| C | -1.06515300 | 0.01149500 | 2.09774200 |
| O | -1.79489300 | -0.25402700 | 3.05280800 |
| N | -0.82713700 | -0.78397700 | 0.99545900 |
| C | -1.26677000 | -2.05458800 | 0.91963700 |
| C | -1.88274000 | -2.86014400 | 1.90831000 |
| C | -1.33324800 | -3.94694700 | -0.56950200 |
| C | -2.19556800 | -4.17968500 | 1.64466600 |
| H | -2.09135500 | -2.39023000 | 2.85781000 |
| C | -1.91350300 | -4.74519500 | 0.39001900 |
| H | -1.07635200 | -4.26102900 | -1.57220000 |
| H | -2.65961200 | -4.78205000 | 2.41953300 |
| H | -2.14191700 | -5.77868100 | 0.15987400 |
| O | -0.52136600 | -1.90717500 | -1.30933800 |
| N | -1.04116200 | -2.65395400 | -0.30449800 |
| Co | 0.51137300 | -0.23901100 | -0.54820000 |
| O | 2.27588200 | 0.49068200 | -1.35113400 |
| C | 2.92621800 | -0.36310900 | -0.65428700 |
| O | 2.27236000 | -1.20370200 | 0.04591400 |
| C | 4.44806100 | -0.33247900 | -0.59482500 |
| C | 4.99054500 | -1.77167000 | -0.63004700 |
| C | 5.02035600 | 0.49336200 | -1.75443200 |
| C | 4.80751000 | 0.32777200 | 0.75718800 |
| H | 4.56252200 | -2.36843900 | 0.17900100 |
| H | 4.74662900 | -2.26014100 | -1.58042300 |
| H | 6.08137900 | -1.76144300 | -0.52375300 |
| H | 4.63258600 | 1.51522500 | -1.74013700 |
| H | 6.11326200 | 0.53124000 | -1.67912000 |
| H | 4.75768300 | 0.05142800 | -2.72125000 |
| H | 5.89678800 | 0.39044800 | 0.86072400 |
| H | 4.39713800 | 1.34184200 | 0.82046500 |
| H | 4.40855300 | -0.25598000 | 1.59205700 |
| C | -1.98801100 | 0.83026500 | -1.73569800 |
| O | -0.76147400 | 1.00039000 | -1.63558700 |
| O | -2.51851200 | -0.36056600 | -1.89408300 |
| H | -1.76546000 | -1.04388300 | -1.80650400 |
| C | -2.97065800 | 1.98091100 | -1.61109100 |
| C | -4.10690200 | 1.83407000 | -2.63771000 |
| C | -3.53821300 | 1.88961600 | -0.17198900 |
| C | -2.23138700 | 3.31393600 | -1.79264600 |
| H | -3.72161800 | 1.87569200 | -3.66263300 |
| H | -4.63938500 | 0.88834300 | -2.50966700 |
| H | -4.82108600 | 2.65492900 | -2.51139100 |
| H | -2.74113600 | 1.98858000 | 0.57141300 |

| | | | |
|---|-------------|------------|-------------|
| H | -4.25425000 | 2.70379100 | -0.01633700 |
| H | -4.05228900 | 0.93809400 | -0.00764500 |
| H | -2.93584700 | 4.14232600 | -1.66189500 |
| H | -1.42574700 | 3.41887700 | -1.06159200 |
| H | -1.79144100 | 3.39079000 | -2.79234700 |

proton-transfer TS(doublet)

| | | | |
|----|-------------|-------------|-------------|
| C | 2.42487500 | -3.94124200 | 0.01420400 |
| C | 1.71830300 | -3.35022000 | 1.06657000 |
| C | 0.97289300 | -2.20811200 | 0.80704500 |
| C | 0.89325700 | -1.64643700 | -0.49172000 |
| C | 1.63135800 | -2.24624100 | -1.52511400 |
| C | 2.38729600 | -3.39151600 | -1.27377000 |
| H | 3.01933100 | -4.83140000 | 0.20017200 |
| H | 1.76440200 | -3.74677400 | 2.07591500 |
| H | -0.30856600 | -1.38872200 | -0.80813800 |
| H | 1.59072900 | -1.81906900 | -2.52270700 |
| H | 2.94942400 | -3.86294000 | -2.07522500 |
| C | 0.31243000 | -1.44138700 | 1.89740200 |
| O | 0.19632600 | -1.77896400 | 3.05869100 |
| N | -0.02235600 | -0.14718200 | 1.40458600 |
| C | -0.49808200 | 0.85844100 | 2.16443200 |
| C | -1.32217000 | 0.77235500 | 3.29788900 |
| C | -0.55498900 | 3.23880300 | 2.27345900 |
| C | -1.76775000 | 1.93509800 | 3.89977000 |
| H | -1.59889700 | -0.21505300 | 3.63694000 |
| C | -1.38293600 | 3.18024500 | 3.37827300 |
| H | -0.20456300 | 4.14537700 | 1.79976200 |
| H | -2.42201400 | 1.88377600 | 4.76312600 |
| H | -1.72487100 | 4.10762600 | 3.82254500 |
| N | -0.11589300 | 2.09986000 | 1.69752100 |
| O | 0.70175700 | 2.17838000 | 0.65877400 |
| Co | 0.89890200 | 0.39965900 | -0.12130200 |
| O | -2.10308600 | 1.45615000 | -0.12173300 |
| O | 2.67667400 | 0.18506800 | 0.71675200 |
| C | -1.53143800 | 1.35700200 | -1.20811600 |
| O | -0.35844600 | 0.82783300 | -1.40904800 |
| C | 3.20661700 | 0.55697200 | -0.38804100 |
| O | 2.39698500 | 0.84084300 | -1.32919600 |
| C | 4.71275900 | 0.59630600 | -0.55272500 |
| C | 5.30929400 | 1.42236700 | 0.60339000 |
| C | 5.08267500 | 1.20932000 | -1.90946100 |
| C | 5.21056500 | -0.86387900 | -0.46388800 |
| H | 5.02834100 | 0.99916600 | 1.57152800 |
| H | 4.95802700 | 2.45968000 | 0.56705200 |
| H | 6.40229400 | 1.42943500 | 0.52686800 |
| H | 4.65186500 | 0.63383100 | -2.73374200 |
| H | 6.17236800 | 1.22077600 | -2.02391600 |
| H | 4.71498900 | 2.23665400 | -1.99300500 |
| H | 6.30234700 | -0.88740400 | -0.55402700 |
| H | 4.78479200 | -1.47319200 | -1.26810300 |
| H | 4.92539600 | -1.31423000 | 0.49104600 |
| C | -2.13722200 | 1.92180300 | -2.51304600 |
| C | -1.93512900 | 0.92831400 | -3.67031500 |
| C | -1.38033300 | 3.23289800 | -2.81499200 |
| C | -3.62787100 | 2.21743500 | -2.30879400 |
| H | -2.37000000 | -0.04702300 | -3.43183500 |
| H | -0.87162200 | 0.77679200 | -3.86981400 |
| H | -2.41288000 | 1.31071600 | -4.58069000 |
| H | -1.51839900 | 3.95959100 | -2.00557800 |
| H | -1.75770500 | 3.68087500 | -3.74226600 |
| H | -0.30895700 | 3.04272900 | -2.92804800 |
| H | -4.04088100 | 2.69253700 | -3.20669200 |
| H | -3.78155200 | 2.88261900 | -1.45515200 |

| | | | |
|---|-------------|-------------|-------------|
| H | -4.19421800 | 1.30006000 | -2.11964500 |
| C | -2.41070500 | -1.62812500 | -0.08517000 |
| O | -2.02288500 | -1.48470400 | 1.10694600 |
| O | -1.66160100 | -1.59128000 | -1.10811100 |
| C | -3.92201800 | -1.89040000 | -0.27731300 |
| C | -4.27887900 | -1.91916800 | -1.76758400 |
| C | -4.24265500 | -3.25115300 | 0.37175300 |
| C | -4.68834200 | -0.76417000 | 0.44273300 |
| H | -4.07469600 | -0.95657100 | -2.24294900 |
| H | -3.70668900 | -2.68350600 | -2.30054800 |
| H | -5.34717200 | -2.13956600 | -1.88182000 |
| H | -3.96266100 | -3.25337500 | 1.42901600 |
| H | -5.31644200 | -3.45751500 | 0.29373600 |
| H | -3.70453400 | -4.06422500 | -0.12956500 |
| H | -5.76587300 | -0.88651100 | 0.28085300 |
| H | -4.49016800 | -0.79067800 | 1.51774200 |
| H | -4.38014600 | 0.21749900 | 0.07174100 |

proton-transfer TS(quartet)

| | | | |
|----|-------------|-------------|-------------|
| C | -4.55284700 | -2.95933100 | -0.10277400 |
| C | -3.25524100 | -3.19667800 | -0.54380600 |
| C | -2.20686700 | -2.30517000 | -0.23911500 |
| C | -2.54303300 | -1.24749700 | 0.58480300 |
| C | -3.82182400 | -0.94525500 | 1.01581600 |
| C | -4.84552600 | -1.83470500 | 0.67459400 |
| H | -5.34596200 | -3.64824500 | -0.37761100 |
| H | -3.00948100 | -4.06451700 | -1.14683900 |
| H | -1.63663300 | -0.45629800 | 1.16167500 |
| H | -4.01349800 | -0.05742600 | 1.60920800 |
| H | -5.86052400 | -1.64317900 | 1.01129300 |
| C | -0.85491400 | -2.63948200 | -0.81308100 |
| O | -0.64610200 | -3.80513900 | -1.14941800 |
| N | 0.03406600 | -1.59179800 | -1.00817200 |
| C | 1.22325800 | -1.86927000 | -1.58610300 |
| C | 1.95722400 | -3.08262000 | -1.58008500 |
| C | 3.01754400 | -0.90538800 | -2.91527000 |
| C | 3.17257500 | -3.18528800 | -2.22117800 |
| H | 1.52189000 | -3.91973100 | -1.05877200 |
| C | 3.71632600 | -2.08239300 | -2.91079700 |
| H | 3.33667500 | 0.01993300 | -3.37266500 |
| H | 3.71608300 | -4.12417200 | -2.18610500 |
| H | 4.67054800 | -2.14027800 | -3.42036800 |
| N | 1.81524100 | -0.80890300 | -2.27614600 |
| O | 1.22285900 | 0.36900700 | -2.30771200 |
| Co | -0.04508800 | 0.49210500 | -0.57063900 |
| O | 2.85783300 | 1.51082100 | -1.15290400 |
| O | -2.02944600 | 0.88092200 | -1.20470200 |
| C | 2.71860100 | 1.10760000 | 0.02928500 |
| O | 1.71174600 | 0.48054300 | 0.47880800 |
| C | -1.74612800 | 2.12487400 | -1.17641600 |
| O | -0.54939800 | 2.47883900 | -0.93504000 |
| C | -2.85659200 | 3.14918600 | -1.39366200 |
| C | -3.48699200 | 2.89474800 | -2.77680900 |
| C | -2.30535700 | 4.57727200 | -1.30648400 |
| C | -3.91314600 | 2.91212500 | -0.29373200 |
| H | -3.85411600 | 1.86736300 | -2.85059400 |
| H | -2.75549500 | 3.05672600 | -3.57694100 |
| H | -4.32565700 | 3.58220300 | -2.93901500 |
| H | -1.84501400 | 4.76175900 | -0.33152800 |
| H | -3.11646600 | 5.30059100 | -1.45355800 |
| H | -1.54174600 | 4.75133800 | -2.07046700 |
| H | -4.74522000 | 3.61587400 | -0.41383300 |
| H | -3.47928800 | 3.06192400 | 0.70196400 |
| H | -4.30291500 | 1.89166600 | -0.35001100 |

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|---|-------------|-------------|-------------|
| C | 3.87418200 | 1.40725200 | 1.01959700 |
| C | 5.12014700 | 1.90901000 | 0.27932000 |
| C | 4.19394400 | 0.11261400 | 1.78585300 |
| C | 3.34839300 | 2.48663900 | 1.98712300 |
| H | 4.90757000 | 2.82479800 | -0.27843100 |
| H | 5.49024100 | 1.16095500 | -0.42997000 |
| H | 5.91708400 | 2.11935800 | 1.00177200 |
| H | 3.31650800 | -0.24967200 | 2.32495500 |
| H | 4.99607700 | 0.30336600 | 2.50821700 |
| H | 4.53227500 | -0.67942100 | 1.10704900 |
| H | 4.11861700 | 2.70750400 | 2.73604600 |
| H | 2.44022500 | 2.15620600 | 2.49583500 |
| H | 3.12019200 | 3.41341800 | 1.44976400 |
| C | -0.28986500 | 0.54539600 | 2.60345200 |
| O | 0.13638600 | 1.63217100 | 2.92378200 |
| O | -1.00914200 | 0.50674700 | 1.44667200 |
| C | -0.09964500 | -0.73459800 | 3.41518300 |
| C | -1.45807200 | -1.12701300 | 4.03800500 |
| C | 0.42652300 | -1.87521800 | 2.52151900 |
| C | 0.91178800 | -0.43835200 | 4.53373600 |
| H | -1.84946700 | -0.32091300 | 4.66819500 |
| H | -2.20499300 | -1.36767900 | 3.27679000 |
| H | -1.32329600 | -2.01455900 | 4.66586800 |
| H | 1.29747600 | -1.55465700 | 1.94436500 |
| H | 0.71209200 | -2.72264900 | 3.15406200 |
| H | -0.33503000 | -2.22891200 | 1.82399400 |
| H | 1.03583400 | -1.32891400 | 5.15909900 |
| H | 1.88742700 | -0.16675100 | 4.12031700 |
| H | 0.57558300 | 0.38900800 | 5.16397900 |

proton-transfer TS(sextet)

| | | | |
|----|-------------|-------------|-------------|
| C | -3.66037000 | -3.88173700 | 1.15291100 |
| C | -2.28453600 | -3.80487800 | 1.34642700 |
| C | -1.58645700 | -2.59977000 | 1.13336900 |
| C | -2.36384500 | -1.48683200 | 0.84460600 |
| C | -3.72389300 | -1.53430200 | 0.58103600 |
| C | -4.38473900 | -2.75208600 | 0.76201300 |
| H | -4.16845700 | -4.83192200 | 1.28792000 |
| H | -1.70810300 | -4.67371200 | 1.64635200 |
| H | -1.80446800 | -0.29889600 | 1.12857400 |
| H | -4.27031200 | -0.64795300 | 0.28135400 |
| H | -5.45650400 | -2.81217200 | 0.59509600 |
| C | -0.08206800 | -2.69385000 | 1.25812100 |
| O | 0.37970800 | -3.50834000 | 2.05336400 |
| N | 0.65694500 | -1.94220800 | 0.35331500 |
| C | 1.89764200 | -2.33955800 | 0.01110800 |
| C | 2.68957400 | -3.40079400 | 0.52836000 |
| C | 3.67362700 | -1.93577900 | -1.60061200 |
| C | 3.91448400 | -3.70861300 | -0.02173600 |
| H | 2.29141000 | -3.93606700 | 1.37541900 |
| C | 4.42519400 | -2.96806600 | -1.10684200 |
| H | 3.96035400 | -1.27119700 | -2.40285400 |
| H | 4.49571400 | -4.52297700 | 0.39951700 |
| H | 5.39328700 | -3.18285000 | -1.54271800 |
| N | 2.45755000 | -1.64107100 | -1.06166100 |
| O | 1.81427000 | -0.61396500 | -1.58889400 |
| Co | 0.32646800 | 0.04363700 | -0.27274900 |
| O | 3.32454200 | 1.02894400 | -0.94053700 |
| O | -1.47903900 | -0.41192100 | -1.44088900 |
| C | 2.85884200 | 1.40092500 | 0.16558700 |
| O | 1.79476800 | 0.96870200 | 0.70366700 |
| C | -1.28515600 | 0.68743500 | -2.05548300 |
| O | -0.33712300 | 1.45173700 | -1.68888800 |
| C | -2.13044400 | 1.03403800 | -3.28238400 |

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|---|-------------|-------------|-------------|
| C | -3.56348600 | 0.50722600 | -3.10716600 |
| C | -1.45517400 | 0.31266300 | -4.47230500 |
| C | -2.13358500 | 2.54923700 | -3.52850500 |
| H | -4.08184200 | 1.03299000 | -2.29708600 |
| H | -3.55961600 | -0.55985500 | -2.87215000 |
| H | -4.13579700 | 0.66578600 | -4.02859500 |
| H | -0.42214600 | 0.65438700 | -4.59639900 |
| H | -2.00412900 | 0.52352600 | -5.39754700 |
| H | -1.44420700 | -0.77033600 | -4.31253700 |
| H | -2.68969100 | 2.77867800 | -4.44519700 |
| H | -1.11487800 | 2.93091400 | -3.62882100 |
| H | -2.61194700 | 3.08375200 | -2.70043800 |
| C | 3.60888100 | 2.51792500 | 0.93228600 |
| C | 5.02648200 | 2.71571800 | 0.38362100 |
| C | 3.64135400 | 2.14681700 | 2.42385200 |
| C | 2.76187400 | 3.79316200 | 0.72944300 |
| H | 5.00879800 | 2.97834600 | -0.67780400 |
| H | 5.62544500 | 1.80536500 | 0.49623200 |
| H | 5.52629800 | 3.52221000 | 0.93250800 |
| H | 2.62842000 | 1.99937000 | 2.80362000 |
| H | 4.12238900 | 2.95345700 | 2.99015300 |
| H | 4.21533700 | 1.22771400 | 2.59200600 |
| H | 3.22446900 | 4.62758800 | 1.27050100 |
| H | 1.74781300 | 3.64362200 | 1.10903500 |
| H | 2.70637500 | 4.06269700 | -0.33130200 |
| C | -1.25289900 | 1.80014300 | 1.79057900 |
| O | -0.32783300 | 2.48463500 | 2.16308100 |
| O | -0.96879400 | 0.54008200 | 1.35313700 |
| C | -2.70990900 | 2.25758300 | 1.77554100 |
| C | -3.24592800 | 2.15366200 | 0.33436300 |
| C | -3.53092000 | 1.37998500 | 2.74373300 |
| C | -2.76469400 | 3.72004500 | 2.24105300 |
| H | -2.68733600 | 2.81942200 | -0.33075900 |
| H | -3.15500100 | 1.14460700 | -0.06885400 |
| H | -4.30141000 | 2.44713400 | 0.30993600 |
| H | -3.14597300 | 1.46644200 | 3.76559400 |
| H | -4.57271400 | 1.71948100 | 2.74506200 |
| H | -3.52307700 | 0.32361800 | 2.46716600 |
| H | -3.80279100 | 4.07023300 | 2.22840100 |
| H | -2.37307100 | 3.82741500 | 3.25642200 |
| H | -2.17184100 | 4.36313600 | 1.58466900 |

TS-S7(doublet)

| | | | |
|---|-------------|-------------|-------------|
| C | 4.17335900 | -0.88482200 | -2.25572100 |
| C | 4.15864800 | 0.48115500 | -2.52597600 |
| C | 2.96574600 | 1.18721700 | -2.38531900 |
| C | 1.79385400 | 0.55822100 | -1.95810300 |
| C | 3.00697700 | -1.54298100 | -1.86083400 |
| H | 5.09220500 | -1.45490800 | -2.35642100 |
| H | 5.06206900 | 0.99207200 | -2.84267900 |
| H | 2.92826300 | 2.25140900 | -2.59496800 |
| H | 3.03758900 | -2.60719400 | -1.66864800 |
| C | 0.57509600 | 1.43216100 | -1.80455800 |
| O | 0.12683800 | 2.06138200 | -2.75061400 |
| N | 0.10351300 | 1.48092700 | -0.49275700 |
| C | -0.99746900 | 2.25208200 | -0.13943800 |
| C | -1.54637300 | 3.33683400 | -0.82788400 |
| C | -2.65981700 | 2.50844800 | 1.55058600 |
| C | -2.65138100 | 4.00638200 | -0.31661500 |
| H | -1.09147500 | 3.61131200 | -1.76767500 |
| C | -3.21284400 | 3.58885400 | 0.89263600 |
| H | -3.02232200 | 2.09091400 | 2.47964100 |
| H | -3.06942400 | 4.84851500 | -0.85787900 |
| H | -4.07541400 | 4.08350300 | 1.32400100 |

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|----|-------------|-------------|-------------|
| O | -1.10622200 | 0.82101000 | 1.70889400 |
| N | -1.58093300 | 1.86179200 | 1.04757900 |
| Co | -0.40662800 | -0.49514600 | 0.30713000 |
| C | 1.81577200 | -0.82808100 | -1.71684000 |
| O | 0.62480600 | -1.43796000 | -1.36831900 |
| C | 0.62250500 | -2.87075500 | -1.23763500 |
| H | 0.92986600 | -3.32834100 | -2.18250800 |
| H | 1.28388300 | -3.17271800 | -0.42046900 |
| H | -0.40070900 | -3.13583700 | -0.98428100 |
| C | 2.10894700 | 0.07539200 | 1.48730100 |
| O | 1.24155200 | -0.81666200 | 1.24982900 |
| C | 3.36717000 | -0.31730100 | 2.26202200 |
| C | 3.20019600 | 0.22976400 | 3.69626100 |
| C | 3.52550900 | -1.84352600 | 2.29044700 |
| C | 4.59064700 | 0.33267700 | 1.59018000 |
| H | 3.07516300 | 1.31673800 | 3.68539700 |
| H | 2.32628800 | -0.21419200 | 4.18580700 |
| H | 4.08767500 | -0.01311900 | 4.29177300 |
| H | 3.62947400 | -2.24268000 | 1.27559300 |
| H | 4.42384700 | -2.11248200 | 2.85781600 |
| H | 2.66074900 | -2.32490200 | 2.75388500 |
| H | 5.49861600 | 0.07778400 | 2.14883300 |
| H | 4.70842900 | -0.02416600 | 0.56111200 |
| H | 4.48862100 | 1.41997600 | 1.56121700 |
| O | 1.99652900 | 1.29189600 | 1.12341900 |
| H | 1.00948700 | 1.42236600 | 0.35356500 |
| C | -2.55483100 | -1.55096900 | 0.02286200 |
| O | -1.74028800 | -2.23067200 | 0.70386800 |
| O | -2.13641400 | -0.47113900 | -0.54302700 |
| C | -4.02639400 | -1.92044700 | -0.12565700 |
| C | -4.30176600 | -3.28861300 | 0.50953900 |
| C | -4.83922900 | -0.82090000 | 0.59308000 |
| C | -4.38603900 | -1.93367900 | -1.62367000 |
| H | -3.71862800 | -4.07501400 | 0.01962200 |
| H | -4.03494100 | -3.29126000 | 1.56999000 |
| H | -5.36499900 | -3.53772300 | 0.41423100 |
| H | -4.63246400 | 0.16035600 | 0.15585300 |
| H | -5.91189300 | -1.02815600 | 0.50322700 |
| H | -4.58638500 | -0.78406500 | 1.65905400 |
| H | -5.45340200 | -2.14899200 | -1.75067900 |
| H | -4.16352200 | -0.96845700 | -2.08598200 |
| H | -3.81984700 | -2.70634000 | -2.15706400 |

TS-S7(quartet)

| | | | |
|---|-------------|-------------|-------------|
| C | 4.06617000 | 1.15547900 | 2.24973900 |
| C | 4.08713700 | -0.18311100 | 2.63447700 |
| C | 2.91999700 | -0.93655400 | 2.52966800 |
| C | 1.74232000 | -0.37948000 | 2.02689800 |
| C | 2.88997200 | 1.74259500 | 1.77934800 |
| H | 4.96548700 | 1.76028000 | 2.31987900 |
| H | 4.99852400 | -0.63619200 | 3.01073100 |
| H | 2.90934000 | -1.98085600 | 2.82483000 |
| H | 2.89310800 | 2.78760900 | 1.49978900 |
| C | 0.55457100 | -1.29238200 | 1.90768700 |
| O | 0.10263700 | -1.87597500 | 2.87997800 |
| N | 0.11303300 | -1.44498700 | 0.58812700 |
| C | -0.89218300 | -2.35133300 | 0.25815900 |
| C | -1.39486600 | -3.40197000 | 1.03006800 |
| C | -2.38821600 | -2.95262700 | -1.49820700 |
| C | -2.39376300 | -4.22577200 | 0.52611100 |
| H | -0.99419200 | -3.52756900 | 2.02416600 |
| C | -2.89522600 | -4.00157600 | -0.75790200 |
| H | -2.70808900 | -2.67722500 | -2.49357300 |
| H | -2.77798100 | -5.03792600 | 1.13415500 |

| | | | |
|----|-------------|-------------|-------------|
| H | -3.67565200 | -4.62073500 | -1.18462100 |
| O | -0.96828000 | -1.15952000 | -1.74823400 |
| N | -1.41485200 | -2.15592200 | -0.99943900 |
| Co | -0.51847000 | 0.41807900 | -0.52613400 |
| C | 1.72392600 | 0.98006000 | 1.67120000 |
| O | 0.52163200 | 1.50891200 | 1.25523700 |
| C | 0.46930600 | 2.93001100 | 1.04022500 |
| H | 0.75262000 | 3.45387200 | 1.95811000 |
| H | 1.12921000 | 3.20673800 | 0.21253300 |
| H | -0.56044500 | 3.13950500 | 0.76494200 |
| C | 2.18820800 | -0.04807000 | -1.42832600 |
| O | 1.27018600 | 0.82376400 | -1.36339800 |
| C | 3.48508100 | 0.31121200 | -2.16001300 |
| C | 4.67745900 | -0.37439600 | -1.47265400 |
| C | 3.33372800 | -0.21415900 | -3.60477400 |
| C | 3.68243500 | 1.83400400 | -2.17223700 |
| H | 4.77772400 | -0.03735400 | -0.43525400 |
| H | 4.55312300 | -1.45959400 | -1.46236100 |
| H | 5.60399200 | -0.13031100 | -2.00548400 |
| H | 2.48084600 | 0.25763600 | -4.10489200 |
| H | 4.23881300 | 0.01149600 | -4.18051800 |
| H | 3.18134900 | -1.29825000 | -3.61043000 |
| H | 4.59768200 | 2.08662500 | -2.72000400 |
| H | 2.83780200 | 2.33858700 | -2.64735200 |
| H | 3.77827100 | 2.22144200 | -1.15185500 |
| O | 2.09721200 | -1.22089000 | -0.93843500 |
| H | 1.03700600 | -1.37185400 | -0.20480400 |
| C | -2.75945300 | 1.35116000 | -0.08463300 |
| O | -1.81092200 | 1.98948700 | -0.67698100 |
| O | -2.53984700 | 0.19088800 | 0.35578400 |
| C | -4.12250900 | 2.02634300 | 0.05229800 |
| C | -5.07842200 | 1.14557000 | 0.86627700 |
| C | -3.92315400 | 3.38816600 | 0.74621500 |
| C | -4.67744700 | 2.24855700 | -1.37022500 |
| H | -5.21680700 | 0.17116600 | 0.38894200 |
| H | -4.69009600 | 0.96777100 | 1.87373400 |
| H | -6.05596000 | 1.63467100 | 0.95150400 |
| H | -3.24021100 | 4.01993200 | 0.17157600 |
| H | -4.88442600 | 3.90672900 | 0.83898300 |
| H | -3.51083800 | 3.25974900 | 1.75422100 |
| H | -5.64629300 | 2.75909700 | -1.31929400 |
| H | -3.98964900 | 2.85676500 | -1.96411000 |
| H | -4.82419900 | 1.29274000 | -1.88674200 |

TS-S7(sextet)

| | | | |
|---|-------------|-------------|-------------|
| C | 4.00180900 | -1.60055600 | -2.08270100 |
| C | 4.08270400 | -0.32029100 | -2.62519500 |
| C | 2.95082400 | 0.49259900 | -2.61982300 |
| C | 1.74681000 | 0.05419700 | -2.06369800 |
| C | 2.79934300 | -2.07281800 | -1.55239000 |
| H | 4.87268200 | -2.24929400 | -2.07443400 |
| H | 5.01384400 | 0.04287800 | -3.04784700 |
| H | 2.98801300 | 1.49275100 | -3.03962300 |
| H | 2.75433700 | -3.07655200 | -1.15082500 |
| C | 0.59620700 | 1.02508600 | -2.06487600 |
| O | 0.15170400 | 1.48906900 | -3.10361400 |
| N | 0.18776900 | 1.38531100 | -0.77780800 |
| C | -0.77002600 | 2.36754300 | -0.55672300 |
| C | -1.47685500 | 3.16072400 | -1.42260500 |
| C | -1.81040100 | 3.58647300 | 1.35608600 |
| C | -2.36701300 | 4.14185500 | -0.93432600 |
| H | -1.29824100 | 3.03362800 | -2.48062400 |
| C | -2.48974800 | 4.35537200 | 0.47083600 |
| H | -1.81750100 | 3.68114400 | 2.43300200 |

| | | | |
|----|-------------|-------------|-------------|
| H | -2.92748300 | 4.75548900 | -1.62913100 |
| H | -3.11188200 | 5.16098200 | 0.84906500 |
| O | -1.24312600 | 1.34964400 | 1.51154500 |
| N | -1.03517500 | 2.48421300 | 0.87292300 |
| Co | -0.56259800 | -0.31311400 | 0.43770500 |
| C | 1.67033400 | -1.25075100 | -1.54792500 |
| O | 0.44243700 | -1.67453200 | -1.07523100 |
| C | 0.31370000 | -3.06424800 | -0.72703300 |
| H | 0.56974000 | -3.68502200 | -1.59049200 |
| H | 0.95621300 | -3.29893700 | 0.12690000 |
| H | -0.72478500 | -3.19674600 | -0.43807100 |
| C | 2.14250900 | 0.22609400 | 1.42186600 |
| O | 1.17976800 | -0.59530500 | 1.41483600 |
| C | 3.40363200 | -0.11578900 | 2.21650400 |
| C | 3.30382500 | 0.64791300 | 3.55588700 |
| C | 3.47453100 | -1.62755700 | 2.47350000 |
| C | 4.64392500 | 0.35210800 | 1.43547800 |
| H | 3.24014000 | 1.72709600 | 3.38466700 |
| H | 2.42076600 | 0.33271600 | 4.12284700 |
| H | 4.19208000 | 0.44542200 | 4.16502300 |
| H | 3.53297900 | -2.17938400 | 1.52900600 |
| H | 4.36820300 | -1.86190600 | 3.06281200 |
| H | 2.59376100 | -1.97991500 | 3.01589200 |
| H | 5.54969200 | 0.12249900 | 2.00836400 |
| H | 4.71125100 | -0.15536600 | 0.46709500 |
| H | 4.60818600 | 1.42811000 | 1.25033600 |
| O | 2.12004200 | 1.34830800 | 0.81178000 |
| H | 1.14035600 | 1.40897400 | 0.03838000 |
| C | -2.76345200 | -1.35046900 | 0.21954200 |
| O | -1.86070800 | -1.82651500 | 0.99775100 |
| O | -2.48138400 | -0.34269700 | -0.49417100 |
| C | -4.14232000 | -2.00247700 | 0.18368000 |
| C | -4.76998100 | -1.83921300 | 1.58411500 |
| C | -5.02558300 | -1.33644600 | -0.87865100 |
| C | -3.96058700 | -3.50118700 | -0.12783700 |
| H | -4.13473400 | -2.29367900 | 2.34946400 |
| H | -4.90370500 | -0.77995000 | 1.83181600 |
| H | -5.75377100 | -2.32186700 | 1.60982200 |
| H | -4.58588400 | -1.43395900 | -1.87592800 |
| H | -6.01585600 | -1.80677400 | -0.88797800 |
| H | -5.14827700 | -0.26902900 | -0.67474800 |
| H | -4.93436000 | -4.00421900 | -0.12808100 |
| H | -3.50728300 | -3.64570300 | -1.11609000 |
| H | -3.32150500 | -3.97872900 | 0.62011200 |

int-S8(doublet)

| | | | |
|---|-------------|-------------|-------------|
| C | 3.40527800 | -0.86613200 | -1.37891900 |
| C | 3.85256200 | 0.15935800 | -0.51016100 |
| C | 5.06913800 | -0.01962800 | 0.16453800 |
| C | 5.81921100 | -1.17992400 | 0.02071000 |
| C | 5.35015000 | -2.19341600 | -0.81641000 |
| C | 4.15520100 | -2.03932200 | -1.51520000 |
| H | 5.38990100 | 0.77907000 | 0.82363700 |
| H | 6.75112000 | -1.29954300 | 0.56355800 |
| H | 5.91620500 | -3.11321500 | -0.93263500 |
| H | 3.80696000 | -2.83030000 | -2.16766100 |
| C | 3.10300000 | 1.40490900 | -0.15720600 |
| O | 3.60355500 | 2.29020900 | 0.52957200 |
| N | 1.79084200 | 1.45983700 | -0.59414400 |
| H | 1.43766400 | 0.68964800 | -1.16763700 |
| C | 0.84915500 | 2.39102800 | -0.26379900 |
| C | 1.01183200 | 3.54262300 | 0.51712600 |
| C | -1.46632800 | 2.89457000 | -0.53633500 |
| C | -0.08455100 | 4.35417100 | 0.76509700 |

| | | | |
|----|-------------|-------------|-------------|
| H | 1.99605100 | 3.74597700 | 0.91165700 |
| C | -1.34062700 | 4.02900700 | 0.23803600 |
| H | -2.38728900 | 2.52292600 | -0.96595400 |
| H | 0.03771900 | 5.24203500 | 1.37678300 |
| H | -2.21496100 | 4.64001300 | 0.42740000 |
| O | -0.51400500 | 1.01444900 | -1.53824100 |
| Co | -1.50978500 | -0.37078300 | -0.59406600 |
| C | -3.79302800 | -0.75017700 | -0.36009000 |
| O | -2.93621600 | -1.61239900 | 0.01698500 |
| O | -3.33747200 | 0.29774700 | -0.94673400 |
| C | 0.09955000 | -0.73280300 | 1.20055500 |
| O | 0.08945200 | -1.31491300 | 0.05040800 |
| O | -0.69832300 | 0.21743700 | 1.41982100 |
| C | -5.28096900 | -0.90982900 | -0.10296500 |
| C | -5.68850500 | 0.19552000 | 0.89614900 |
| C | -6.03240900 | -0.70910000 | -1.43340200 |
| C | -5.57645800 | -2.29563900 | 0.48460200 |
| H | -5.15340500 | 0.08287800 | 1.84559200 |
| H | -5.46587700 | 1.18668200 | 0.49041500 |
| H | -6.76362700 | 0.13323100 | 1.09907900 |
| H | -5.76148400 | -1.48408100 | -2.15953100 |
| H | -7.11316500 | -0.76798200 | -1.26194100 |
| H | -5.79882700 | 0.26574600 | -1.86974800 |
| H | -6.65040300 | -2.39330400 | 0.68025600 |
| H | -5.27745900 | -3.08982800 | -0.20651300 |
| H | -5.03502200 | -2.44983500 | 1.42203200 |
| C | 1.01810500 | -1.24007700 | 2.31378700 |
| C | 1.71805800 | -0.03864400 | 2.97538700 |
| C | 0.09303800 | -1.92552000 | 3.34543300 |
| C | 2.04932500 | -2.24722300 | 1.79051700 |
| H | 2.41093500 | 0.45621800 | 2.28744900 |
| H | 0.98164700 | 0.69843100 | 3.30551800 |
| H | 2.29528900 | -0.37527900 | 3.84446300 |
| H | -0.43695700 | -2.77139500 | 2.89311900 |
| H | 0.68690000 | -2.30163900 | 4.18673100 |
| H | -0.65020300 | -1.21922300 | 3.72606700 |
| H | 2.64132900 | -2.63757800 | 2.62677400 |
| H | 1.55992500 | -3.08743800 | 1.28997200 |
| H | 2.73657400 | -1.78366800 | 1.07951600 |
| N | -0.38850100 | 2.11525200 | -0.78096300 |
| O | 2.25621900 | -0.65485400 | -2.07533300 |
| C | 1.54525200 | -1.76988300 | -2.61637400 |
| H | 1.35787600 | -2.51266200 | -1.83760700 |
| H | 0.59783600 | -1.35849900 | -2.96337500 |
| H | 2.09099400 | -2.20646800 | -3.46017000 |

int-S8(quartet)

| | | | |
|---|-------------|-------------|-------------|
| C | 2.59817900 | -1.63703800 | -1.32976000 |
| C | 3.38224200 | -0.46690400 | -1.16582500 |
| C | 4.74478800 | -0.61352100 | -0.86262200 |
| C | 5.32841900 | -1.86271000 | -0.70056300 |
| C | 4.53639600 | -3.00388900 | -0.83602700 |
| C | 3.18412200 | -2.89535800 | -1.14922200 |
| H | 5.32043100 | 0.29611700 | -0.73553600 |
| H | 6.38275500 | -1.94723400 | -0.45852800 |
| H | 4.96955000 | -3.99060000 | -0.69929900 |
| H | 2.58549400 | -3.79103900 | -1.25430000 |
| C | 2.88630500 | 0.94336400 | -1.17681100 |
| O | 3.63380300 | 1.89592700 | -0.97549900 |
| N | 1.52327100 | 1.10648600 | -1.36223800 |
| H | 0.95989200 | 0.27165700 | -1.53411600 |
| C | 0.79386600 | 2.23099100 | -1.09328600 |
| C | 1.26471100 | 3.52190600 | -0.82565200 |
| C | -1.44781000 | 2.97220700 | -0.76776500 |

| | | | |
|----|-------------|-------------|-------------|
| C | 0.35681800 | 4.52562300 | -0.52288100 |
| H | 2.33230400 | 3.68109900 | -0.84690100 |
| C | -1.01601100 | 4.25177000 | -0.48759300 |
| H | -2.47361300 | 2.62880100 | -0.73642900 |
| H | 0.71979400 | 5.52496400 | -0.30654600 |
| H | -1.74437000 | 5.01374200 | -0.23775900 |
| O | -0.99243200 | 0.76787100 | -1.33883300 |
| Co | -1.37087200 | -0.30110500 | 0.32131800 |
| C | -3.72715700 | -0.78250700 | 0.04729500 |
| O | -2.84359600 | -1.61719600 | -0.34065000 |
| O | -3.35883400 | 0.29232500 | 0.63375200 |
| C | 0.61783600 | -0.05256200 | 1.75680100 |
| O | 0.22768500 | -1.15301700 | 1.21378900 |
| O | -0.03907800 | 1.00244400 | 1.53060700 |
| C | -5.21361000 | -1.03859500 | -0.18561600 |
| C | -5.91386800 | -1.04921900 | 1.18873300 |
| C | -5.76278700 | 0.12633000 | -1.03493100 |
| C | -5.43109400 | -2.37404700 | -0.90737400 |
| H | -5.54036100 | -1.86884200 | 1.81343700 |
| H | -5.74263300 | -0.10836500 | 1.71862700 |
| H | -6.99309500 | -1.18834700 | 1.05636100 |
| H | -5.27087900 | 0.16491000 | -2.01398400 |
| H | -6.83813500 | -0.00646600 | -1.20058100 |
| H | -5.60115600 | 1.08247000 | -0.52960600 |
| H | -6.50304000 | -2.54060100 | -1.06604100 |
| H | -4.93019400 | -2.38287200 | -1.87993700 |
| H | -5.03330300 | -3.20795000 | -0.32162500 |
| C | 1.80590600 | -0.04837300 | 2.71599800 |
| C | 2.58475600 | 1.27037600 | 2.57343000 |
| C | 1.19943100 | -0.13930400 | 4.13641100 |
| C | 2.72485100 | -1.25263800 | 2.46580900 |
| H | 3.04569200 | 1.36344400 | 1.58496500 |
| H | 1.92340200 | 2.12792800 | 2.72029600 |
| H | 3.38509600 | 1.31089900 | 3.32147900 |
| H | 0.62751400 | -1.06576800 | 4.25867700 |
| H | 2.00169500 | -0.12959200 | 4.88314500 |
| H | 0.53321700 | 0.70745400 | 4.32954800 |
| H | 3.52568600 | -1.26728400 | 3.21446800 |
| H | 2.16866500 | -2.19123800 | 2.53018200 |
| H | 3.18820900 | -1.20151300 | 1.47721600 |
| N | -0.55567800 | 2.00556300 | -1.07764000 |
| O | 1.29247600 | -1.49355500 | -1.68324800 |
| C | 0.40181400 | -2.60857900 | -1.56736000 |
| H | 0.43512700 | -3.01116800 | -0.55219100 |
| H | -0.59318700 | -2.21316700 | -1.77222200 |
| H | 0.65104500 | -3.37828400 | -2.30570900 |

int-S8(sextet)

| | | | |
|---|-------------|-------------|-------------|
| C | -1.67270300 | -1.64793300 | -1.92117200 |
| C | -0.42598500 | -2.11253300 | -1.44394700 |
| C | -0.37583700 | -3.35689800 | -0.80356100 |
| C | -1.52112900 | -4.11893400 | -0.60491600 |
| C | -2.74721700 | -3.63709100 | -1.06189900 |
| C | -2.82603900 | -2.41191700 | -1.72292600 |
| H | 0.58837900 | -3.69734500 | -0.44781400 |
| H | -1.45978900 | -5.07284500 | -0.09130600 |
| H | -3.65424100 | -4.21550000 | -0.91096700 |
| H | -3.78385700 | -2.06038600 | -2.08530800 |
| C | 0.86392000 | -1.36938900 | -1.52349200 |
| O | 1.95571000 | -1.91499400 | -1.39804800 |
| N | 0.75351800 | 0.00766100 | -1.68470800 |
| H | -0.19143900 | 0.36576600 | -1.81563600 |
| C | 1.78610700 | 0.91494000 | -1.71048600 |
| C | 3.13840100 | 0.70148300 | -1.84430400 |

| | | | |
|----|-------------|-------------|-------------|
| C | 2.16441500 | 3.35629900 | -1.87429800 |
| C | 4.01474800 | 1.79422700 | -1.95310000 |
| H | 3.48366000 | -0.31979200 | -1.91653000 |
| C | 3.49297100 | 3.12024800 | -2.01261200 |
| H | 1.67178800 | 4.31764100 | -1.91787000 |
| H | 5.08012800 | 1.62437100 | -2.05020000 |
| H | 4.15476000 | 3.95963900 | -2.20362300 |
| O | 0.59400100 | 2.48661800 | -0.42735400 |
| Co | 0.14284900 | 1.07571300 | 0.99449600 |
| C | -2.28922200 | 1.26267600 | 1.15237900 |
| O | -1.45109700 | 1.69683100 | 2.02291200 |
| O | -1.84750400 | 0.77953800 | 0.06971400 |
| C | 1.83927200 | -0.50981600 | 1.66357700 |
| O | 0.65465500 | -0.91297000 | 1.42068900 |
| O | 2.09150900 | 0.74207200 | 1.54609600 |
| C | -3.78990300 | 1.31653100 | 1.42951200 |
| C | -4.42627500 | 2.27746600 | 0.40379200 |
| C | -4.35743300 | -0.10496200 | 1.24202800 |
| C | -4.06484000 | 1.81489400 | 2.85445300 |
| H | -4.03211400 | 3.29340000 | 0.52094900 |
| H | -4.22632300 | 1.95139700 | -0.62070200 |
| H | -5.51163000 | 2.31525400 | 0.55121400 |
| H | -3.92699100 | -0.79667700 | 1.97468200 |
| H | -5.44492200 | -0.09463000 | 1.37937700 |
| H | -4.12851500 | -0.49382700 | 0.24664400 |
| H | -5.14579600 | 1.84488500 | 3.03521000 |
| H | -3.60736100 | 1.15486300 | 3.59726400 |
| H | -3.65863300 | 2.81866000 | 3.00783100 |
| C | 2.93549800 | -1.46247400 | 2.12067200 |
| C | 4.22466600 | -1.15455700 | 1.33672100 |
| C | 3.15760100 | -1.18742600 | 3.62528200 |
| C | 2.51631200 | -2.92152900 | 1.89911300 |
| H | 4.07766600 | -1.35455100 | 0.27141000 |
| H | 4.51517300 | -0.10789400 | 1.45733800 |
| H | 5.03865000 | -1.79297300 | 1.69937100 |
| H | 2.24933100 | -1.39687000 | 4.20174400 |
| H | 3.95852800 | -1.83317800 | 4.00305000 |
| H | 3.44142800 | -0.14408300 | 3.79269000 |
| H | 3.29006400 | -3.59126300 | 2.29242000 |
| H | 1.57149900 | -3.14372400 | 2.40262500 |
| H | 2.39388600 | -3.12303600 | 0.83161000 |
| N | 1.30061900 | 2.26825800 | -1.52211900 |
| O | -1.68354200 | -0.46285000 | -2.60231500 |
| C | -2.93454700 | 0.15545500 | -2.88130000 |
| H | -3.50466800 | 0.29461100 | -1.96001900 |
| H | -2.69209800 | 1.12765100 | -3.31251200 |
| H | -3.50898100 | -0.43176600 | -3.60717900 |

int-S9(doublet)

| | | | |
|---|-------------|-------------|-------------|
| C | 4.11332200 | -0.72097400 | -2.34450400 |
| C | 4.06178000 | 0.64541600 | -2.60694300 |
| C | 2.85729400 | 1.32423800 | -2.43375400 |
| C | 1.71282400 | 0.66285800 | -1.98453700 |
| C | 2.97309400 | -1.40870200 | -1.92429200 |
| H | 5.04264700 | -1.26876000 | -2.46910900 |
| H | 4.94600200 | 1.17831100 | -2.94077300 |
| H | 2.79306400 | 2.38930800 | -2.63298500 |
| H | 3.03464100 | -2.47179000 | -1.73428900 |
| C | 0.47078300 | 1.49065600 | -1.79557800 |
| O | -0.09632300 | 2.03990400 | -2.72290000 |
| C | -1.03352800 | 2.31122800 | -0.04055000 |
| C | -1.63328400 | 3.38141100 | -0.70118300 |
| C | -2.65775700 | 2.47064900 | 1.68899400 |
| C | -2.75188400 | 3.99952800 | -0.15419500 |

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|----|-------------|-------------|-------------|
| H | -1.21116200 | 3.68757000 | -1.64678200 |
| C | -3.26450800 | 3.54057900 | 1.06123400 |
| H | -2.98149800 | 2.02578800 | 2.61972700 |
| H | -3.21542900 | 4.83335700 | -0.67015100 |
| H | -4.13335900 | 3.99620600 | 1.52204800 |
| O | -1.04314900 | 0.83483200 | 1.77096300 |
| N | -1.57014200 | 1.87056000 | 1.14725200 |
| Co | -0.38508100 | -0.47019200 | 0.35427200 |
| C | 1.77014500 | -0.72280200 | -1.74773800 |
| O | 0.60043700 | -1.35800800 | -1.37121400 |
| C | 0.63546300 | -2.79351900 | -1.25078800 |
| H | 0.93450700 | -3.23450500 | -2.20597000 |
| H | 1.32026200 | -3.08163700 | -0.44872800 |
| H | -0.37571300 | -3.08444500 | -0.97900300 |
| C | 2.17629900 | 0.05326000 | 1.46125700 |
| O | 1.26895900 | -0.82232100 | 1.23576100 |
| C | 3.43948900 | -0.43013700 | 2.18822200 |
| C | 4.66792700 | 0.24842600 | 1.55826600 |
| C | 3.29599900 | 0.00651400 | 3.66191800 |
| C | 3.57442500 | -1.95637000 | 2.10166700 |
| H | 4.77516200 | -0.03687700 | 0.50571200 |
| H | 4.57574800 | 1.33589200 | 1.60353000 |
| H | 5.57750200 | -0.05362500 | 2.09090500 |
| H | 2.41815500 | -0.45916700 | 4.12365000 |
| H | 4.18359900 | -0.29394400 | 4.23117800 |
| H | 3.18810100 | 1.09326200 | 3.73383400 |
| H | 4.47337900 | -2.28239500 | 2.63821700 |
| H | 2.70547900 | -2.45717800 | 2.53547400 |
| H | 3.66424600 | -2.28034700 | 1.05874500 |
| O | 2.09388900 | 1.26624200 | 1.14136300 |
| C | -2.53796100 | -1.52937400 | 0.02048600 |
| O | -1.72509100 | -2.22834200 | 0.68576800 |
| O | -2.13448700 | -0.41219900 | -0.47397500 |
| C | -3.97682300 | -1.98712900 | -0.20001700 |
| C | -4.76773600 | -0.94297100 | -0.99846700 |
| C | -3.93060700 | -3.32749300 | -0.96153800 |
| C | -4.61654900 | -2.20228700 | 1.18639300 |
| H | -4.79318300 | 0.01690900 | -0.47307200 |
| H | -4.31739900 | -0.77019800 | -1.98029200 |
| H | -5.79858400 | -1.28705000 | -1.14345400 |
| H | -3.34692200 | -4.06668600 | -0.40542400 |
| H | -4.94577800 | -3.71606200 | -1.10190700 |
| H | -3.47718900 | -3.20101700 | -1.95196300 |
| H | -5.64075900 | -2.57650900 | 1.07352100 |
| H | -4.03843500 | -2.92257000 | 1.77103600 |
| H | -4.65766600 | -1.26167100 | 1.74823100 |
| N | 0.08497400 | 1.58726300 | -0.45326300 |
| H | 0.91082500 | 1.50134700 | 0.27257300 |

int-S9(quartet)

| | | | |
|---|-------------|-------------|-------------|
| C | 4.06257000 | -0.57525100 | -2.43445500 |
| C | 3.99070400 | 0.79273600 | -2.68410900 |
| C | 2.78078100 | 1.45520400 | -2.48573200 |
| C | 1.65554900 | 0.77316600 | -2.02134500 |
| C | 2.93801700 | -1.28181000 | -2.00298800 |
| H | 4.99642600 | -1.11015000 | -2.57991100 |
| H | 4.86265500 | 1.33859100 | -3.02920000 |
| H | 2.69833200 | 2.52083500 | -2.67530600 |
| H | 3.01540700 | -2.34610900 | -1.82659800 |
| C | 0.40495400 | 1.57045200 | -1.79495000 |
| O | -0.18898900 | 2.12983400 | -2.70054200 |
| C | -1.04727900 | 2.37407500 | 0.01298100 |
| C | -1.71539600 | 3.39782200 | -0.65994200 |
| C | -2.53168500 | 2.62395800 | 1.85490500 |

| | | | |
|----|-------------|-------------|-------------|
| C | -2.79569400 | 4.03346800 | -0.06072300 |
| H | -1.37512000 | 3.65153800 | -1.65239900 |
| C | -3.20528000 | 3.64622000 | 1.21716200 |
| H | -2.76952400 | 2.23212300 | 2.83411500 |
| H | -3.31154300 | 4.82890800 | -0.58779000 |
| H | -4.04189400 | 4.11961700 | 1.71762800 |
| O | -0.88230700 | 1.01684500 | 1.89979300 |
| N | -1.48432000 | 2.00653800 | 1.26074700 |
| Co | -0.45283300 | -0.51319500 | 0.61353500 |
| C | 1.73026300 | -0.61146600 | -1.79576400 |
| O | 0.57571200 | -1.24964900 | -1.39780100 |
| C | 0.61290100 | -2.68729100 | -1.34187800 |
| H | 0.89622600 | -3.08805300 | -2.31985500 |
| H | 1.31274800 | -3.01169200 | -0.56654300 |
| H | -0.39354200 | -2.99137200 | -1.06736800 |
| C | 2.25688600 | -0.09971800 | 1.41883800 |
| O | 1.31842600 | -0.97510800 | 1.33584000 |
| C | 3.56986100 | -0.57090200 | 2.06328300 |
| C | 4.72880200 | 0.32941800 | 1.61309300 |
| C | 3.37349200 | -0.46323100 | 3.59078000 |
| C | 3.85518800 | -2.03260300 | 1.68060800 |
| H | 4.85328000 | 0.28804200 | 0.52548600 |
| H | 4.54487700 | 1.37098700 | 1.88669700 |
| H | 5.66395800 | 0.00050000 | 2.08219200 |
| H | 2.53827000 | -1.09032300 | 3.91944500 |
| H | 4.28092000 | -0.79203600 | 4.11128900 |
| H | 3.16482600 | 0.57148300 | 3.88392400 |
| H | 4.77186200 | -2.37761000 | 2.17358900 |
| H | 3.02999600 | -2.68422000 | 1.97769200 |
| H | 3.99629400 | -2.13050400 | 0.59829000 |
| O | 2.15713400 | 1.09011300 | 1.03774900 |
| C | -2.65215100 | -1.44163000 | 0.00578100 |
| O | -1.71189300 | -2.12955000 | 0.54818300 |
| O | -2.44416200 | -0.22568900 | -0.26592700 |
| C | -3.98436600 | -2.12205500 | -0.29967500 |
| C | -4.96822200 | -1.12204000 | -0.91940300 |
| C | -3.70977400 | -3.28117900 | -1.27993200 |
| C | -4.54697500 | -2.68609800 | 1.02040600 |
| H | -5.16014200 | -0.28708600 | -0.23863200 |
| H | -4.57352500 | -0.70528200 | -1.85061600 |
| H | -5.92055500 | -1.62021300 | -1.13557000 |
| H | -3.01219200 | -4.00165500 | -0.84331500 |
| H | -4.64504800 | -3.80148300 | -1.51614200 |
| H | -3.28313800 | -2.90945800 | -2.21913500 |
| H | -5.48640400 | -3.21825800 | 0.83047000 |
| H | -3.83625800 | -3.37804300 | 1.47994700 |
| H | -4.75235300 | -1.88066800 | 1.73534000 |
| N | 0.04060200 | 1.63719000 | -0.44589400 |
| H | 0.85743100 | 1.46993200 | 0.24287100 |

int-S9(sextet)

| | | | |
|---|-------------|-------------|-------------|
| C | 4.02284800 | -1.26002600 | -2.23220100 |
| C | 3.99072100 | 0.03167000 | -2.75203200 |
| C | 2.79957600 | 0.75418500 | -2.70435400 |
| C | 1.65188700 | 0.20760200 | -2.12924100 |
| C | 2.87724700 | -1.83457000 | -1.67727600 |
| H | 4.94191800 | -1.83782800 | -2.25815200 |
| H | 4.88010300 | 0.47356400 | -3.18908600 |
| H | 2.75097300 | 1.76220700 | -3.10432100 |
| H | 2.92262800 | -2.84282200 | -1.28813400 |
| C | 0.41056800 | 1.05347200 | -2.08635100 |
| O | -0.22076500 | 1.36171500 | -3.08031600 |
| C | -0.93880300 | 2.36540200 | -0.48984100 |
| C | -1.79856600 | 3.03302400 | -1.31817900 |

| | | | |
|----|-------------|-------------|-------------|
| C | -1.95078600 | 3.51252600 | 1.46566500 |
| C | -2.75799200 | 3.91922800 | -0.78058500 |
| H | -1.69208500 | 2.88900900 | -2.38403300 |
| C | -2.78516700 | 4.16956200 | 0.62232000 |
| H | -1.87802000 | 3.64608700 | 2.53599600 |
| H | -3.44074500 | 4.43990100 | -1.44086400 |
| H | -3.45838900 | 4.91675300 | 1.03140800 |
| O | -1.19873400 | 1.33298300 | 1.60334200 |
| N | -1.10924000 | 2.47521600 | 0.94825700 |
| Co | -0.49361500 | -0.33428200 | 0.54698900 |
| C | 1.68887200 | -1.10327000 | -1.62633600 |
| O | 0.51227900 | -1.61250000 | -1.11605500 |
| C | 0.51563100 | -2.99517400 | -0.71705500 |
| H | 0.78279800 | -3.62519500 | -1.57063600 |
| H | 1.21293300 | -3.14181000 | 0.11279600 |
| H | -0.49534800 | -3.20106800 | -0.37658100 |
| C | 2.21642200 | 0.26839300 | 1.39738700 |
| O | 1.25480500 | -0.58607100 | 1.40019500 |
| C | 3.49845500 | -0.13464400 | 2.14156300 |
| C | 4.71301900 | 0.51419000 | 1.45953400 |
| C | 3.35352600 | 0.39849300 | 3.58367800 |
| C | 3.65555300 | -1.66239600 | 2.16344000 |
| H | 4.81368500 | 0.16272500 | 0.42659600 |
| H | 4.61150400 | 1.60147100 | 1.43423800 |
| H | 5.63012400 | 0.25620800 | 2.00233100 |
| H | 2.48304600 | -0.04624800 | 4.07847700 |
| H | 4.24657900 | 0.14872000 | 4.16849800 |
| H | 3.23409300 | 1.48707000 | 3.58486800 |
| H | 4.56085700 | -1.93738200 | 2.71755000 |
| H | 2.79511900 | -2.14138700 | 2.63667500 |
| H | 3.74823000 | -2.05757500 | 1.14573800 |
| O | 2.15788500 | 1.39576100 | 0.85224300 |
| C | -2.65599100 | -1.42645500 | 0.24688100 |
| O | -1.75662500 | -1.90428500 | 1.02658500 |
| O | -2.39152400 | -0.37622300 | -0.41194800 |
| C | -4.00957300 | -2.12111800 | 0.14421200 |
| C | -4.87644000 | -1.45352300 | -0.93077200 |
| C | -3.76902500 | -3.60425000 | -0.19997300 |
| C | -4.68974900 | -2.01507800 | 1.52572600 |
| H | -5.04410800 | -0.39756800 | -0.70081000 |
| H | -4.39743000 | -1.50592900 | -1.91325900 |
| H | -5.84846800 | -1.95686900 | -0.99067100 |
| H | -3.14377600 | -4.08275800 | 0.55882700 |
| H | -4.72581400 | -4.13613800 | -0.25113100 |
| H | -3.27394800 | -3.70701200 | -1.17315000 |
| H | -5.65729100 | -2.52984500 | 1.50520400 |
| H | -4.06629500 | -2.46888400 | 2.30117300 |
| H | -4.86710900 | -0.96752400 | 1.79512600 |
| N | 0.09858100 | 1.48310300 | -0.78811200 |
| H | 0.94448200 | 1.52301400 | -0.11401200 |

S10

| | | | |
|---|------------|-------------|-------------|
| C | 2.27185200 | 0.58806300 | -0.00022200 |
| C | 1.77589800 | -0.73836700 | -0.00025100 |
| C | 2.70336600 | -1.78846700 | -0.00002800 |
| C | 4.07439300 | -1.55855500 | 0.00030600 |
| C | 4.54392400 | -0.24609600 | 0.00049600 |
| C | 3.65080300 | 0.82373600 | 0.00024200 |
| H | 2.30198200 | -2.79547200 | -0.00008200 |
| H | 4.76829100 | -2.39304900 | 0.00045400 |
| H | 5.61147000 | -0.04457300 | 0.00084900 |
| H | 4.02960400 | 1.83837000 | 0.00041300 |
| C | 0.33230500 | -1.15702400 | -0.00033400 |
| O | 0.02101600 | -2.34641700 | -0.00054600 |

| | | | |
|---|-------------|-------------|-------------|
| N | -0.60443300 | -0.14937600 | -0.00000600 |
| H | -0.30882100 | 0.82996300 | -0.00000600 |
| C | -1.97320300 | -0.28666600 | 0.00003400 |
| C | -2.72470900 | -1.46081100 | 0.00018000 |
| C | -4.11466200 | -1.39403700 | 0.00025700 |
| H | -2.18455400 | -2.39619900 | 0.00014000 |
| C | -3.96954300 | 1.00190100 | 0.00009900 |
| C | -4.73980700 | -0.14635500 | 0.00021500 |
| H | -4.69907200 | -2.30776300 | 0.00038000 |
| H | -4.35712300 | 2.01140700 | 0.00008800 |
| H | -5.81993100 | -0.05012400 | 0.00024100 |
| N | -2.60848900 | 0.94788100 | 0.00004900 |
| O | -1.89885900 | 2.02961600 | -0.00003100 |
| O | 1.35929800 | 1.59899600 | -0.00060900 |
| C | 1.78396400 | 2.95507300 | 0.00003100 |
| H | 2.37242300 | 3.18296100 | 0.89662200 |
| H | 2.37306000 | 3.18361500 | -0.89597300 |
| H | 0.86399400 | 3.53940600 | -0.00009000 |

Co(OPiv)₃⁻ (doublet)

| | | | |
|----|-------------|-------------|-------------|
| Co | 0.32830000 | 0.00191600 | -0.00960900 |
| O | -1.05592200 | 1.12370300 | -0.80463100 |
| O | 2.03674800 | 0.82119100 | -0.75822900 |
| O | -1.03632100 | -1.13076900 | 0.80179700 |
| C | -1.15803300 | 2.00666100 | 0.12354400 |
| O | -0.40394000 | 2.02466200 | 1.11956000 |
| C | 2.68896700 | 0.01617500 | -0.02260800 |
| O | 2.04988200 | -0.79836900 | 0.71805700 |
| C | -1.15028300 | -2.01067200 | -0.12805100 |
| O | -0.41106500 | -2.02407000 | -1.13498600 |
| C | 4.21927700 | 0.01158600 | -0.00436000 |
| C | 4.77499200 | 1.04101000 | -0.99518700 |
| C | 4.67081900 | 0.34785200 | 1.43052600 |
| C | 4.69467700 | -1.40610900 | -0.37558500 |
| H | 4.44479400 | 0.82004700 | -2.01472900 |
| H | 4.42610500 | 2.04816700 | -0.74896900 |
| H | 5.87285700 | 1.03266600 | -0.97208600 |
| H | 4.24376300 | -0.36489800 | 2.14139600 |
| H | 5.76571600 | 0.31222200 | 1.50419700 |
| H | 4.34022700 | 1.35296000 | 1.71732100 |
| H | 5.78962600 | -1.46750600 | -0.32257400 |
| H | 4.26327900 | -2.14358600 | 0.30651000 |
| H | 4.38585400 | -1.66636800 | -1.39475400 |
| C | -2.29620200 | -3.02795600 | 0.04150700 |
| C | -2.21482600 | -4.11012300 | -1.04057200 |
| C | -2.20712900 | -3.65813800 | 1.44198900 |
| C | -3.61747100 | -2.24309300 | -0.08754200 |
| H | -2.25160700 | -3.66333600 | -2.03790800 |
| H | -1.27377700 | -4.66520900 | -0.96664700 |
| H | -3.04747900 | -4.81971700 | -0.93742400 |
| H | -2.22508500 | -2.88045800 | 2.20959300 |
| H | -3.04626600 | -4.34736400 | 1.61010400 |
| H | -1.27430500 | -4.22357900 | 1.55687300 |
| H | -4.47960800 | -2.90940100 | 0.05432400 |
| H | -3.65771700 | -1.44395500 | 0.65787300 |
| H | -3.69794200 | -1.78262000 | -1.07921700 |
| C | -2.30613700 | 3.02335400 | -0.03416100 |
| C | -2.22709400 | 3.65694300 | -1.43384000 |
| C | -3.62637500 | 2.23823200 | 0.10239400 |
| C | -2.21684400 | 4.10307200 | 1.04970300 |
| H | -1.29509600 | 4.22263500 | -1.55397200 |
| H | -2.25056600 | 2.88107300 | -2.20314700 |
| H | -3.06742000 | 4.34651800 | -1.59433900 |
| H | -3.70029700 | 1.77590500 | 1.09374600 |

| | | | |
|---|-------------|------------|-------------|
| H | -4.48945800 | 2.90479900 | -0.03231300 |
| H | -3.67167900 | 1.44053100 | -0.64423100 |
| H | -3.05004500 | 4.81305300 | 0.95391000 |
| H | -2.24690100 | 3.65421200 | 2.04637500 |
| H | -1.27615300 | 4.65792800 | 0.97043400 |

Co(OPiv)₃⁻ (quartet)

| | | | |
|----|-------------|-------------|-------------|
| Co | -0.46895000 | 0.34828400 | -0.35838200 |
| O | 0.34686700 | -1.28702100 | -0.98395900 |
| O | 1.21962700 | 0.75547200 | 1.06956700 |
| O | -2.46545300 | 0.55083500 | -1.24161500 |
| C | 1.58266900 | -1.62107500 | -0.73388900 |
| O | 2.58221900 | -1.05938600 | -1.18539200 |
| C | 1.57414600 | 1.58870700 | 0.19391200 |
| O | 0.76229200 | 1.92867100 | -0.74093900 |
| C | -2.92053900 | 0.33175700 | -0.08109000 |
| O | -2.13659500 | 0.15749000 | 0.91179600 |
| C | 2.98130600 | 2.19708300 | 0.20376200 |
| C | 2.87697900 | 3.62200400 | 0.78263300 |
| C | 3.90942800 | 1.32967000 | 1.06559000 |
| C | 3.50435000 | 2.24795400 | -1.24266300 |
| H | 2.19079000 | 4.23190500 | 0.18516900 |
| H | 2.50823400 | 3.60068800 | 1.81532700 |
| H | 3.86270400 | 4.10583600 | 0.78117100 |
| H | 3.95963700 | 0.31839300 | 0.65165700 |
| H | 4.92018600 | 1.75950700 | 1.08317200 |
| H | 3.53851000 | 1.25795600 | 2.09207400 |
| H | 4.52547000 | 2.65323400 | -1.26012200 |
| H | 3.50733600 | 1.24082400 | -1.66903600 |
| H | 2.86163300 | 2.87844600 | -1.86293200 |
| C | -4.43376700 | 0.26160600 | 0.17088600 |
| C | -4.79101900 | 1.33042200 | 1.22148200 |
| C | -5.21519900 | 0.50371300 | -1.12548500 |
| C | -4.75140900 | -1.13732600 | 0.73461300 |
| H | -4.20371700 | 1.18103500 | 2.13137600 |
| H | -4.58082800 | 2.33736900 | 0.84135300 |
| H | -5.85848500 | 1.27718300 | 1.47260700 |
| H | -4.95479900 | -0.24091700 | -1.88334500 |
| H | -6.29487700 | 0.44727000 | -0.93286300 |
| H | -4.98537500 | 1.48881000 | -1.54248400 |
| H | -5.81975300 | -1.21837400 | 0.97434500 |
| H | -4.50561100 | -1.91722300 | 0.00415800 |
| H | -4.16831800 | -1.32480900 | 1.64020900 |
| C | 1.72420300 | -2.85346300 | 0.19733600 |
| C | 1.03081400 | -2.53262700 | 1.53555700 |
| C | 1.02637100 | -4.05269800 | -0.47021200 |
| C | 3.20514400 | -3.16692100 | 0.43665900 |
| H | 1.46122400 | -1.63392000 | 1.98764500 |
| H | -0.03580000 | -2.34413600 | 1.38339300 |
| H | 1.14369800 | -3.37369600 | 2.23427400 |
| H | 1.51596000 | -4.31649300 | -1.41643100 |
| H | 1.05984300 | -4.93391200 | 0.18544800 |
| H | -0.01816300 | -3.80952900 | -0.68314700 |
| H | 3.31082500 | -4.06059400 | 1.06751100 |
| H | 3.72636200 | -3.34053700 | -0.50982100 |
| H | 3.70244600 | -2.32930300 | 0.93538900 |

HOPIV

| | | | |
|---|-------------|-------------|-------------|
| C | -0.94147100 | 0.18715600 | -0.00001600 |
| O | -1.52425200 | 1.24935300 | -0.00002000 |
| C | 0.57194000 | -0.01045000 | -0.00000500 |
| C | 0.96957800 | -0.80423500 | 1.26187900 |
| C | 0.96960900 | -0.80456100 | -1.26166800 |

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|---|-------------|-------------|-------------|
| C | 1.25115100 | 1.36456600 | -0.00016900 |
| H | 0.68389200 | -0.26617800 | 2.17270600 |
| H | 0.49340300 | -1.78822900 | 1.27901600 |
| H | 2.05624200 | -0.94381900 | 1.27926900 |
| H | 0.68385700 | -0.26679000 | -2.17264400 |
| H | 2.05628400 | -0.94406000 | -1.27904800 |
| H | 0.49351300 | -1.78859800 | -1.27851700 |
| H | 2.33944300 | 1.23937700 | -0.00008200 |
| H | 0.96727200 | 1.94453600 | -0.88303900 |
| H | 0.96715100 | 1.94480500 | 0.88248200 |
| O | -1.61393100 | -0.99515400 | -0.00001300 |
| H | -2.56044100 | -0.75948900 | 0.00000000 |

O⁻Piv

| | | | |
|---|-------------|-------------|-------------|
| C | -1.06431400 | 0.03083100 | 0.00045700 |
| O | -1.60855100 | 1.16207600 | 0.00007700 |
| O | -1.59327100 | -1.11127600 | 0.00002600 |
| C | 0.52882700 | 0.01319800 | -0.00000200 |
| C | 0.99216300 | -0.74953700 | 1.24988900 |
| C | 0.99148400 | -0.75026500 | -1.24968500 |
| C | 1.10321000 | 1.43167900 | -0.00056700 |
| H | 0.71213200 | -0.20625200 | 2.16296000 |
| H | 0.49847400 | -1.72544400 | 1.27603000 |
| H | 2.08528100 | -0.89424900 | 1.26680000 |
| H | 0.71093800 | -0.20753800 | -2.16293200 |
| H | 2.08459500 | -0.89494800 | -1.26710300 |
| H | 0.49782500 | -1.72621300 | -1.27497900 |
| H | 2.20620000 | 1.42226300 | -0.00075000 |
| H | 0.75532500 | 1.98499100 | -0.87893600 |
| H | 0.75558100 | 1.98555700 | 0.87754000 |

MeOH

| | | | |
|---|-------------|-------------|-------------|
| C | 0.66226700 | -0.01950700 | 0.00000100 |
| H | 1.07958000 | 0.99101900 | -0.00061900 |
| H | 1.03666000 | -0.54420700 | -0.89284100 |
| H | 1.03675800 | -0.54316200 | 0.89342100 |
| O | -0.74912000 | 0.12249900 | 0.00000300 |
| H | -1.13363800 | -0.76659600 | 0.00001000 |

int13-tBu (doublet)

| | | | |
|----|-------------|-------------|-------------|
| C | 2.97515800 | -0.99258500 | -1.82941600 |
| C | 1.91564000 | -0.08963600 | -1.98157700 |
| C | 0.59347100 | -0.52658000 | -2.02930800 |
| C | 0.29931500 | -1.89119800 | -1.99158000 |
| C | 1.34292000 | -2.80040300 | -1.85829000 |
| C | 2.66442600 | -2.35641600 | -1.76244800 |
| H | 2.10104800 | 0.97561400 | -2.02130600 |
| H | -0.72578800 | -2.22624100 | -2.07580700 |
| H | 1.12910400 | -3.86541400 | -1.82577100 |
| H | 3.45308500 | -3.09096200 | -1.64501200 |
| C | -0.48588100 | 0.49581100 | -2.17960800 |
| O | -0.71491200 | 1.04096200 | -3.24158700 |
| C | -2.23999900 | 1.70369700 | -1.00406300 |
| C | -2.63709900 | 2.60517800 | -2.01217700 |
| C | -3.97845500 | 2.56615700 | 0.40856500 |
| C | -3.69743900 | 3.46696200 | -1.79536700 |
| H | -2.08318400 | 2.58981900 | -2.93659000 |
| C | -4.38264900 | 3.44716300 | -0.57221000 |
| H | -4.42291300 | 2.46736000 | 1.38945600 |
| H | -3.99077700 | 4.16133400 | -2.57528500 |
| H | -5.21475500 | 4.11202200 | -0.37288900 |
| O | -2.60894500 | 0.88174200 | 1.14451900 |
| N | -2.94011300 | 1.72891100 | 0.18474000 |
| Co | -0.90180900 | 0.14116700 | 0.79025400 |

| | | | |
|---|-------------|-------------|-------------|
| O | -1.67685300 | -1.56736000 | 0.54081500 |
| O | -0.41233000 | -0.54574200 | 2.55015200 |
| O | -0.10802300 | 1.77360600 | 1.31889900 |
| C | 0.66686600 | -0.98043900 | 2.03203900 |
| O | 0.84089200 | -0.68097700 | 0.80130300 |
| C | -2.55110600 | -1.81681500 | -0.36498100 |
| O | -2.88085200 | -1.06129600 | -1.29604300 |
| C | 0.66439700 | 2.46660200 | 0.55002500 |
| O | 0.73339500 | 2.38818800 | -0.68444000 |
| C | 1.63740700 | -1.87666900 | 2.76569800 |
| C | 1.51191900 | -1.66351000 | 4.28014900 |
| C | 1.23479200 | -3.32168200 | 2.38428700 |
| C | 3.06610100 | -1.58920800 | 2.27668300 |
| H | 1.78148200 | -0.63882600 | 4.55778800 |
| H | 0.48886500 | -1.84605800 | 4.61972800 |
| H | 2.18425700 | -2.34994200 | 4.80664800 |
| H | 1.30036800 | -3.46547400 | 1.30150400 |
| H | 1.90798200 | -4.03224600 | 2.87691800 |
| H | 0.20892800 | -3.53632600 | 2.70074200 |
| H | 3.76819500 | -2.27866100 | 2.75883900 |
| H | 3.13651300 | -1.71374100 | 1.19323500 |
| H | 3.36831600 | -0.56579900 | 2.52489700 |
| C | 1.55806100 | 3.46275400 | 1.32693700 |
| C | 2.47015400 | 2.62720000 | 2.24801500 |
| C | 2.39841700 | 4.29605800 | 0.35345600 |
| C | 0.65311700 | 4.37570100 | 2.17432700 |
| H | 1.87350500 | 2.03567300 | 2.94775800 |
| H | 3.09529900 | 1.94339300 | 1.66338000 |
| H | 3.13163700 | 3.28907300 | 2.81928200 |
| H | 1.76193600 | 4.86652100 | -0.32969100 |
| H | 3.02608100 | 4.99951000 | 0.91316900 |
| H | 3.04942000 | 3.66019400 | -0.25309600 |
| H | 1.26689900 | 5.06903500 | 2.76156100 |
| H | -0.01070800 | 4.97181000 | 1.53653800 |
| H | 0.03738700 | 3.78555100 | 2.85769500 |
| C | -3.20394000 | -3.21551400 | -0.22697600 |
| C | -2.08709000 | -4.27632400 | -0.24168600 |
| C | -3.93699100 | -3.24758100 | 1.12802400 |
| C | -4.18754200 | -3.46136000 | -1.37638400 |
| H | -1.56212300 | -4.28690900 | -1.20373700 |
| H | -1.35439600 | -4.08325800 | 0.54534400 |
| H | -2.52011800 | -5.27165500 | -0.08722200 |
| H | -4.72695900 | -2.48848400 | 1.16467100 |
| H | -4.40284400 | -4.22918600 | 1.27550900 |
| H | -3.24204400 | -3.05754000 | 1.94999200 |
| H | -4.64147900 | -4.45345600 | -1.26894300 |
| H | -4.98565900 | -2.71339600 | -1.38121600 |
| H | -3.68302300 | -3.41488200 | -2.34614000 |
| N | -1.23036600 | 0.78944600 | -0.99587300 |
| C | 4.41043400 | -0.45317100 | -1.76514000 |
| C | 4.51604600 | 0.62454100 | -0.66397300 |
| C | 5.43476500 | -1.55655200 | -1.45491300 |
| C | 4.76388900 | 0.17809500 | -3.12954100 |
| H | 3.82842600 | 1.45624900 | -0.84116100 |
| H | 4.28009000 | 0.20170000 | 0.31726500 |
| H | 5.53406700 | 1.03061700 | -0.62790400 |
| H | 5.45565600 | -2.32384000 | -2.23650700 |
| H | 6.43823100 | -1.12125400 | -1.39282100 |
| H | 5.22321600 | -2.04610300 | -0.49743300 |
| H | 5.78326600 | 0.58276000 | -3.11266600 |
| H | 4.70358000 | -0.56756200 | -3.93015700 |
| H | 4.07851700 | 0.99431100 | -3.37985300 |

TS14-tBu (doublet)

| | | | |
|----|-------------|-------------|-------------|
| C | 3.06736900 | -2.43949900 | -1.26136900 |
| C | 1.75674900 | -2.92244500 | -1.16451200 |
| C | 0.74270400 | -2.06498800 | -1.53970600 |
| C | 0.93265800 | -0.74605300 | -1.89466900 |
| C | 2.25179800 | -0.30296000 | -2.01820200 |
| C | 3.33044100 | -1.11996900 | -1.66378400 |
| H | 1.56038700 | -3.93901400 | -0.83880900 |
| H | -0.51848500 | -2.56526500 | -1.61015700 |
| H | 2.39755700 | 0.73063200 | -2.30509300 |
| C | -0.18691000 | 0.20905800 | -2.18297100 |
| O | -0.21575900 | 0.81397900 | -3.24908500 |
| N | -1.14125800 | 0.28722800 | -1.18750400 |
| C | -2.23627600 | 1.08963900 | -1.32255100 |
| C | -2.65656400 | 1.89128300 | -2.40382400 |
| C | -3.81744100 | 2.64127900 | -2.30278400 |
| H | -2.03264900 | 1.90032000 | -3.28375600 |
| C | -4.15554900 | 1.82856300 | -0.08197600 |
| C | -4.58308300 | 2.61716400 | -1.12891900 |
| H | -4.12376700 | 3.26048000 | -3.13981000 |
| H | -4.64810400 | 1.73149200 | 0.87605600 |
| H | -5.48652800 | 3.20469800 | -1.01957000 |
| N | -3.03125100 | 1.09114600 | -0.20237700 |
| O | -2.67548300 | 0.30139700 | 0.82416900 |
| Co | -0.81939300 | -0.05010900 | 0.70205800 |
| C | -1.97625100 | -2.66844400 | -0.21415100 |
| O | -1.61411700 | -2.96968000 | -1.42841100 |
| O | -1.27033300 | -2.03392100 | 0.58376400 |
| C | -3.37551200 | -3.17500200 | 0.16523600 |
| C | -3.61150100 | -2.94081200 | 1.66310100 |
| C | -4.38704200 | -2.35307700 | -0.66526700 |
| C | -3.49595200 | -4.67003300 | -0.18304100 |
| H | -2.88499400 | -3.49008400 | 2.26983000 |
| H | -3.52478500 | -1.88067400 | 1.91045500 |
| H | -4.61625800 | -3.28913600 | 1.92819200 |
| H | -4.22831300 | -2.49467500 | -1.73812500 |
| H | -5.40374100 | -2.67742300 | -0.41704900 |
| H | -4.29978600 | -1.28904400 | -0.43014000 |
| H | -4.49668700 | -5.02610200 | 0.08504300 |
| H | -3.33788500 | -4.84508800 | -1.25027800 |
| H | -2.76598800 | -5.26610900 | 0.37641800 |
| C | 0.37840200 | 2.45583000 | 0.34041600 |
| O | -0.52092400 | 1.74906900 | 0.98630400 |
| O | 1.15028700 | 2.05313000 | -0.52089800 |
| C | 0.33720200 | 3.93777000 | 0.78374000 |
| C | -1.06925100 | 4.48875000 | 0.47404300 |
| C | 0.60965600 | 4.01625200 | 2.29713800 |
| C | 1.39887600 | 4.72623600 | 0.00857900 |
| H | -1.30309200 | 4.38836600 | -0.59275000 |
| H | -1.83121800 | 3.94931400 | 1.04321500 |
| H | -1.12509400 | 5.55285600 | 0.73385300 |
| H | 1.60564300 | 3.62337300 | 2.53370100 |
| H | 0.57013500 | 5.05859800 | 2.63607000 |
| H | -0.12891100 | 3.43537000 | 2.85589000 |
| H | 1.37871400 | 5.77978200 | 0.31238900 |
| H | 2.39973400 | 4.32774600 | 0.19954800 |
| H | 1.22223300 | 4.66860900 | -1.06929900 |
| C | 0.85035600 | -0.54548600 | 2.20534200 |
| O | 1.05366000 | -0.46440700 | 0.94742700 |
| O | -0.35588700 | -0.37765900 | 2.57922700 |
| C | 2.00651300 | -0.75117300 | 3.15922100 |
| C | 1.49179000 | -1.13449400 | 4.55202900 |
| C | 2.92948000 | -1.84263700 | 2.58725700 |
| C | 2.75916800 | 0.59924700 | 3.21033300 |
| H | 0.81997300 | -0.36826100 | 4.94845400 |

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|---|------------|-------------|-------------|
| H | 0.94168700 | -2.08085600 | 4.52307900 |
| H | 2.33740100 | -1.24815300 | 5.23966200 |
| H | 3.25546500 | -1.58661500 | 1.57627300 |
| H | 3.81039400 | -1.95632000 | 3.22902000 |
| H | 2.41325400 | -2.80821900 | 2.53963100 |
| H | 3.64087100 | 0.50648400 | 3.85440200 |
| H | 3.08149000 | 0.90017300 | 2.20907200 |
| H | 2.11669900 | 1.38799900 | 3.61580600 |
| H | 3.88054900 | -3.10798300 | -1.00204300 |
| C | 4.73905000 | -0.51282600 | -1.65263200 |
| C | 4.76940100 | 0.62272000 | -0.60307300 |
| C | 5.81874400 | -1.54373300 | -1.28625500 |
| C | 5.06723100 | 0.06084900 | -3.04777100 |
| H | 3.99600700 | 1.37347900 | -0.79057000 |
| H | 4.59896400 | 0.22034900 | 0.40160600 |
| H | 5.74743200 | 1.11906100 | -0.61123600 |
| H | 5.84762100 | -2.37475400 | -2.00048100 |
| H | 6.80305400 | -1.06339300 | -1.29520300 |
| H | 5.66269100 | -1.95578700 | -0.28303400 |
| H | 6.07198800 | 0.49936100 | -3.04749700 |
| H | 5.03730400 | -0.72534800 | -3.81056500 |
| H | 4.36113800 | 0.84276700 | -3.34243300 |

int13-Me (doublet)

| | | | |
|----|-------------|-------------|-------------|
| C | -1.81339800 | -2.15728500 | 2.77353900 |
| C | -1.35531100 | -0.84965800 | 2.58624800 |
| C | -0.00445200 | -0.59741600 | 2.34770800 |
| C | 0.91961000 | -1.64553500 | 2.34080700 |
| C | 0.47193300 | -2.94941500 | 2.53582000 |
| C | -0.88522500 | -3.20368300 | 2.74125300 |
| H | -2.05455100 | -0.02116800 | 2.58126000 |
| H | 1.97130700 | -1.43432400 | 2.19258400 |
| H | 1.18343000 | -3.77060000 | 2.53269400 |
| H | -1.22724500 | -4.22549900 | 2.88814700 |
| C | 0.45982600 | 0.81300600 | 2.16624400 |
| O | 0.69998900 | 1.53806800 | 3.11119300 |
| C | 1.06840900 | 2.49750400 | 0.52015700 |
| C | 1.24995800 | 3.61199200 | 1.36258400 |
| C | 1.78884100 | 3.82572800 | -1.34359500 |
| C | 1.70092100 | 4.81119200 | 0.84006000 |
| H | 1.02476100 | 3.48467800 | 2.40879400 |
| C | 1.97952800 | 4.92222600 | -0.52943500 |
| H | 1.96156300 | 3.79485700 | -2.41067300 |
| H | 1.83171300 | 5.66531100 | 1.49567500 |
| H | 2.33154300 | 5.84878100 | -0.96735600 |
| O | 1.20676500 | 1.62763600 | -1.63708500 |
| N | 1.34654900 | 2.65938400 | -0.82058900 |
| Co | 0.20586600 | 0.26213200 | -0.79015500 |
| O | 1.72492400 | -0.86205300 | -0.74873000 |
| O | -0.33371100 | -0.82454700 | -2.32339000 |
| O | -1.37886600 | 1.26227700 | -1.07419400 |
| C | -0.91345200 | -1.60881500 | -1.50501000 |
| O | -0.87973100 | -1.24194200 | -0.28085700 |
| C | 2.80544200 | -0.56778700 | -0.12128200 |
| O | 2.96454000 | 0.38450800 | 0.66217900 |
| C | -2.13890800 | 1.66336300 | -0.11197600 |
| O | -1.81196600 | 1.79611100 | 1.07713500 |
| C | -1.52090400 | -2.93367600 | -1.90249100 |
| C | -1.91632900 | -2.91122600 | -3.38478600 |
| C | -0.41543100 | -3.98711100 | -1.64873300 |
| C | -2.73353100 | -3.22642000 | -1.00291400 |
| H | -2.69132000 | -2.16073100 | -3.57465100 |
| H | -1.05696800 | -2.67520700 | -4.01810100 |
| H | -2.30908300 | -3.89135700 | -3.67726800 |

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|---|-------------|-------------|-------------|
| H | -0.11444900 | -3.98163700 | -0.59651200 |
| H | -0.79252700 | -4.98387300 | -1.90402200 |
| H | 0.46747200 | -3.78100900 | -2.26271000 |
| H | -3.14820600 | -4.20953700 | -1.25201600 |
| H | -2.44323900 | -3.22280900 | 0.05071100 |
| H | -3.51966700 | -2.47696200 | -1.14506700 |
| C | -3.58782400 | 1.96843800 | -0.56004100 |
| C | -4.19760700 | 0.62713400 | -1.01720900 |
| C | -4.39422700 | 2.54990500 | 0.60649700 |
| C | -3.55142600 | 2.95739500 | -1.73836400 |
| H | -3.63572700 | 0.21570900 | -1.86019900 |
| H | -4.18424500 | -0.10689000 | -0.20305200 |
| H | -5.23908100 | 0.77578700 | -1.32563300 |
| H | -3.95159700 | 3.48366500 | 0.96671500 |
| H | -5.42098400 | 2.75615700 | 0.28221900 |
| H | -4.42896200 | 1.85315000 | 1.44877700 |
| H | -4.57022600 | 3.15090100 | -2.09476700 |
| H | -3.11488800 | 3.91600500 | -1.43320600 |
| H | -2.95906400 | 2.55624900 | -2.56430900 |
| C | 3.97520300 | -1.53987400 | -0.41648400 |
| C | 3.51108900 | -2.97444900 | -0.10311000 |
| C | 4.30444900 | -1.41366700 | -1.91687700 |
| C | 5.19807500 | -1.17677500 | 0.43330600 |
| H | 3.28265400 | -3.09410200 | 0.96187900 |
| H | 2.61488500 | -3.22840700 | -0.67383100 |
| H | 4.30730700 | -3.68428300 | -0.35681400 |
| H | 4.62344900 | -0.39444600 | -2.16394600 |
| H | 5.12126600 | -2.09719300 | -2.17752900 |
| H | 3.43093000 | -1.65631700 | -2.52756900 |
| H | 6.02040100 | -1.86715500 | 0.21184700 |
| H | 5.53528000 | -0.15713900 | 0.22627000 |
| H | 4.97206300 | -1.24093400 | 1.50210200 |
| N | 0.62649300 | 1.24171600 | 0.81438300 |
| C | -3.28720900 | -2.42184900 | 2.96483700 |
| H | -3.46868500 | -3.43539200 | 3.33671800 |
| H | -3.73248200 | -1.71453900 | 3.67335500 |
| H | -3.83034800 | -2.31490900 | 2.01657000 |

TS14-Me (doublet)

| | | | |
|----|-------------|-------------|-------------|
| C | -2.69926500 | -2.82769600 | 2.30204600 |
| C | -1.42194900 | -3.10452800 | 1.81089000 |
| C | -0.48700400 | -2.08827400 | 1.89559300 |
| C | -0.77199800 | -0.79564100 | 2.28611400 |
| C | -2.05159800 | -0.55163200 | 2.79860500 |
| C | -3.02634200 | -1.55166800 | 2.79395100 |
| H | -1.16905200 | -4.08553400 | 1.42161000 |
| H | 0.81103300 | -2.41671600 | 1.68314600 |
| H | -2.28126100 | 0.45488000 | 3.13133800 |
| C | 0.24059200 | 0.31096600 | 2.26540000 |
| O | 0.41801800 | 0.98819900 | 3.27201400 |
| N | 0.94762200 | 0.42485700 | 1.08357800 |
| C | 1.93882200 | 1.35257000 | 0.94616400 |
| C | 2.48532400 | 2.25473200 | 1.88256100 |
| C | 3.49650300 | 3.12307200 | 1.50363300 |
| H | 2.07218600 | 2.24376600 | 2.87886200 |
| C | 3.43795500 | 2.23280700 | -0.71185600 |
| C | 3.98524600 | 3.12022900 | 0.19004900 |
| H | 3.90054800 | 3.81755300 | 2.23322600 |
| H | 3.71728600 | 2.13866300 | -1.75251700 |
| H | 4.76555500 | 3.79771700 | -0.13478100 |
| N | 2.46392300 | 1.38269800 | -0.32304200 |
| O | 1.99083200 | 0.50532900 | -1.22294000 |
| Co | 0.26365200 | -0.04711600 | -0.67738200 |
| C | 1.91841900 | -2.44867400 | -0.00287800 |

| | | | |
|---|-------------|-------------|-------------|
| O | 1.88690700 | -2.70219300 | 1.27230000 |
| O | 0.96946600 | -1.95893700 | -0.63584400 |
| C | 3.24502700 | -2.81266600 | -0.68562200 |
| C | 3.09899100 | -2.64459700 | -2.20350500 |
| C | 4.30869600 | -1.83062100 | -0.14480800 |
| C | 3.62907400 | -4.25985000 | -0.32621700 |
| H | 2.32848300 | -3.31045400 | -2.60418400 |
| H | 2.82326300 | -1.61856400 | -2.45619000 |
| H | 4.05203300 | -2.88898700 | -2.68638300 |
| H | 4.41643000 | -1.91920300 | 0.93997600 |
| H | 5.27465500 | -2.05381600 | -0.61129600 |
| H | 4.03760800 | -0.80102800 | -0.39252800 |
| H | 4.58061600 | -4.51328100 | -0.80624000 |
| H | 3.73862400 | -4.38684700 | 0.75396200 |
| H | 2.87341300 | -4.96942800 | -0.68222400 |
| C | -1.09942000 | 2.32589300 | -0.09823800 |
| O | -0.30568200 | 1.68967900 | -0.93054100 |
| O | -1.60265100 | 1.87790200 | 0.92369100 |
| C | -1.31034200 | 3.79113000 | -0.54993700 |
| C | 0.06227400 | 4.49396200 | -0.52038500 |
| C | -1.87636500 | 3.80600900 | -1.98137500 |
| C | -2.27914400 | 4.48312700 | 0.41552000 |
| H | 0.50360600 | 4.44859200 | 0.48247900 |
| H | 0.75613400 | 4.02140200 | -1.22102500 |
| H | -0.04700000 | 5.55034500 | -0.79434700 |
| H | -2.84951000 | 3.30194800 | -2.02064400 |
| H | -2.01892200 | 4.83890800 | -2.32199400 |
| H | -1.20009100 | 3.29704600 | -2.67297500 |
| H | -2.43159800 | 5.52528000 | 0.10965000 |
| H | -3.24969500 | 3.97804700 | 0.42583800 |
| H | -1.89096700 | 4.47015700 | 1.43784300 |
| C | -1.62530500 | -0.80780800 | -1.74462000 |
| O | -1.54793600 | -0.68727000 | -0.47543200 |
| O | -0.56565900 | -0.51917800 | -2.38991500 |
| C | -2.92962800 | -1.19779300 | -2.40397800 |
| C | -2.69104900 | -1.59915700 | -3.86479700 |
| C | -3.56122200 | -2.35242700 | -1.60513300 |
| C | -3.83572800 | 0.05344500 | -2.32573600 |
| H | -2.22541900 | -0.78442100 | -4.42600500 |
| H | -2.03304400 | -2.47186500 | -3.93224200 |
| H | -3.64609900 | -1.85023000 | -4.33982500 |
| H | -3.68881200 | -2.07632200 | -0.55536000 |
| H | -4.53983800 | -2.60428700 | -2.02916000 |
| H | -2.93060500 | -3.24791700 | -1.64519800 |
| H | -4.81238200 | -0.16975200 | -2.76988500 |
| H | -3.98135300 | 0.36067000 | -1.28580900 |
| H | -3.39044100 | 0.89130900 | -2.87294200 |
| H | -3.45386000 | -3.61084400 | 2.29591500 |
| C | -4.41694900 | -1.26224400 | 3.30338300 |
| H | -5.16525900 | -1.88247000 | 2.79930200 |
| H | -4.49135900 | -1.46752100 | 4.37954600 |
| H | -4.68238300 | -0.21177700 | 3.15102000 |

int13-OMe (doublet)

| | | | |
|---|------------|-------------|-------------|
| C | 2.55684300 | 1.21346000 | -2.30413700 |
| C | 1.23492300 | 0.76829400 | -2.18239500 |
| C | 0.96707600 | -0.59342300 | -2.18968600 |
| C | 1.99989900 | -1.52671100 | -2.38489200 |
| C | 3.30581400 | -1.07293700 | -2.50912600 |
| C | 3.59868000 | 0.29616100 | -2.46111700 |
| H | 0.44068200 | 1.48866300 | -2.04767400 |
| H | 1.76568100 | -2.58445000 | -2.41297300 |
| H | 4.11563900 | -1.78403300 | -2.64586400 |
| H | 4.62673700 | 0.62598800 | -2.55228700 |

| | | | |
|----|-------------|-------------|-------------|
| C | -0.41982800 | -1.12981200 | -2.07068500 |
| O | -0.93240400 | -1.77151100 | -2.96850400 |
| C | -2.32592800 | -1.46611200 | -0.63121800 |
| C | -3.31063400 | -1.79376500 | -1.58195500 |
| C | -3.83085800 | -2.11617500 | 1.11843100 |
| C | -4.53652800 | -2.28571700 | -1.16826500 |
| H | -3.07363100 | -1.64415800 | -2.62248400 |
| C | -4.79869300 | -2.46051400 | 0.19787700 |
| H | -3.92794600 | -2.18827700 | 2.19298800 |
| H | -5.29466100 | -2.52622800 | -1.90567500 |
| H | -5.74890500 | -2.84310100 | 0.55131400 |
| O | -1.73112500 | -1.32778900 | 1.61125600 |
| N | -2.63993200 | -1.63140900 | 0.70019800 |
| Co | -0.45840900 | -0.15664100 | 0.83656000 |
| O | 0.94741100 | -1.37924700 | 1.11583700 |
| O | 0.21160700 | 0.75601500 | 2.43067100 |
| O | -1.80587500 | 1.17319500 | 0.73642600 |
| C | 0.97948000 | 1.42795600 | 1.67005600 |
| O | 0.85414800 | 1.18541200 | 0.42117200 |
| C | 0.95296300 | -2.56287700 | 0.61917400 |
| O | 0.09935700 | -3.04110800 | -0.14847800 |
| C | -2.10713400 | 1.75285600 | -0.37889600 |
| O | -1.78481500 | 1.37044500 | -1.51352100 |
| C | 2.02777900 | 2.39826300 | 2.16222000 |
| C | 1.75024000 | 2.78857100 | 3.61924600 |
| C | 3.38125700 | 1.65801200 | 2.04334400 |
| C | 2.02758200 | 3.63312700 | 1.24176400 |
| H | 0.78765700 | 3.30228800 | 3.71232900 |
| H | 1.72419400 | 1.90767400 | 4.26669400 |
| H | 2.53608300 | 3.46293700 | 3.97722300 |
| H | 3.56375900 | 1.34799400 | 1.00985900 |
| H | 4.19155000 | 2.32286700 | 2.36341700 |
| H | 3.39680500 | 0.76416900 | 2.67610600 |
| H | 2.82957000 | 4.31612200 | 1.54427100 |
| H | 2.18001100 | 3.34456600 | 0.19825300 |
| H | 1.07666300 | 4.17267000 | 1.31207300 |
| C | -2.95327600 | 3.03356500 | -0.19335100 |
| C | -2.09243500 | 4.03745100 | 0.59898900 |
| C | -3.33681400 | 3.61761500 | -1.55738400 |
| C | -4.21504600 | 2.67165700 | 0.61174900 |
| H | -1.81721000 | 3.62567400 | 1.57381600 |
| H | -1.17276400 | 4.27813900 | 0.05309800 |
| H | -2.64941800 | 4.96918400 | 0.75341500 |
| H | -3.92732500 | 2.90428800 | -2.14042000 |
| H | -3.93161300 | 4.52790400 | -1.41743100 |
| H | -2.44798200 | 3.86796300 | -2.14318000 |
| H | -4.82566200 | 3.56789400 | 0.77318600 |
| H | -4.82837000 | 1.94038000 | 0.07108600 |
| H | -3.94787100 | 2.24738700 | 1.58284900 |
| C | 2.14390200 | -3.43237100 | 1.09206500 |
| C | 3.42923000 | -2.58774700 | 1.09327500 |
| C | 1.80696800 | -3.88173400 | 2.52884300 |
| C | 2.30415000 | -4.65161400 | 0.17585800 |
| H | 3.65154800 | -2.20843400 | 0.09075500 |
| H | 3.33164000 | -1.73034400 | 1.76281900 |
| H | 4.27399700 | -3.20278400 | 1.42642000 |
| H | 0.89189700 | -4.48426600 | 2.54759500 |
| H | 2.62555800 | -4.49105000 | 2.93009000 |
| H | 1.66365300 | -3.01500600 | 3.18107000 |
| H | 3.11958200 | -5.28636300 | 0.54203800 |
| H | 1.38653600 | -5.24433600 | 0.14072200 |
| H | 2.54433400 | -4.34628100 | -0.84793100 |
| N | -1.07776200 | -0.94544700 | -0.81759300 |
| O | 2.72232000 | 2.56985500 | -2.23840700 |

| | | | |
|---|------------|------------|-------------|
| C | 4.04205900 | 3.07902900 | -2.30540900 |
| H | 3.95065900 | 4.16325900 | -2.22164400 |
| H | 4.66068400 | 2.70197800 | -1.47974600 |
| H | 4.52411900 | 2.82724600 | -3.25941000 |

TS14-OMe (doublet)

| | | | |
|----|-------------|-------------|-------------|
| C | 2.78876400 | -2.85918400 | -1.86620600 |
| C | 1.45826900 | -3.09450800 | -1.54877800 |
| C | 0.54631800 | -2.07061100 | -1.78483200 |
| C | 0.92589100 | -0.77987300 | -2.11115500 |
| C | 2.25728000 | -0.55074300 | -2.46434700 |
| C | 3.19026400 | -1.58097900 | -2.31264000 |
| H | 1.13965300 | -4.06535800 | -1.18186300 |
| H | -0.85265800 | -2.38670100 | -1.77916200 |
| H | 2.53545100 | 0.44719900 | -2.77368600 |
| C | -0.05051000 | 0.35534700 | -2.21077200 |
| O | -0.06997100 | 1.05425500 | -3.21872100 |
| N | -0.90463300 | 0.47312100 | -1.13274200 |
| C | -1.88157900 | 1.42456500 | -1.10983500 |
| C | -2.27506200 | 2.35702500 | -2.09197700 |
| C | -3.30828500 | 3.24387800 | -1.83497900 |
| H | -1.73064900 | 2.35212200 | -3.02317200 |
| C | -3.56963200 | 2.31350100 | 0.34942700 |
| C | -3.97011400 | 3.23010200 | -0.59944500 |
| H | -3.59431100 | 3.96086100 | -2.59785200 |
| H | -3.98948200 | 2.20811900 | 1.34066600 |
| H | -4.77225000 | 3.92057200 | -0.36880500 |
| N | -2.57119000 | 1.44650700 | 0.07785300 |
| O | -2.24384900 | 0.54177100 | 1.01468100 |
| Co | -0.47675400 | -0.05416100 | 0.69222500 |
| C | -2.09961200 | -2.39148300 | -0.24463100 |
| O | -1.93705800 | -2.62514100 | -1.51324600 |
| O | -1.19902000 | -1.94529500 | 0.48840900 |
| C | -3.49350800 | -2.72422000 | 0.29727300 |
| C | -3.50164000 | -2.57628800 | 1.82393600 |
| C | -4.47734200 | -1.71513800 | -0.33673000 |
| C | -3.87097300 | -4.15922000 | -0.11718200 |
| H | -2.79159500 | -3.26455500 | 2.29274200 |
| H | -3.23026000 | -1.56008500 | 2.11737000 |
| H | -4.50448100 | -2.80236000 | 2.20399000 |
| H | -4.46346100 | -1.77932200 | -1.42850000 |
| H | -5.49253100 | -1.93335000 | 0.01322700 |
| H | -4.22226200 | -0.69551300 | -0.03635700 |
| H | -4.87140600 | -4.39571200 | 0.26123500 |
| H | -3.87269900 | -4.27223000 | -1.20439100 |
| H | -3.17060300 | -4.88936300 | 0.30445600 |
| C | 1.02667500 | 2.28267900 | 0.35575400 |
| O | 0.10528500 | 1.66100900 | 1.05600500 |
| O | 1.66002500 | 1.83153600 | -0.59027500 |
| C | 1.21215100 | 3.73552200 | 0.85622500 |
| C | -0.12827900 | 4.47487600 | 0.66958800 |
| C | 1.59384700 | 3.71180000 | 2.34750500 |
| C | 2.31117200 | 4.41785000 | 0.03385900 |
| H | -0.44450200 | 4.45385500 | -0.38023700 |
| H | -0.91421400 | 4.01176700 | 1.27231300 |
| H | -0.02762700 | 5.52436000 | 0.97173400 |
| H | 2.53875700 | 3.17640300 | 2.49927100 |
| H | 1.72269600 | 4.73447800 | 2.72278800 |
| H | 0.82060400 | 3.21455200 | 2.93887600 |
| H | 2.44221400 | 5.45339000 | 0.37051100 |
| H | 3.26546300 | 3.89367900 | 0.14321600 |
| H | 2.05877900 | 4.42396900 | -1.03031100 |
| C | 1.22288500 | -0.88462800 | 1.99930700 |
| O | 1.32987000 | -0.74621500 | 0.73419400 |

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|---|------------|-------------|-------------|
| O | 0.08930400 | -0.57648400 | 2.49213300 |
| C | 2.40990800 | -1.31528300 | 2.83207700 |
| C | 1.95945800 | -1.69878300 | 4.24715700 |
| C | 3.10426200 | -2.49655800 | 2.13021300 |
| C | 3.36127600 | -0.09640400 | 2.87704100 |
| H | 1.44927300 | -0.86522600 | 4.73758300 |
| H | 1.26866200 | -2.54803100 | 4.22508300 |
| H | 2.83123200 | -1.97880600 | 4.84907600 |
| H | 3.38520300 | -2.23343500 | 1.10733200 |
| H | 4.00604800 | -2.77877400 | 2.68514200 |
| H | 2.44316700 | -3.36963400 | 2.08609400 |
| H | 4.26020900 | -0.34982900 | 3.45027200 |
| H | 3.65732400 | 0.19986300 | 1.86633400 |
| H | 2.87487600 | 0.75939900 | 3.35743700 |
| H | 3.54244900 | -3.63381400 | -1.76611700 |
| O | 4.51768700 | -1.43961500 | -2.54474400 |
| C | 5.00163700 | -0.13826500 | -2.86298600 |
| H | 6.08425500 | -0.23836300 | -2.95048900 |
| H | 4.58787600 | 0.21597300 | -3.81511900 |
| H | 4.75463200 | 0.57842500 | -2.07123300 |

int13-SMe (doublet)

| | | | |
|----|-------------|-------------|-------------|
| C | 2.86610800 | -0.59403500 | -2.09685900 |
| C | 1.68381700 | 0.15513600 | -2.13837600 |
| C | 0.45226000 | -0.49221400 | -2.17072300 |
| C | 0.38112000 | -1.88853300 | -2.20945000 |
| C | 1.55918100 | -2.62730200 | -2.18105600 |
| C | 2.80120100 | -1.99154100 | -2.11834700 |
| H | 1.71445700 | 1.23671000 | -2.08291800 |
| H | -0.58412900 | -2.37772200 | -2.25432500 |
| H | 1.51643600 | -3.71269700 | -2.20548300 |
| H | 3.70344200 | -2.59152200 | -2.09132400 |
| C | -0.81187000 | 0.30938800 | -2.19572400 |
| O | -1.33031500 | 0.66225700 | -3.23600400 |
| C | -2.54035500 | 1.30600900 | -0.81091300 |
| C | -3.22947000 | 2.05912000 | -1.78100300 |
| C | -4.19346400 | 1.93146100 | 0.80978000 |
| C | -4.39098900 | 2.73055200 | -1.44197700 |
| H | -2.81787400 | 2.08367600 | -2.77672200 |
| C | -4.88575700 | 2.66313700 | -0.13203900 |
| H | -4.47151600 | 1.81650600 | 1.84846700 |
| H | -4.91190600 | 3.31295300 | -2.19421900 |
| H | -5.79166100 | 3.17910200 | 0.16342000 |
| O | -2.44198700 | 0.57289200 | 1.39807700 |
| N | -3.05802100 | 1.28182100 | 0.46556300 |
| Co | -0.70243600 | 0.10308000 | 0.81720500 |
| O | -1.19088700 | -1.71907400 | 0.72238900 |
| O | 0.13867000 | -0.39165600 | 2.51332900 |
| O | -0.11259200 | 1.87499400 | 1.15801200 |
| C | 1.19427000 | -0.66701300 | 1.85795800 |
| O | 1.13316400 | -0.42979700 | 0.60297500 |
| C | -2.10940600 | -2.16931700 | -0.05396300 |
| O | -2.69493800 | -1.53329700 | -0.94711200 |
| C | 0.34827400 | 2.65411100 | 0.24045100 |
| O | 0.16671300 | 2.53786800 | -0.98275200 |
| C | 2.42863000 | -1.29875000 | 2.46009300 |
| C | 2.34435000 | -1.28344300 | 3.99093300 |
| C | 2.46736100 | -2.75025500 | 1.92721900 |
| C | 3.66748400 | -0.53034500 | 1.96220500 |
| H | 2.28941400 | -0.25892400 | 4.37270100 |
| H | 1.45853100 | -1.81990000 | 4.34268600 |
| H | 3.23410900 | -1.76264900 | 4.41425600 |
| H | 2.50528700 | -2.75909900 | 0.83417300 |
| H | 3.35366000 | -3.26143800 | 2.32018800 |

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|---|-------------|-------------|-------------|
| H | 1.57927100 | -3.30746600 | 2.24489800 |
| H | 4.57704200 | -1.03913400 | 2.30139800 |
| H | 3.67836400 | -0.46950100 | 0.87102300 |
| H | 3.68289600 | 0.49135200 | 2.35568800 |
| C | 1.22259000 | 3.80785900 | 0.78479200 |
| C | 2.48198000 | 3.15082300 | 1.38657700 |
| C | 1.61216300 | 4.76319000 | -0.34895800 |
| C | 0.44328800 | 4.55686500 | 1.87964800 |
| H | 2.21113400 | 2.49308300 | 2.21688000 |
| H | 3.01464800 | 2.55666000 | 0.63529000 |
| H | 3.16377700 | 3.92518000 | 1.75762800 |
| H | 0.72685800 | 5.19869700 | -0.82256700 |
| H | 2.22718000 | 5.57815800 | 0.05024200 |
| H | 2.18373300 | 4.24555700 | -1.12438900 |
| H | 1.07003500 | 5.34935700 | 2.30541500 |
| H | -0.45869000 | 5.02670400 | 1.46916000 |
| H | 0.14353900 | 3.87552800 | 2.67954700 |
| C | -2.46573400 | -3.65392800 | 0.21012300 |
| C | -1.17786600 | -4.49287600 | 0.11756700 |
| C | -3.04177700 | -3.73637200 | 1.63737300 |
| C | -3.49648200 | -4.14403900 | -0.81303500 |
| H | -0.74997200 | -4.45341600 | -0.89038700 |
| H | -0.42434200 | -4.13014400 | 0.82053600 |
| H | -1.40180600 | -5.54144800 | 0.34683700 |
| H | -3.95345400 | -3.13444200 | 1.72743400 |
| H | -3.29680300 | -4.77560000 | 1.87691900 |
| H | -2.31713700 | -3.37145600 | 2.36992600 |
| H | -3.74487600 | -5.19327900 | -0.61462600 |
| H | -4.41567300 | -3.55360600 | -0.76258400 |
| H | -3.10932200 | -4.06832300 | -1.83379900 |
| N | -1.38392400 | 0.59049000 | -0.92068200 |
| S | 4.38219300 | 0.33590400 | -1.98543900 |
| C | 5.61637400 | -0.94839200 | -1.60998200 |
| H | 6.55742900 | -0.41972500 | -1.43981900 |
| H | 5.34746200 | -1.49866800 | -0.70382200 |
| H | 5.74845700 | -1.64213000 | -2.44457500 |

TS14-SMe (doublet)

| | | | |
|----|-------------|-------------|-------------|
| C | 3.41263100 | -2.03539200 | -1.43280400 |
| C | 2.16681200 | -2.61318900 | -1.19131200 |
| C | 1.04110500 | -1.89800500 | -1.56537000 |
| C | 1.07858000 | -0.57327600 | -1.96883400 |
| C | 2.32440100 | -0.00350000 | -2.22385200 |
| C | 3.49396300 | -0.72379700 | -1.93912700 |
| H | 2.09398000 | -3.61270300 | -0.77329600 |
| H | -0.20933600 | -2.58234300 | -1.58620400 |
| H | 2.36330100 | 1.02376400 | -2.56934000 |
| C | -0.16763900 | 0.22682000 | -2.21648900 |
| O | -0.31635300 | 0.81555600 | -3.28095300 |
| N | -1.09364800 | 0.16086200 | -1.19318100 |
| C | -2.29975900 | 0.78944400 | -1.29386100 |
| C | -2.87167300 | 1.50702000 | -2.36469800 |
| C | -4.12805300 | 2.07533100 | -2.22804400 |
| H | -2.28531200 | 1.60146500 | -3.26522100 |
| C | -4.26497700 | 1.24765400 | 0.00860600 |
| C | -4.84177200 | 1.94979100 | -1.02827200 |
| H | -4.55155400 | 2.63241900 | -3.05757700 |
| H | -4.70398600 | 1.09067600 | 0.98459000 |
| H | -5.81946200 | 2.39564400 | -0.89145700 |
| N | -3.04681800 | 0.68686100 | -0.14574200 |
| O | -2.53979600 | -0.02366700 | 0.87520500 |
| Co | -0.65696700 | -0.09319500 | 0.68606600 |
| C | -1.49277600 | -2.85910300 | -0.10233100 |
| O | -1.19614200 | -3.10915600 | -1.34427100 |

| | | | |
|---|-------------|-------------|-------------|
| O | -0.80775700 | -2.12553700 | 0.63128800 |
| C | -2.75967700 | -3.55521200 | 0.40603800 |
| C | -2.90425000 | -3.31855700 | 1.91479600 |
| C | -3.95467500 | -2.92419400 | -0.34362300 |
| C | -2.67496900 | -5.06075100 | 0.09106000 |
| H | -2.05516500 | -3.73562700 | 2.46500900 |
| H | -2.95786200 | -2.25058800 | 2.13677400 |
| H | -3.81964200 | -3.80440100 | 2.27132300 |
| H | -3.86079800 | -3.05722300 | -1.42517800 |
| H | -4.88173700 | -3.40483800 | -0.01178000 |
| H | -4.02269400 | -1.85621600 | -0.12025300 |
| H | -3.58459500 | -5.55830600 | 0.44481800 |
| H | -2.57522800 | -5.23774600 | -0.98297100 |
| H | -1.82020000 | -5.52304300 | 0.59808800 |
| C | 0.10973300 | 2.55615100 | 0.21562800 |
| O | -0.62390600 | 1.73573700 | 0.93451500 |
| O | 0.89335300 | 2.25147700 | -0.67383800 |
| C | -0.16588800 | 4.02796300 | 0.60634400 |
| C | -1.64791500 | 4.32573400 | 0.30024300 |
| C | 0.10662100 | 4.21481400 | 2.10984800 |
| C | 0.73940500 | 4.94836400 | -0.22002800 |
| H | -1.87135100 | 4.15049400 | -0.75893700 |
| H | -2.30435900 | 3.68768200 | 0.89825600 |
| H | -1.87773700 | 5.37421800 | 0.52550100 |
| H | 1.15607400 | 4.00103600 | 2.34495100 |
| H | -0.09979200 | 5.25048000 | 2.40672400 |
| H | -0.51995200 | 3.54608400 | 2.70581200 |
| H | 0.54297900 | 5.99606000 | 0.03811900 |
| H | 1.79529700 | 4.73476900 | -0.02893900 |
| H | 0.56510600 | 4.81175400 | -1.29094800 |
| C | 1.13181700 | -0.29098100 | 2.11928000 |
| O | 1.26579700 | -0.21671700 | 0.85153000 |
| O | -0.06772900 | -0.30357000 | 2.54692200 |
| C | 2.34339800 | -0.27145600 | 3.02489400 |
| C | 1.97343900 | -0.78468100 | 4.42230100 |
| C | 3.45505200 | -1.12770100 | 2.39266200 |
| C | 2.79275000 | 1.20767400 | 3.09097200 |
| H | 1.16632300 | -0.18979100 | 4.85807300 |
| H | 1.63952700 | -1.82711100 | 4.38446600 |
| H | 2.84658700 | -0.72694900 | 5.08193200 |
| H | 3.68562100 | -0.77924300 | 1.38256800 |
| H | 4.36094300 | -1.06989000 | 3.00673000 |
| H | 3.15227500 | -2.17882900 | 2.32616000 |
| H | 3.68460800 | 1.29467000 | 3.72192900 |
| H | 3.02867200 | 1.58493600 | 2.09115000 |
| H | 2.00327900 | 1.83496900 | 3.51790900 |
| H | 4.30906500 | -2.60593000 | -1.21888100 |
| S | 5.02297500 | 0.12483100 | -2.21912300 |
| C | 6.23919800 | -0.91938700 | -1.35470200 |
| H | 7.18612600 | -0.37668800 | -1.40545800 |
| H | 5.96190500 | -1.05725800 | -0.30623800 |
| H | 6.36384000 | -1.88995300 | -1.84269000 |

int13-Cl (doublet)

| | | | |
|---|-------------|-------------|-------------|
| C | 2.64886700 | -1.24982000 | -2.38398400 |
| C | 1.69395500 | -0.24226300 | -2.31606200 |
| C | 0.34733200 | -0.60297800 | -2.23810000 |
| C | -0.03176500 | -1.94653600 | -2.27444600 |
| C | 0.94508500 | -2.93757800 | -2.34873300 |
| C | 2.29736400 | -2.59819600 | -2.39575000 |
| H | 1.98306600 | 0.79906100 | -2.27229300 |
| H | -1.08249600 | -2.20637500 | -2.23934300 |
| H | 0.65392600 | -3.98365200 | -2.36810800 |
| H | 3.06614400 | -3.36144400 | -2.44571000 |

| | | | |
|----|-------------|-------------|-------------|
| C | -0.70576300 | 0.46213600 | -2.18162300 |
| O | -1.17086400 | 0.95155400 | -3.19156100 |
| C | -2.12351600 | 1.75773000 | -0.69800200 |
| C | -2.69414600 | 2.65500800 | -1.62150900 |
| C | -3.52567600 | 2.67360700 | 1.01894600 |
| C | -3.67414600 | 3.54183600 | -1.21162900 |
| H | -2.33763600 | 2.61549300 | -2.63786000 |
| C | -4.10178200 | 3.55007800 | 0.12350000 |
| H | -3.76655900 | 2.59708100 | 2.07040200 |
| H | -4.10423300 | 4.23353500 | -1.92784400 |
| H | -4.86547400 | 4.23435000 | 0.47380200 |
| O | -2.06319800 | 0.97181700 | 1.49392800 |
| N | -2.56800900 | 1.81229900 | 0.60598100 |
| Co | -0.47902700 | 0.18605200 | 0.81450800 |
| O | -1.31207100 | -1.50877100 | 0.73999700 |
| O | 0.34512100 | -0.48304400 | 2.45291900 |
| O | 0.44601100 | 1.81171500 | 1.12877300 |
| C | 1.29160100 | -0.94433300 | 1.73754300 |
| O | 1.20693000 | -0.67664900 | 0.48888600 |
| C | -2.35672400 | -1.75356200 | 0.03492100 |
| O | -2.85944500 | -1.00249300 | -0.81904900 |
| C | 1.04001100 | 2.46697500 | 0.19036100 |
| O | 0.82993100 | 2.35628400 | -1.02821200 |
| C | 2.40468200 | -1.81684500 | 2.26762800 |
| C | 2.44847700 | -1.75160200 | 3.79927300 |
| C | 2.07682700 | -3.25184800 | 1.79026700 |
| C | 3.73896000 | -1.35645200 | 1.65194600 |
| H | 2.65911600 | -0.73438700 | 4.14539800 |
| H | 1.49544700 | -2.06336300 | 4.23575800 |
| H | 3.23768300 | -2.41290100 | 4.17356100 |
| H | 2.01981000 | -3.29083000 | 0.69859700 |
| H | 2.85971300 | -3.93903900 | 2.13009900 |
| H | 1.11815800 | -3.59009600 | 2.19846900 |
| H | 4.54321200 | -2.02487500 | 1.97857100 |
| H | 3.69583600 | -1.36963600 | 0.56011800 |
| H | 3.99029200 | -0.33955400 | 1.97117800 |
| C | 2.12153200 | 3.44509000 | 0.70395100 |
| C | 3.24784900 | 2.57166100 | 1.29503300 |
| C | 2.65833500 | 4.29854600 | -0.45054700 |
| C | 1.51586500 | 4.33729900 | 1.80117300 |
| H | 2.87401900 | 1.97777700 | 2.13381400 |
| H | 3.65214600 | 1.88769100 | 0.54017300 |
| H | 4.06564900 | 3.20859500 | 1.65198300 |
| H | 1.86094200 | 4.89481600 | -0.90530700 |
| H | 3.43104200 | 4.98151000 | -0.07900500 |
| H | 3.09478100 | 3.67439400 | -1.23508000 |
| H | 2.28452400 | 5.00937800 | 2.20071600 |
| H | 0.70381800 | 4.95608000 | 1.40081900 |
| H | 1.11701400 | 3.73236400 | 2.61899300 |
| C | -2.98873400 | -3.13727200 | 0.32890300 |
| C | -1.91721800 | -4.22108900 | 0.10705900 |
| C | -3.42896600 | -3.13368100 | 1.80581000 |
| C | -4.19158500 | -3.38066900 | -0.58954700 |
| H | -1.59661700 | -4.25346600 | -0.94030000 |
| H | -1.03758800 | -4.03422600 | 0.72761700 |
| H | -2.32845400 | -5.20495700 | 0.36184900 |
| H | -4.18054900 | -2.35724900 | 1.98957800 |
| H | -3.87225700 | -4.10261200 | 2.06445400 |
| H | -2.57657500 | -2.94678900 | 2.46393200 |
| H | -4.63180600 | -4.36057400 | -0.37086900 |
| H | -4.96003200 | -2.61545500 | -0.44700600 |
| H | -3.89715700 | -3.36239500 | -1.64333200 |
| N | -1.14854300 | 0.82200700 | -0.87823900 |
| Cl | 4.35182600 | -0.80509100 | -2.42161600 |

TS14-Cl (doublet)

| | | | |
|----|-------------|-------------|-------------|
| C | 3.16414900 | -2.47243100 | -1.78326200 |
| C | 1.87528500 | -2.91346700 | -1.48129000 |
| C | 0.83401300 | -2.03219900 | -1.71673200 |
| C | 0.99213300 | -0.71319400 | -2.08839100 |
| C | 2.28357400 | -0.28065300 | -2.41443500 |
| C | 3.34558600 | -1.16116400 | -2.24168400 |
| H | 1.70293700 | -3.92146000 | -1.11852800 |
| H | -0.42503100 | -2.53326100 | -1.64402700 |
| H | 2.43597100 | 0.74562000 | -2.72346600 |
| C | -0.16372200 | 0.23721600 | -2.23447600 |
| O | -0.31741400 | 0.84125900 | -3.28933300 |
| N | -1.00540500 | 0.28084100 | -1.14333200 |
| C | -2.12091700 | 1.06769100 | -1.14770500 |
| C | -2.66885400 | 1.87350300 | -2.16601700 |
| C | -3.82157800 | 2.60537200 | -1.92758100 |
| H | -2.14736100 | 1.90219000 | -3.10995400 |
| C | -3.89858300 | 1.76551400 | 0.30778200 |
| C | -4.45128300 | 2.55739100 | -0.67647900 |
| H | -4.22733000 | 3.22884600 | -2.71775400 |
| H | -4.27892700 | 1.65331700 | 1.31405800 |
| H | -5.34489800 | 3.13019900 | -0.46046000 |
| N | -2.78420500 | 1.04723800 | 0.05455200 |
| O | -2.30113500 | 0.25674600 | 1.02706000 |
| Co | -0.46197200 | -0.05066000 | 0.69774800 |
| C | -1.67670000 | -2.67955000 | -0.07586700 |
| O | -1.48561500 | -2.95887000 | -1.33317100 |
| O | -0.86413500 | -2.05283700 | 0.62094200 |
| C | -3.00323800 | -3.20635400 | 0.49198300 |
| C | -3.03820700 | -2.96504800 | 2.00656200 |
| C | -4.13691100 | -2.41602100 | -0.19884800 |
| C | -3.13379700 | -4.70718600 | 0.17050100 |
| H | -2.22675800 | -3.49708400 | 2.51240400 |
| H | -2.93855500 | -1.90170800 | 2.23426300 |
| H | -3.99172300 | -3.32837700 | 2.40651300 |
| H | -4.11604100 | -2.55656600 | -1.28329100 |
| H | -5.10227300 | -2.76910300 | 0.18039500 |
| H | -4.05063400 | -1.34942200 | 0.02393000 |
| H | -4.08054600 | -5.08335400 | 0.57299200 |
| H | -3.11760300 | -4.88674800 | -0.90765600 |
| H | -2.32135800 | -5.28208700 | 0.62935100 |
| C | 0.60653800 | 2.47753200 | 0.17985700 |
| O | -0.17037100 | 1.75144200 | 0.95311300 |
| O | 1.25262600 | 2.08660800 | -0.78360100 |
| C | 0.59286900 | 3.95964200 | 0.62266500 |
| C | -0.85997200 | 4.46988200 | 0.54230500 |
| C | 1.10147400 | 4.05139800 | 2.07348800 |
| C | 1.49375300 | 4.77488100 | -0.31186700 |
| H | -1.25704600 | 4.36257500 | -0.47444600 |
| H | -1.50700300 | 3.91016500 | 1.22305500 |
| H | -0.90280700 | 5.53220100 | 0.81143200 |
| H | 2.13432800 | 3.69094500 | 2.14789900 |
| H | 1.08381600 | 5.09327400 | 2.41569200 |
| H | 0.47993200 | 3.45041400 | 2.74267300 |
| H | 1.48861700 | 5.82908300 | -0.00956000 |
| H | 2.52392600 | 4.40838800 | -0.28193400 |
| H | 1.15023800 | 4.70591600 | -1.34806200 |
| C | 1.37789000 | -0.51804100 | 1.99476200 |
| O | 1.43363500 | -0.42684600 | 0.72150200 |
| O | 0.21894200 | -0.37171800 | 2.50362200 |
| C | 2.63460800 | -0.71440500 | 2.81206600 |
| C | 2.27960800 | -1.14479700 | 4.24078700 |
| C | 3.51779800 | -1.76589000 | 2.11599700 |

| | | | |
|----|------------|-------------|-------------|
| C | 3.35518800 | 0.65444900 | 2.81954700 |
| H | 1.63450900 | -0.40703500 | 4.72567500 |
| H | 1.75322100 | -2.10512400 | 4.24490700 |
| H | 3.19523400 | -1.25174800 | 4.83309800 |
| H | 3.74276700 | -1.46787300 | 1.08895100 |
| H | 4.45871800 | -1.88107900 | 2.66539700 |
| H | 3.01746000 | -2.74055200 | 2.08536700 |
| H | 4.29392000 | 0.57351800 | 3.37897600 |
| H | 3.57977800 | 0.97857000 | 1.79889000 |
| H | 2.73350500 | 1.41984000 | 3.29593800 |
| H | 4.01782700 | -3.13080000 | -1.66337500 |
| Cl | 4.97607100 | -0.60477200 | -2.56765700 |

int13-CO₂Me (doublet)

| | | | |
|----|-------------|-------------|-------------|
| C | 2.55286400 | -0.89587000 | -2.04110500 |
| C | 1.36155200 | -0.16745800 | -1.99809300 |
| C | 0.14529800 | -0.81757800 | -2.18204200 |
| C | 0.11817400 | -2.19018400 | -2.46015200 |
| C | 1.30824600 | -2.91517100 | -2.50328600 |
| C | 2.52754000 | -2.27405400 | -2.28530000 |
| H | 1.39226600 | 0.89316900 | -1.79609500 |
| H | -0.83778700 | -2.67830700 | -2.61727400 |
| H | 1.28406900 | -3.98197200 | -2.70483700 |
| H | 3.45610200 | -2.83276400 | -2.30189200 |
| C | -1.15235500 | -0.08000200 | -2.16463800 |
| O | -1.84468000 | 0.01237700 | -3.16003000 |
| C | -2.74536500 | 1.11426100 | -0.80241100 |
| C | -3.48825200 | 1.76982100 | -1.80137500 |
| C | -4.36019500 | 1.81081200 | 0.82481000 |
| C | -4.66092600 | 2.42778000 | -1.47327900 |
| H | -3.11201600 | 1.73658000 | -2.81062600 |
| C | -5.10973000 | 2.44273400 | -0.14518200 |
| H | -4.59724900 | 1.76997500 | 1.87908000 |
| H | -5.22463900 | 2.93759200 | -2.24699600 |
| H | -6.02300400 | 2.95000300 | 0.14251400 |
| O | -2.53724600 | 0.56253200 | 1.44766200 |
| N | -3.21476300 | 1.17453600 | 0.48876500 |
| Co | -0.78706600 | 0.17617700 | 0.85347100 |
| O | -1.08560500 | -1.68226900 | 0.93310300 |
| O | 0.09371400 | -0.04466700 | 2.57116900 |
| O | -0.32973200 | 2.02301200 | 0.96841600 |
| C | 1.18171800 | -0.28173400 | 1.95128700 |
| O | 1.10584900 | -0.21601300 | 0.67819100 |
| C | -1.94858500 | -2.30208300 | 0.20950100 |
| O | -2.67158200 | -1.79783200 | -0.66555000 |
| C | 0.08068900 | 2.68893900 | -0.05490000 |
| O | -0.13974900 | 2.40929900 | -1.24723600 |
| C | 2.45628400 | -0.66914300 | 2.66682500 |
| C | 2.67657600 | 0.29569500 | 3.84612500 |
| C | 2.24259000 | -2.10768500 | 3.19078000 |
| C | 3.64233500 | -0.62739700 | 1.69252500 |
| H | 2.84190000 | 1.31867200 | 3.49097600 |
| H | 1.81120700 | 0.30187500 | 4.51416400 |
| H | 3.55926400 | -0.01402100 | 4.41669500 |
| H | 2.05435300 | -2.79912800 | 2.36239300 |
| H | 3.14024500 | -2.44178800 | 3.72303100 |
| H | 1.39084400 | -2.15061700 | 3.87577600 |
| H | 4.56210400 | -0.88991300 | 2.22758300 |
| H | 3.50581200 | -1.33799700 | 0.87298500 |
| H | 3.76545000 | 0.36803800 | 1.25579300 |
| C | 0.95781900 | 3.91257600 | 0.29343500 |
| C | 2.28810200 | 3.34036900 | 0.83054000 |
| C | 1.21557300 | 4.75781300 | -0.95925200 |
| C | 0.26148800 | 4.74734300 | 1.38100700 |

| | | | |
|---|-------------|-------------|-------------|
| H | 2.11323000 | 2.75223400 | 1.73615700 |
| H | 2.77557100 | 2.70223100 | 0.08582400 |
| H | 2.96851400 | 4.16427400 | 1.07696100 |
| H | 0.27894200 | 5.13336000 | -1.38411200 |
| H | 1.84583600 | 5.61699000 | -0.70184000 |
| H | 1.72338100 | 4.17244400 | -1.73017600 |
| H | 0.90121800 | 5.59060900 | 1.66714400 |
| H | -0.68915300 | 5.15574000 | 1.01722100 |
| H | 0.05894400 | 4.14216500 | 2.26790100 |
| C | -2.05933900 | -3.81153800 | 0.53761200 |
| C | -0.65422600 | -4.39727000 | 0.75794500 |
| C | -2.88241400 | -3.91474300 | 1.83822800 |
| C | -2.77315900 | -4.54600700 | -0.60375000 |
| H | -0.02842400 | -4.26578100 | -0.13135000 |
| H | -0.15373400 | -3.90748000 | 1.59620700 |
| H | -0.72945300 | -5.47060500 | 0.96995100 |
| H | -3.88925700 | -3.50535400 | 1.69840100 |
| H | -2.97996900 | -4.96536400 | 2.13658700 |
| H | -2.39453500 | -3.36467000 | 2.64852700 |
| H | -2.89511600 | -5.60442200 | -0.34562300 |
| H | -3.75834300 | -4.11444800 | -0.79661000 |
| H | -2.19609900 | -4.48802500 | -1.53306300 |
| N | -1.56182200 | 0.43906600 | -0.90377100 |
| C | 3.80610600 | -0.15878900 | -1.74098300 |
| O | 3.87801000 | 1.03887600 | -1.53454700 |
| O | 4.88501800 | -0.97412000 | -1.68977000 |
| C | 6.11949900 | -0.32758000 | -1.35436900 |
| H | 6.05827400 | 0.11628700 | -0.35701300 |
| H | 6.35224400 | 0.45762000 | -2.07820700 |
| H | 6.87647700 | -1.11189300 | -1.37916300 |

TS14-CO₂Me (doublet)

| | | | |
|----|-------------|-------------|-------------|
| C | 3.23941600 | -2.20580800 | -1.25655100 |
| C | 1.96584100 | -2.76766400 | -1.16763000 |
| C | 0.90396700 | -1.96063600 | -1.53437000 |
| C | 0.99627200 | -0.63438600 | -1.89203600 |
| C | 2.28344500 | -0.09651800 | -2.01391400 |
| C | 3.39283900 | -0.87322900 | -1.67590000 |
| H | 1.82419100 | -3.79669800 | -0.85464600 |
| H | -0.29695600 | -2.53970800 | -1.58440300 |
| H | 2.40378100 | 0.94234900 | -2.29471100 |
| C | -0.20665300 | 0.21562600 | -2.18816400 |
| O | -0.28786600 | 0.79883200 | -3.26215000 |
| N | -1.17020600 | 0.19842300 | -1.19949300 |
| C | -2.33592800 | 0.89353600 | -1.34255400 |
| C | -2.82341500 | 1.64978100 | -2.42777800 |
| C | -4.04925200 | 2.28949700 | -2.33343300 |
| H | -2.19916100 | 1.71612200 | -3.30515000 |
| C | -4.31894300 | 1.45678400 | -0.11062000 |
| C | -4.81385000 | 2.19830400 | -1.16241400 |
| H | -4.40764400 | 2.87605400 | -3.17323600 |
| H | -4.80294900 | 1.31998200 | 0.84693500 |
| H | -5.76795600 | 2.70050400 | -1.05836900 |
| N | -3.13106100 | 0.82591900 | -0.22457700 |
| O | -2.70575700 | 0.07872600 | 0.80761300 |
| Co | -0.82148900 | -0.08421300 | 0.69588300 |
| C | -1.73158900 | -2.80708200 | -0.17864200 |
| O | -1.36104600 | -3.06350900 | -1.40157400 |
| O | -1.08015200 | -2.11177400 | 0.61271500 |
| C | -3.07142000 | -3.45105200 | 0.21407100 |
| C | -3.30229100 | -3.25177000 | 1.71758800 |
| C | -4.16879100 | -2.71977400 | -0.59153900 |
| C | -3.05322400 | -4.94731800 | -0.14812200 |
| H | -2.51810800 | -3.73582400 | 2.30771900 |

| | | | |
|---|-------------|-------------|-------------|
| H | -3.31044200 | -2.18994000 | 1.97242900 |
| H | -4.26596500 | -3.69440800 | 1.99410200 |
| H | -4.01457300 | -2.83312300 | -1.66840900 |
| H | -5.14558100 | -3.14294300 | -0.33230600 |
| H | -4.17801100 | -1.65555000 | -0.34257300 |
| H | -4.00937700 | -5.40042400 | 0.13533600 |
| H | -2.90072000 | -5.09722000 | -1.22009900 |
| H | -2.25837300 | -5.47517000 | 0.39102500 |
| C | 0.08835900 | 2.52374100 | 0.27277700 |
| O | -0.70644000 | 1.73594600 | 0.96373100 |
| O | 0.87946700 | 2.18450000 | -0.59687100 |
| C | -0.12327000 | 4.00449800 | 0.66817400 |
| C | -1.58314400 | 4.37605800 | 0.33741600 |
| C | 0.12962100 | 4.16789100 | 2.17793700 |
| C | 0.84142500 | 4.88416300 | -0.13514200 |
| H | -1.79613200 | 4.21640600 | -0.72640800 |
| H | -2.28083400 | 3.76935400 | 0.92115500 |
| H | -1.76407700 | 5.43376600 | 0.56341200 |
| H | 1.16333700 | 3.90391000 | 2.43068900 |
| H | -0.03398600 | 5.21012300 | 2.47825200 |
| H | -0.53909200 | 3.52566500 | 2.75719200 |
| H | 0.69143500 | 5.93842500 | 0.12726500 |
| H | 1.88191800 | 4.61774200 | 0.07241500 |
| H | 0.68049700 | 4.76339900 | -1.21004200 |
| C | 0.89207900 | -0.38811400 | 2.19898000 |
| O | 1.08269600 | -0.30954900 | 0.93827000 |
| O | -0.32515400 | -0.34060000 | 2.57293000 |
| C | 2.05992100 | -0.44366900 | 3.15783300 |
| C | 1.59630000 | -0.94331400 | 4.53212100 |
| C | 3.15031700 | -1.35791500 | 2.57158700 |
| C | 2.58877000 | 1.00730900 | 3.25818600 |
| H | 0.80599000 | -0.30530200 | 4.93660800 |
| H | 1.20498000 | -1.96436200 | 4.46958100 |
| H | 2.44049200 | -0.94098400 | 5.23068700 |
| H | 3.46492000 | -1.01188400 | 1.58399500 |
| H | 4.02114600 | -1.36617200 | 3.23664800 |
| H | 2.78799800 | -2.38715600 | 2.46989600 |
| H | 3.45415800 | 1.03851300 | 3.92974500 |
| H | 2.89269700 | 1.37699200 | 2.27403900 |
| H | 1.81794200 | 1.67652000 | 3.65444100 |
| H | 4.11348200 | -2.79513100 | -1.00439700 |
| C | 4.73311400 | -0.22617500 | -1.74135800 |
| O | 4.94111800 | 0.89393500 | -2.15949100 |
| O | 5.71278500 | -1.03343100 | -1.26888000 |
| C | 7.02983800 | -0.46679200 | -1.30099600 |
| H | 7.07003500 | 0.44190600 | -0.69463900 |
| H | 7.68814700 | -1.23321200 | -0.89118100 |
| H | 7.31613800 | -0.21960300 | -2.32672100 |

int13-CO₂Et (doublet)

| | | | |
|---|-------------|-------------|-------------|
| C | 2.50967600 | -0.63608500 | -1.93017700 |
| C | 1.25053200 | -0.03184700 | -1.93405700 |
| C | 0.11258300 | -0.80095400 | -2.15638200 |
| C | 0.23394800 | -2.16876000 | -2.43313100 |
| C | 1.49222100 | -2.76941400 | -2.43318200 |
| C | 2.63212700 | -2.00942100 | -2.17098000 |
| H | 1.16796800 | 1.02697700 | -1.73713200 |
| H | -0.66104200 | -2.75122800 | -2.62446800 |
| H | 1.58298600 | -3.83277100 | -2.63408200 |
| H | 3.61221200 | -2.47185600 | -2.15128500 |
| C | -1.25105700 | -0.19595100 | -2.18355100 |
| O | -1.92408400 | -0.18668800 | -3.19630100 |
| C | -2.98318100 | 0.86586300 | -0.88323600 |
| C | -3.75239200 | 1.43970500 | -1.91224600 |

| | | | |
|----|-------------|-------------|-------------|
| C | -4.70103600 | 1.43360300 | 0.68755000 |
| C | -4.98845400 | 1.99301100 | -1.62697500 |
| H | -3.34499500 | 1.42883500 | -2.90982000 |
| C | -5.47541200 | 1.98356200 | -0.31227700 |
| H | -4.96419500 | 1.38440000 | 1.73524600 |
| H | -5.57281900 | 2.44058000 | -2.42353500 |
| H | -6.43859600 | 2.40986900 | -0.05790700 |
| O | -2.79303800 | 0.36100200 | 1.37942400 |
| N | -3.49406500 | 0.89833100 | 0.39307000 |
| Co | -0.99840100 | 0.12578500 | 0.84143800 |
| O | -1.13327700 | -1.75048000 | 0.93705800 |
| O | -0.15590000 | 0.00056700 | 2.58731600 |
| O | -0.71133700 | 2.00571000 | 0.95048000 |
| C | 0.96821800 | -0.14443400 | 2.00457400 |
| O | 0.92812500 | -0.09811600 | 0.72908200 |
| C | -1.90781200 | -2.45522700 | 0.19152900 |
| O | -2.64376000 | -2.02913000 | -0.71358900 |
| C | -0.33966400 | 2.70421100 | -0.06607500 |
| O | -0.50283500 | 2.40207100 | -1.26186900 |
| C | 2.24830300 | -0.40814600 | 2.76565700 |
| C | 2.34208500 | 0.58409300 | 3.93918000 |
| C | 2.14820200 | -1.85461000 | 3.30137600 |
| C | 3.45709600 | -0.26842700 | 1.82936900 |
| H | 2.42567500 | 1.61458500 | 3.57721500 |
| H | 1.45874400 | 0.51803300 | 4.57983800 |
| H | 3.23050600 | 0.36041700 | 4.54012400 |
| H | 2.05401500 | -2.56909900 | 2.47649600 |
| H | 3.05269800 | -2.09930900 | 3.86941400 |
| H | 1.27955300 | -1.96859200 | 3.95634600 |
| H | 4.37939000 | -0.43429100 | 2.39785300 |
| H | 3.41609800 | -0.99975000 | 1.01792300 |
| H | 3.49957200 | 0.72827400 | 1.38045000 |
| C | 0.40721500 | 4.00706400 | 0.30018000 |
| C | 1.76286800 | 3.56780200 | 0.89518100 |
| C | 0.63367500 | 4.86181900 | -0.95203600 |
| C | -0.40747200 | 4.78183700 | 1.34954400 |
| H | 1.60789500 | 2.97309900 | 1.80008800 |
| H | 2.33738500 | 2.97293100 | 0.17717600 |
| H | 2.35219400 | 4.45454500 | 1.15726800 |
| H | -0.31632000 | 5.14142600 | -1.41896800 |
| H | 1.16763000 | 5.77984300 | -0.68026300 |
| H | 1.22693100 | 4.32131200 | -1.69422800 |
| H | 0.13946200 | 5.68290000 | 1.65134500 |
| H | -1.37614900 | 5.09713800 | 0.94323500 |
| H | -0.58889200 | 4.16677100 | 2.23422300 |
| C | -1.88302600 | -3.96565100 | 0.53243100 |
| C | -0.42908500 | -4.41598000 | 0.75736900 |
| C | -2.69246300 | -4.13548400 | 1.83430200 |
| C | -2.52409700 | -4.77199200 | -0.60326800 |
| H | 0.18140500 | -4.24020200 | -0.13502300 |
| H | 0.02399300 | -3.86923000 | 1.58740000 |
| H | -0.40460800 | -5.48849500 | 0.98463600 |
| H | -3.73329000 | -3.82278200 | 1.69311300 |
| H | -2.69138100 | -5.18862100 | 2.13995000 |
| H | -2.25792300 | -3.53662500 | 2.64018000 |
| H | -2.54508800 | -5.83549200 | -0.33802800 |
| H | -3.54624000 | -4.43776800 | -0.79769000 |
| H | -1.95607800 | -4.66501400 | -1.53364500 |
| N | -1.74063000 | 0.30078700 | -0.94164000 |
| C | 3.66971100 | 0.22369900 | -1.58213000 |
| O | 3.61382200 | 1.42740400 | -1.40517200 |
| O | 4.81206400 | -0.48516800 | -1.44554400 |
| C | 5.97525800 | 0.27025500 | -1.05040600 |
| C | 7.11374100 | -0.71616600 | -0.87909800 |

| | | | |
|---|------------|-------------|-------------|
| H | 5.74885600 | 0.80315100 | -0.12192600 |
| H | 6.18795400 | 1.01971700 | -1.81943300 |
| H | 8.02425300 | -0.18714500 | -0.57792700 |
| H | 6.87226300 | -1.45568800 | -0.10885000 |
| H | 7.31557100 | -1.24609400 | -1.81545200 |

TS14-CO₂Et (doublet)

| | | | |
|----|-------------|-------------|-------------|
| C | 3.17500100 | -1.97187400 | -1.22744900 |
| C | 1.94317500 | -2.62247000 | -1.15930200 |
| C | 0.83301500 | -1.89124800 | -1.54152600 |
| C | 0.83830500 | -0.56165400 | -1.89853200 |
| C | 2.08669600 | 0.06439100 | -2.00477300 |
| C | 3.24150000 | -0.63183500 | -1.64518200 |
| H | 1.86940500 | -3.65888800 | -0.84724600 |
| H | -0.32958100 | -2.54926100 | -1.58974700 |
| H | 2.13854300 | 1.10945200 | -2.28328500 |
| C | -0.41766700 | 0.20655000 | -2.19988000 |
| O | -0.54026100 | 0.77169900 | -3.27946600 |
| N | -1.37368300 | 0.13961600 | -1.20615100 |
| C | -2.57883200 | 0.76413800 | -1.34668400 |
| C | -3.11153300 | 1.49295900 | -2.42929800 |
| C | -4.37284700 | 2.05908400 | -2.33150300 |
| H | -2.49357500 | 1.59741000 | -3.30745900 |
| C | -4.58968400 | 1.20581700 | -0.11051400 |
| C | -5.12927800 | 1.91901700 | -1.16000300 |
| H | -4.76644400 | 2.62587100 | -3.16911000 |
| H | -5.06329900 | 1.03845800 | 0.84738800 |
| H | -6.11165300 | 2.36284400 | -1.05367200 |
| N | -3.36625700 | 0.64782700 | -0.22728100 |
| O | -2.89371200 | -0.07302300 | 0.80318400 |
| Co | -1.00239300 | -0.11436600 | 0.68879000 |
| C | -1.73573300 | -2.89412800 | -0.17383200 |
| O | -1.35603500 | -3.13636600 | -1.39694700 |
| O | -1.12353500 | -2.15480400 | 0.60907700 |
| C | -3.03175700 | -3.61528300 | 0.23103600 |
| C | -3.26332800 | -3.42384200 | 1.73537700 |
| C | -4.17648600 | -2.95365700 | -0.56882000 |
| C | -2.92709800 | -5.10921400 | -0.12635100 |
| H | -2.44824600 | -3.85925900 | 2.32157500 |
| H | -3.33137900 | -2.36315600 | 1.98584500 |
| H | -4.19781600 | -3.92029800 | 2.02060400 |
| H | -4.02095100 | -3.05703700 | -1.64651500 |
| H | -5.12376800 | -3.43663900 | -0.30469500 |
| H | -4.24996200 | -1.89228900 | -0.31871500 |
| H | -3.85293000 | -5.61741500 | 0.16424700 |
| H | -2.77242200 | -5.25354800 | -1.19882400 |
| H | -2.09908400 | -5.58718000 | 0.40941500 |
| C | -0.26778900 | 2.54646600 | 0.25619700 |
| O | -1.00497200 | 1.71038100 | 0.95418700 |
| O | 0.53171800 | 2.25747000 | -0.62381900 |
| C | -0.56235900 | 4.01080700 | 0.65894700 |
| C | -2.04648000 | 4.29529100 | 0.35045500 |
| C | -0.29721000 | 4.18514300 | 2.16542700 |
| C | 0.33658600 | 4.94834700 | -0.15507700 |
| H | -2.26494700 | 4.12576200 | -0.71075700 |
| H | -2.69834600 | 3.64644700 | 0.94183000 |
| H | -2.28746600 | 5.33973500 | 0.58242900 |
| H | 0.75368400 | 3.98093200 | 2.40212300 |
| H | -0.51628300 | 5.21539000 | 2.47162600 |
| H | -0.91872200 | 3.50377700 | 2.75249600 |
| H | 0.12977900 | 5.99109800 | 0.11454400 |
| H | 1.39384200 | 4.74190200 | 0.03522500 |
| H | 0.16608800 | 4.82261300 | -1.22795400 |
| C | 0.73128100 | -0.30215200 | 2.18905000 |

| | | | |
|---|-------------|-------------|-------------|
| O | 0.91312700 | -0.21297900 | 0.92787600 |
| O | -0.48548100 | -0.33500800 | 2.56600700 |
| C | 1.90279000 | -0.27846300 | 3.14511800 |
| C | 1.47555200 | -0.80456900 | 4.52145500 |
| C | 3.05073800 | -1.12016400 | 2.55966200 |
| C | 2.33551300 | 1.20406300 | 3.24138000 |
| H | 0.64328100 | -0.22127900 | 4.92436200 |
| H | 1.15558000 | -1.85037500 | 4.46243000 |
| H | 2.31770700 | -0.74185700 | 5.21964200 |
| H | 3.34774100 | -0.75237300 | 1.57450200 |
| H | 3.91772200 | -1.07539500 | 3.22841100 |
| H | 2.75484600 | -2.16994900 | 2.45344000 |
| H | 3.19943700 | 1.29278000 | 3.90971000 |
| H | 2.61114100 | 1.59100900 | 2.25551200 |
| H | 1.52394100 | 1.82203200 | 3.63935400 |
| H | 4.08415700 | -2.49725100 | -0.95842000 |
| C | 4.53328500 | 0.11096600 | -1.67460700 |
| O | 4.67450100 | 1.23282400 | -2.11647800 |
| O | 5.54390800 | -0.60799300 | -1.13449900 |
| C | 6.83077300 | 0.04449400 | -1.11330400 |
| C | 7.80716000 | -0.90749600 | -0.45066100 |
| H | 6.73702100 | 0.98802300 | -0.56682800 |
| H | 7.12066100 | 0.28593600 | -2.14088400 |
| H | 8.80216700 | -0.45169700 | -0.40910700 |
| H | 7.49055100 | -1.14027100 | 0.57112600 |
| H | 7.87998300 | -1.84475600 | -1.01170700 |

int13-CF₃ (doublet)

| | | | |
|----|-------------|-------------|-------------|
| C | 2.75012800 | -0.91614000 | -1.90930600 |
| C | 1.70737200 | 0.00215500 | -1.97150000 |
| C | 0.39687300 | -0.45657800 | -2.10915100 |
| C | 0.13949800 | -1.82186600 | -2.23857100 |
| C | 1.19368700 | -2.73467600 | -2.19143300 |
| C | 2.50072600 | -2.28734200 | -2.01509500 |
| H | 1.89515900 | 1.06074600 | -1.86132400 |
| H | -0.88160700 | -2.16187600 | -2.36343400 |
| H | 0.99147100 | -3.79773100 | -2.28050200 |
| H | 3.32182900 | -2.99420600 | -1.95282600 |
| C | -0.73322900 | 0.52547300 | -2.16126900 |
| O | -1.13310100 | 0.98596600 | -3.21166100 |
| C | -2.33994500 | 1.74317800 | -0.81377500 |
| C | -2.84477100 | 2.63516800 | -1.77940500 |
| C | -3.94128800 | 2.58188000 | 0.76139900 |
| C | -3.89150600 | 3.48215200 | -1.46066500 |
| H | -2.38730300 | 2.62369800 | -2.75521800 |
| C | -4.45268100 | 3.45433300 | -0.17617100 |
| H | -4.28567000 | 2.47881400 | 1.78131700 |
| H | -4.27043500 | 4.17042800 | -2.20834900 |
| H | -5.27156200 | 4.10674900 | 0.10299400 |
| O | -2.47622700 | 0.92216300 | 1.36193800 |
| N | -2.91703900 | 1.75989700 | 0.43660900 |
| Co | -0.82646900 | 0.16146200 | 0.83490200 |
| O | -1.63295800 | -1.53434500 | 0.61296600 |
| O | -0.21734500 | -0.55216500 | 2.53723800 |
| O | 0.07577500 | 1.76412600 | 1.30465100 |
| C | 0.81016500 | -1.01037700 | 1.94093700 |
| O | 0.89316500 | -0.71180800 | 0.69909300 |
| C | -2.53324400 | -1.80137000 | -0.26288300 |
| O | -2.91723000 | -1.05104600 | -1.17659700 |
| C | 0.71523600 | 2.48915300 | 0.45341600 |
| O | 0.54195600 | 2.50096500 | -0.77734200 |
| C | 1.83018800 | -1.90871200 | 2.60176600 |
| C | 1.59117300 | -1.95518600 | 4.11643300 |
| C | 1.63533100 | -3.30908900 | 1.97544600 |

| | | | |
|---|-------------|-------------|-------------|
| C | 3.24500000 | -1.38957300 | 2.28417600 |
| H | 1.70476200 | -0.96343500 | 4.56566000 |
| H | 0.58426100 | -2.31408700 | 4.34752000 |
| H | 2.31810100 | -2.62991100 | 4.58182500 |
| H | 1.77651000 | -3.26933500 | 0.89171900 |
| H | 2.36303800 | -4.00710000 | 2.40401800 |
| H | 0.62900700 | -3.69104900 | 2.17900000 |
| H | 3.98654500 | -2.05959500 | 2.73346600 |
| H | 3.42639300 | -1.34934500 | 1.20842400 |
| H | 3.40044200 | -0.38738000 | 2.69683900 |
| C | 1.80234400 | 3.38764400 | 1.08798000 |
| C | 2.84957700 | 2.43899700 | 1.70673000 |
| C | 2.45754000 | 4.27004200 | 0.01885700 |
| C | 1.15586000 | 4.25067800 | 2.18538300 |
| H | 2.39656300 | 1.82519600 | 2.48942700 |
| H | 3.27741200 | 1.77630100 | 0.94734200 |
| H | 3.66508900 | 3.02539500 | 2.14609000 |
| H | 1.72102900 | 4.91170700 | -0.47441100 |
| H | 3.21715200 | 4.90863400 | 0.48427900 |
| H | 2.94257200 | 3.66286300 | -0.75091500 |
| H | 1.92185900 | 4.86320400 | 2.67548900 |
| H | 0.40393500 | 4.92773900 | 1.76261600 |
| H | 0.67218500 | 3.62324500 | 2.93824700 |
| C | -3.14123900 | -3.21818600 | -0.10671200 |
| C | -2.00071700 | -4.24783000 | -0.21858400 |
| C | -3.78103100 | -3.29732600 | 1.29268200 |
| C | -4.19327900 | -3.46897700 | -1.19275600 |
| H | -1.54185300 | -4.22468800 | -1.21362100 |
| H | -1.22079400 | -4.05069700 | 0.52080200 |
| H | -2.39578800 | -5.25755600 | -0.05642600 |
| H | -4.58745100 | -2.56219100 | 1.39736200 |
| H | -4.20969100 | -4.29420600 | 1.45006900 |
| H | -3.03871300 | -3.10316400 | 2.07091400 |
| H | -4.61628900 | -4.47320900 | -1.07319300 |
| H | -5.00677900 | -2.74037300 | -1.13063300 |
| H | -3.75688000 | -3.39410000 | -2.19326400 |
| N | -1.31353000 | 0.84939600 | -0.90400800 |
| C | 4.15842900 | -0.43353800 | -1.72248000 |
| F | 4.86515000 | -0.45229200 | -2.87475700 |
| F | 4.83649400 | -1.21358900 | -0.84283900 |
| F | 4.20887500 | 0.83483900 | -1.24983100 |

TS14-CF₃ (doublet)

| | | | |
|---|-------------|-------------|-------------|
| C | 3.07660900 | -2.34807100 | -1.39193900 |
| C | 1.78993100 | -2.88520000 | -1.34368900 |
| C | 0.74967100 | -2.03027200 | -1.65817200 |
| C | 0.87844000 | -0.69624800 | -1.96156500 |
| C | 2.17921400 | -0.17816700 | -2.03767400 |
| C | 3.25677600 | -0.99858100 | -1.72283200 |
| H | 1.62389800 | -3.92651100 | -1.08915600 |
| H | -0.48056400 | -2.55004900 | -1.63789700 |
| H | 2.30846400 | 0.87569600 | -2.24604200 |
| C | -0.30453700 | 0.19941100 | -2.21018900 |
| O | -0.42135300 | 0.76626700 | -3.28921800 |
| N | -1.20447200 | 0.23707000 | -1.16722200 |
| C | -2.34158200 | 0.98831800 | -1.24239800 |
| C | -2.85133700 | 1.77224700 | -2.29626300 |
| C | -4.03479700 | 2.47428500 | -2.12831100 |
| H | -2.27769600 | 1.80877900 | -3.20942800 |
| C | -4.21578700 | 1.64549400 | 0.10585900 |
| C | -4.73233900 | 2.41654500 | -0.91413500 |
| H | -4.41175500 | 3.08243800 | -2.94425300 |
| H | -4.64925800 | 1.52994200 | 1.09003500 |
| H | -5.65136100 | 2.96677700 | -0.75301000 |

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|----|-------------|-------------|-------------|
| N | -3.07069700 | 0.95533200 | -0.07905500 |
| O | -2.62131900 | 0.18335000 | 0.92433500 |
| Co | -0.75408800 | -0.06280900 | 0.70226900 |
| C | -1.83309300 | -2.74057300 | -0.13464800 |
| O | -1.55197100 | -3.01480900 | -1.37989900 |
| O | -1.10339400 | -2.07832500 | 0.61344800 |
| C | -3.17358100 | -3.32744800 | 0.33779600 |
| C | -3.31157300 | -3.10577400 | 1.84985000 |
| C | -4.28777000 | -2.56478500 | -0.41347800 |
| C | -3.23060000 | -4.82712900 | -0.00690700 |
| H | -2.51370500 | -3.61312500 | 2.40060900 |
| H | -3.26734200 | -2.04217600 | 2.09370400 |
| H | -4.27368700 | -3.50987700 | 2.18456400 |
| H | -4.20069800 | -2.69580400 | -1.49583300 |
| H | -5.26238800 | -2.94904400 | -0.09285000 |
| H | -4.24590300 | -1.49801100 | -0.17871000 |
| H | -4.18528300 | -5.24086500 | 0.33541700 |
| H | -3.14540200 | -4.99355500 | -1.08388300 |
| H | -2.42656800 | -5.37896200 | 0.49309600 |
| C | 0.22349900 | 2.51681600 | 0.23188700 |
| O | -0.54429000 | 1.74817300 | 0.97092000 |
| O | 0.91863100 | 2.16725800 | -0.71338400 |
| C | 0.12961600 | 3.99121200 | 0.68964300 |
| C | -1.34485600 | 4.43175400 | 0.59613000 |
| C | 0.61550600 | 4.08787200 | 2.14810600 |
| C | 1.00231900 | 4.86056200 | -0.22269700 |
| H | -1.72594600 | 4.30937200 | -0.42509700 |
| H | -1.97158100 | 3.83934100 | 1.26794400 |
| H | -1.44078200 | 5.48979300 | 0.86827200 |
| H | 1.66433600 | 3.77870600 | 2.22984900 |
| H | 0.54167600 | 5.12242000 | 2.50440000 |
| H | 0.01683400 | 3.44698200 | 2.80102200 |
| H | 0.94576600 | 5.90857100 | 0.09529900 |
| H | 2.04753300 | 4.54053800 | -0.18693400 |
| H | 0.67309700 | 4.79287200 | -1.26374300 |
| C | 1.03463200 | -0.45024600 | 2.09825200 |
| O | 1.14856500 | -0.36730500 | 0.82777100 |
| O | -0.15438300 | -0.35061400 | 2.54529800 |
| C | 2.25793400 | -0.59831500 | 2.97431700 |
| C | 3.12156700 | -1.74968000 | 2.42296600 |
| C | 3.04061900 | 0.73064700 | 2.86118400 |
| C | 1.84180600 | -0.86505500 | 4.42585300 |
| H | 2.56718000 | -2.69516000 | 2.42046500 |
| H | 3.44846300 | -1.53612100 | 1.40321000 |
| H | 4.00850200 | -1.87468700 | 3.05406300 |
| H | 2.43681800 | 1.57299800 | 3.21577300 |
| H | 3.94727800 | 0.67502600 | 3.47408800 |
| H | 3.33024700 | 0.92030100 | 1.82388700 |
| H | 2.73459000 | -0.94932800 | 5.05536400 |
| H | 1.21741900 | -0.05484300 | 4.81284300 |
| H | 1.27173300 | -1.79608300 | 4.50918500 |
| H | 3.93529100 | -2.97317200 | -1.16938600 |
| C | 4.62867900 | -0.40056900 | -1.59328500 |
| F | 4.77666200 | 0.71546200 | -2.33079300 |
| F | 5.59631500 | -1.27031000 | -1.96353400 |
| F | 4.88743000 | -0.06297400 | -0.30237300 |

int13-CN (doublet)

| | | | |
|---|------------|-------------|------------|
| C | 2.16648400 | -1.63381300 | 2.55447700 |
| C | 1.02412800 | -0.86651200 | 2.28612600 |
| C | 1.13310100 | 0.51964600 | 2.23838200 |
| C | 2.35793900 | 1.14275700 | 2.51480800 |
| C | 3.48888700 | 0.37474500 | 2.78436200 |
| C | 3.40241300 | -1.01634000 | 2.79672600 |

| | | | |
|----|-------------|-------------|-------------|
| H | 0.07192500 | -1.34199300 | 2.10198500 |
| H | 2.41316800 | 2.22552000 | 2.49296800 |
| H | 4.43969700 | 0.85983300 | 2.98186300 |
| H | 4.27854500 | -1.62581600 | 2.99161200 |
| C | -0.03988100 | 1.40319300 | 1.97684800 |
| O | -0.36744400 | 2.26464500 | 2.77217100 |
| C | -1.74567100 | 2.05644300 | 0.41749000 |
| C | -2.64551500 | 2.71221100 | 1.27740400 |
| C | -2.97166200 | 2.88596700 | -1.46808500 |
| C | -3.69199400 | 3.45006400 | 0.75079800 |
| H | -2.49302100 | 2.61068600 | 2.33955200 |
| C | -3.85284400 | 3.54831500 | -0.63841200 |
| H | -3.01051200 | 2.87306700 | -2.54865000 |
| H | -4.39078400 | 3.94254600 | 1.41819800 |
| H | -4.66322000 | 4.11724400 | -1.07854300 |
| O | -1.12336300 | 1.55252900 | -1.76202500 |
| N | -1.95777100 | 2.16478000 | -0.93948200 |
| Co | -0.27581700 | 0.14068200 | -0.82199400 |
| O | 1.44085500 | 0.86077600 | -1.11898900 |
| O | 0.10177000 | -1.04805200 | -2.30458900 |
| O | -1.96717100 | -0.70126100 | -0.67268300 |
| C | 0.60845800 | -1.87696800 | -1.48085700 |
| O | 0.57027400 | -1.50502400 | -0.25645700 |
| C | 1.78614100 | 2.03070200 | -0.72297400 |
| O | 1.09291500 | 2.81045700 | -0.04389200 |
| C | -2.45990100 | -1.04450400 | 0.47250200 |
| O | -2.01387700 | -0.72423200 | 1.58473100 |
| C | 1.22692100 | -3.19490200 | -1.88204500 |
| C | 1.10024100 | -3.39599400 | -3.39753900 |
| C | 2.71131700 | -3.15342400 | -1.45702300 |
| C | 0.49645500 | -4.31749200 | -1.11477100 |
| H | 0.05113400 | -3.41081100 | -3.70850600 |
| H | 1.60151100 | -2.59407700 | -3.94781900 |
| H | 1.55876200 | -4.35032500 | -3.67847800 |
| H | 2.80399900 | -3.01132600 | -0.37752900 |
| H | 3.19336500 | -4.09970800 | -1.72532400 |
| H | 3.24324700 | -2.33992700 | -1.96321800 |
| H | 0.93298300 | -5.28522500 | -1.38455800 |
| H | 0.59527200 | -4.18702200 | -0.03417800 |
| H | -0.56839100 | -4.33934400 | -1.37144200 |
| C | -3.73945800 | -1.90254800 | 0.35440600 |
| C | -3.39163500 | -3.16781700 | -0.45184100 |
| C | -4.25447800 | -2.27933100 | 1.74809700 |
| C | -4.79269900 | -1.06653900 | -0.39938000 |
| H | -3.00963500 | -2.90434800 | -1.44162500 |
| H | -2.62938200 | -3.76196700 | 0.06508700 |
| H | -4.28438700 | -3.79279700 | -0.57126300 |
| H | -4.49084100 | -1.38840200 | 2.33729200 |
| H | -5.16208700 | -2.88701700 | 1.65571100 |
| H | -3.50722600 | -2.85462500 | 2.30228800 |
| H | -5.72501100 | -1.63566300 | -0.49291800 |
| H | -5.01805600 | -0.13918800 | 0.14194000 |
| H | -4.43830400 | -0.80578800 | -1.40013000 |
| C | 3.19903800 | 2.45863100 | -1.18937900 |
| C | 4.17194600 | 1.28015400 | -1.01159000 |
| C | 3.07289900 | 2.81792300 | -2.68420900 |
| C | 3.67681500 | 3.67392800 | -0.38565600 |
| H | 4.23556600 | 0.97596500 | 0.03840300 |
| H | 3.84831700 | 0.41442900 | -1.59374200 |
| H | 5.17364000 | 1.57676000 | -1.34485800 |
| H | 2.38291700 | 3.65663400 | -2.82988700 |
| H | 4.05290500 | 3.10957400 | -3.07987000 |
| H | 2.70410400 | 1.96268600 | -3.25808600 |
| H | 4.66085800 | 3.99382100 | -0.74732700 |

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|---|-------------|-------------|-------------|
| H | 2.98004200 | 4.51080500 | -0.47910600 |
| H | 3.76805400 | 3.43155400 | 0.67840000 |
| N | -0.68604100 | 1.25023900 | 0.72130400 |
| C | 2.06595100 | -3.06216300 | 2.51915600 |
| N | 1.98036300 | -4.22085700 | 2.45711500 |

TS14-CN (doublet)

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|----|-------------|-------------|-------------|
| C | 2.91067800 | -2.71464600 | -1.99794700 |
| C | 1.60166200 | -3.07335900 | -1.68411300 |
| C | 0.63317300 | -2.09552300 | -1.83079100 |
| C | 0.87038200 | -0.78299200 | -2.17032300 |
| C | 2.18315900 | -0.43643400 | -2.51085000 |
| C | 3.19566900 | -1.39663400 | -2.40772000 |
| H | 1.35619400 | -4.08235400 | -1.37054100 |
| H | -0.63412400 | -2.48382300 | -1.67497200 |
| H | 2.40324000 | 0.58896000 | -2.77982800 |
| C | -0.21605400 | 0.25554800 | -2.24786000 |
| O | -0.37522700 | 0.87686900 | -3.29166100 |
| N | -0.98921600 | 0.35836200 | -1.11263800 |
| C | -2.02971400 | 1.24193600 | -1.05014300 |
| C | -2.55690800 | 2.10428100 | -2.03185700 |
| C | -3.62476300 | 2.93371000 | -1.72643900 |
| H | -2.08698700 | 2.09651700 | -3.00290100 |
| C | -3.65647700 | 2.07877600 | 0.50441700 |
| C | -4.18776500 | 2.92784400 | -0.44328400 |
| H | -4.01477700 | 3.59965600 | -2.48933800 |
| H | -3.99109000 | 1.98908200 | 1.52902300 |
| H | -5.01390800 | 3.57520600 | -0.17544700 |
| N | -2.62592100 | 1.26689700 | 0.18641300 |
| O | -2.16585900 | 0.42507600 | 1.12628900 |
| Co | -0.38335300 | -0.04651800 | 0.69475400 |
| C | -1.85619300 | -2.55396800 | -0.06143200 |
| O | -1.72349700 | -2.83868300 | -1.32711500 |
| O | -0.98160400 | -2.00195700 | 0.61909600 |
| C | -3.21514500 | -2.96733800 | 0.52830000 |
| C | -3.17538100 | -2.78967800 | 2.05154300 |
| C | -4.26969300 | -2.02106500 | -0.08904700 |
| C | -3.52345100 | -4.42769500 | 0.15052200 |
| H | -2.41043800 | -3.42669700 | 2.50602100 |
| H | -2.95582900 | -1.75355500 | 2.31714900 |
| H | -4.14934500 | -3.06792200 | 2.46978300 |
| H | -4.29527600 | -2.10947400 | -1.17889200 |
| H | -5.25815800 | -2.28087900 | 0.30539600 |
| H | -4.05392400 | -0.98414500 | 0.18009300 |
| H | -4.49244500 | -4.71363900 | 0.57346000 |
| H | -3.56378300 | -4.56110200 | -0.93367600 |
| H | -2.76632600 | -5.10928400 | 0.55445800 |
| C | 0.88509100 | 2.37953800 | 0.14062600 |
| O | 0.08506700 | 1.71857600 | 0.94776400 |
| O | 1.44974600 | 1.93744800 | -0.85189000 |
| C | 1.01172500 | 3.85852800 | 0.57511000 |
| C | -0.38972700 | 4.49679100 | 0.48583700 |
| C | 1.52421500 | 3.92063900 | 2.02554000 |
| C | 1.98240400 | 4.58043000 | -0.36648400 |
| H | -0.79238200 | 4.41720700 | -0.53111400 |
| H | -1.08631900 | 4.00502400 | 1.17042100 |
| H | -0.33650000 | 5.56082900 | 0.74537400 |
| H | 2.52082300 | 3.47101400 | 2.10660600 |
| H | 1.59882700 | 4.96411000 | 2.35477000 |
| H | 0.85124500 | 3.38577200 | 2.70081800 |
| H | 2.07271200 | 5.63310100 | -0.07289700 |
| H | 2.97586800 | 4.12361700 | -0.33251400 |
| H | 1.63404700 | 4.53374200 | -1.40209500 |
| C | 1.47201900 | -0.68746600 | 1.89039900 |

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|---|------------|-------------|-------------|
| O | 1.46639600 | -0.59812200 | 0.61516800 |
| O | 0.35632600 | -0.44852300 | 2.45798700 |
| C | 2.75061900 | -0.97533600 | 2.64316700 |
| C | 3.55319500 | 0.34780300 | 2.63035500 |
| C | 2.43678000 | -1.40076000 | 4.08318300 |
| C | 3.53506100 | -2.06915300 | 1.89673700 |
| H | 3.75382300 | 0.66877400 | 1.60370800 |
| H | 3.00003800 | 1.14399400 | 3.13946500 |
| H | 4.50823000 | 0.20341800 | 3.14741400 |
| H | 1.85489500 | -2.32837100 | 4.10370700 |
| H | 3.37100700 | -1.56896800 | 4.63028600 |
| H | 1.86059800 | -0.63154000 | 4.60445000 |
| H | 4.48919400 | -2.25036000 | 2.40351600 |
| H | 2.97448200 | -3.01072900 | 1.87579600 |
| H | 3.73661400 | -1.76999300 | 0.86516100 |
| H | 3.71187000 | -3.44341200 | -1.93037800 |
| C | 4.55278800 | -1.03351200 | -2.69215300 |
| N | 5.65850100 | -0.75309300 | -2.91770300 |

int13-NO₂ (doublet)

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|----|-------------|-------------|-------------|
| C | 2.52195700 | -1.00786400 | -2.24664700 |
| C | 1.38812400 | -0.21453900 | -2.12364600 |
| C | 0.14053000 | -0.82460000 | -2.22206400 |
| C | 0.04603000 | -2.19553300 | -2.49040700 |
| C | 1.20130300 | -2.96870000 | -2.61259500 |
| C | 2.45707700 | -2.37915700 | -2.48199800 |
| H | 1.47499600 | 0.84281600 | -1.92691200 |
| H | -0.93525500 | -2.64845600 | -2.57961700 |
| H | 1.12244000 | -4.03351800 | -2.80752300 |
| H | 3.37179200 | -2.95329000 | -2.55579900 |
| C | -1.12648600 | -0.03574300 | -2.12342000 |
| O | -1.85975600 | 0.09780300 | -3.08372500 |
| C | -2.59691500 | 1.18594100 | -0.65393900 |
| C | -3.38853400 | 1.86634100 | -1.59739600 |
| C | -4.06893000 | 1.92817500 | 1.08530400 |
| C | -4.51287500 | 2.56090700 | -1.18558300 |
| H | -3.08682100 | 1.82332500 | -2.63112600 |
| C | -4.86424500 | 2.58738100 | 0.17128400 |
| H | -4.23221300 | 1.89175200 | 2.15367400 |
| H | -5.11414400 | 3.09014800 | -1.91676100 |
| H | -5.73739700 | 3.12366300 | 0.52361700 |
| O | -2.25034000 | 0.61631800 | 1.57519100 |
| N | -2.97226700 | 1.25549500 | 0.66813300 |
| Co | -0.55488300 | 0.18868400 | 0.86090700 |
| O | -0.89834800 | -1.66315700 | 0.95908000 |
| O | 0.44146600 | -0.06113600 | 2.50748000 |
| O | -0.05696700 | 2.02482700 | 0.94632400 |
| C | 1.47487000 | -0.33014400 | 1.81181900 |
| O | 1.30729700 | -0.25058700 | 0.54671300 |
| C | -1.82136900 | -2.25789500 | 0.29253600 |
| O | -2.57341400 | -1.73581200 | -0.54844300 |
| C | 0.32163600 | 2.67432300 | -0.10010300 |
| O | 0.05534400 | 2.38000300 | -1.27960400 |
| C | 2.78362300 | -0.76463300 | 2.43049100 |
| C | 3.16236300 | 0.23470700 | 3.53990000 |
| C | 2.53666000 | -2.16261900 | 3.04197500 |
| C | 3.87870200 | -0.83596400 | 1.35712800 |
| H | 3.35733000 | 1.22861800 | 3.12342300 |
| H | 2.36162300 | 0.32222500 | 4.27921200 |
| H | 4.07238600 | -0.10656700 | 4.04522500 |
| H | 2.23354800 | -2.87822100 | 2.26988500 |
| H | 3.45969200 | -2.52671700 | 3.50636000 |
| H | 1.75120700 | -2.12332400 | 3.80220400 |
| H | 4.82667800 | -1.12993600 | 1.82024800 |

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|---|-------------|-------------|-------------|
| H | 3.63269200 | -1.57402100 | 0.58876400 |
| H | 4.02246500 | 0.12940300 | 0.86342400 |
| C | 1.21933300 | 3.89500100 | 0.20095800 |
| C | 2.54986400 | 3.32069200 | 0.73397000 |
| C | 1.46611600 | 4.70403900 | -1.07741300 |
| C | 0.54988400 | 4.76670500 | 1.27688800 |
| H | 2.38287700 | 2.76670800 | 1.66184300 |
| H | 3.01126600 | 2.64789000 | 0.00281000 |
| H | 3.25027900 | 4.13923800 | 0.93662800 |
| H | 0.52697300 | 5.07746800 | -1.49810700 |
| H | 2.10866100 | 5.56302400 | -0.85221500 |
| H | 1.95659600 | 4.09434200 | -1.84086000 |
| H | 1.20409300 | 5.60902900 | 1.53058600 |
| H | -0.40098700 | 5.17739500 | 0.91639100 |
| H | 0.35425100 | 4.18777600 | 2.18272500 |
| C | -1.97149400 | -3.75896300 | 0.64245800 |
| C | -0.58008600 | -4.39497600 | 0.79931100 |
| C | -2.73221100 | -3.81660100 | 1.98350900 |
| C | -2.76918700 | -4.47795600 | -0.45245500 |
| H | 0.00311100 | -4.29985300 | -0.12320100 |
| H | -0.01861100 | -3.91449700 | 1.60354800 |
| H | -0.68466500 | -5.46176800 | 1.03009600 |
| H | -3.72857000 | -3.37056800 | 1.88808300 |
| H | -2.85449100 | -4.85964100 | 2.29855800 |
| H | -2.18458700 | -3.27758100 | 2.76237700 |
| H | -2.91600200 | -5.52814900 | -0.17503100 |
| H | -3.74685700 | -4.01294800 | -0.60043300 |
| H | -2.23866500 | -4.45245000 | -1.41068000 |
| N | -1.44563700 | 0.47403800 | -0.83747100 |
| N | 3.83302100 | -0.37944400 | -2.05464600 |
| O | 4.82552900 | -1.10773900 | -2.07811600 |
| O | 3.86867700 | 0.83718800 | -1.86329700 |

TS14-NO₂ (doublet)

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|----|-------------|-------------|-------------|
| C | 3.14106300 | -2.39453000 | -1.59006500 |
| C | 1.84531100 | -2.88678800 | -1.44886700 |
| C | 0.81027800 | -2.00587100 | -1.71289100 |
| C | 0.95387000 | -0.67662400 | -2.03709700 |
| C | 2.25687900 | -0.19619200 | -2.22070300 |
| C | 3.31430400 | -1.06083000 | -1.97200000 |
| H | 1.66499600 | -3.91777200 | -1.16469900 |
| H | -0.42523300 | -2.50589600 | -1.65957900 |
| H | 2.42402300 | 0.84378400 | -2.46452400 |
| C | -0.21875600 | 0.24876900 | -2.22112300 |
| O | -0.35713000 | 0.84201800 | -3.28325600 |
| N | -1.08274100 | 0.27894200 | -1.14878700 |
| C | -2.20597100 | 1.05612700 | -1.17310000 |
| C | -2.73458300 | 1.86706900 | -2.19659300 |
| C | -3.89753000 | 2.58943000 | -1.97820300 |
| H | -2.19197100 | 1.90792400 | -3.12826500 |
| C | -4.02037900 | 1.72838100 | 0.24750300 |
| C | -4.55518100 | 2.52566500 | -0.74242500 |
| H | -4.28900900 | 3.21783500 | -2.77158500 |
| H | -4.42293500 | 1.60519900 | 1.24380700 |
| H | -5.45710100 | 3.09100600 | -0.54187000 |
| N | -2.89593900 | 1.01934900 | 0.01326100 |
| O | -2.42953900 | 0.22276300 | 0.98920300 |
| Co | -0.57938500 | -0.06233900 | 0.70330200 |
| C | -1.74221600 | -2.70244600 | -0.13534900 |
| O | -1.49916100 | -2.96169300 | -1.39144500 |
| O | -0.97495500 | -2.07081700 | 0.60153900 |
| C | -3.08415900 | -3.26378100 | 0.36395800 |
| C | -3.17475500 | -3.06506200 | 1.88276400 |
| C | -4.19818900 | -2.46084900 | -0.34433400 |

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|---|-------------|-------------|-------------|
| C | -3.18755700 | -4.75538200 | -0.00442800 |
| H | -2.37560900 | -3.60222200 | 2.40249100 |
| H | -3.09707100 | -2.00745500 | 2.14377700 |
| H | -4.13738200 | -3.45080900 | 2.23696500 |
| H | -4.14240300 | -2.57411400 | -1.43075400 |
| H | -5.17298200 | -2.82810800 | -0.00505900 |
| H | -4.12506100 | -1.39991000 | -0.09171100 |
| H | -4.14285600 | -5.15126700 | 0.35653400 |
| H | -3.13557600 | -4.90490900 | -1.08600600 |
| H | -2.38469000 | -5.33551700 | 0.46433300 |
| C | 0.46766000 | 2.48269100 | 0.23292400 |
| O | -0.31286900 | 1.73835000 | 0.98498600 |
| O | 1.13331500 | 2.10827900 | -0.72391200 |
| C | 0.43051200 | 3.95936800 | 0.69001900 |
| C | -1.02758900 | 4.45261300 | 0.59920400 |
| C | 0.92279400 | 4.04194000 | 2.14715900 |
| C | 1.33161600 | 4.79446200 | -0.22676700 |
| H | -1.41301600 | 4.34957800 | -0.42248300 |
| H | -1.67504500 | 3.88005500 | 1.26880000 |
| H | -1.08524200 | 5.51199100 | 0.87657100 |
| H | 1.95895000 | 3.69320700 | 2.22905100 |
| H | 0.88909400 | 5.08005400 | 2.49899800 |
| H | 0.30122900 | 3.42744300 | 2.80405900 |
| H | 1.31176100 | 5.84484700 | 0.08759800 |
| H | 2.36530900 | 4.43895300 | -0.19143900 |
| H | 0.99889300 | 4.73413200 | -1.26702300 |
| C | 1.23363100 | -0.52389100 | 2.04220800 |
| O | 1.31957800 | -0.42314500 | 0.77069800 |
| O | 0.05927100 | -0.39525100 | 2.52011900 |
| C | 2.46911900 | -0.70297800 | 2.89451900 |
| C | 3.42893500 | -1.68058100 | 2.19302900 |
| C | 3.12217000 | 0.69668500 | 2.99115000 |
| C | 2.08159500 | -1.21187900 | 4.28906200 |
| H | 2.97232000 | -2.67095900 | 2.08492500 |
| H | 3.70075000 | -1.32238600 | 1.19713900 |
| H | 4.34333300 | -1.78877800 | 2.78642200 |
| H | 2.44814000 | 1.40913500 | 3.47801000 |
| H | 4.04358800 | 0.63206400 | 3.58028700 |
| H | 3.36835500 | 1.07907200 | 1.99580900 |
| H | 2.97816400 | -1.29744700 | 4.91290600 |
| H | 1.38057400 | -0.52907100 | 4.77652000 |
| H | 1.60722800 | -2.19741200 | 4.23220800 |
| H | 4.00818500 | -3.01778700 | -1.41134900 |
| N | 4.68696600 | -0.54097900 | -2.07204300 |
| O | 5.60065200 | -1.28005900 | -1.70195800 |
| O | 4.83789100 | 0.59511000 | -2.51276800 |