Supplementary Information

Mechanistic insight into the ruthenium-catalysed *anti*-Markovnikov hydration of alkynes using a self-assembled complex: a crucial role for ligand-assisted proton shuttle processes

Bernhard Breit,[b] Urs Gellrich,[b] Timothy Li,[a] Jason M. Lynam,[a]* Lucy M. Milner,[a] Natalie E. Pridmore,[a] John M. Slattery,[a]* and Adrian C. Whitwood.[a]

[a] Department of Chemistry, University of York, Heslington, York, YO10 5DD, UK, Fax: (+) 44(0)1904 432516. Email: john.slattery@york.ac.uk.

[b] Institut für Organische Chemie & Biochemie, Albert-Ludwigs-Universität Freiburg, Albertstr. 21a, 79104 Freiburg i. Brsg., Germany.

This document contains the SCF energies, ZPEs, XYZ coordinates and vibrational frequencies for the stationary points reported in the main section of the publication. Experimental details and procedures are also included.

Contents

Experimental Methods

General Considerations

All experimental procedures were performed under an atmosphere of dinitrogen using standard Schlenk Line and Glove Box techniques. Dichloromethane and pentane were purified with the aid of an Innovative Technologies anhydrous solvent engineering system. Acetone was degassed by bubbling with N_2 before use. The CD_2Cl_2 used for NMR experiments was dried over CaH_2 and degassed with three freeze-pump-thaw cycles. The solvent was then transferred into NMR tubes fitted with PTFE Young's taps or kept under a nitrogen atmosphere in the Glove Box. NMR spectra were acquired on a Jeol ECX-400 (Operating frequencies ^{1}H 399.78 MHz, ^{31}P 161.83 MHz, ^{19}F 376.17 MHz, ^{13}C 100.53 MHz), a Bruker AVANCE 500 (Operating frequencies ^{1}H 500.13 MHz, ^{31}P 202.47 MHz, ^{13}C 125.77 MHz) or a Bruker AVANCE 700 (Operating frequencies ^{1}H 700.13 MHz, ^{31}P 283.46 MHz, ^{13}C 176.07 MHz). ^{31}P and ^{13}C spectra were recorded with proton decoupling. Assignments were confirmed with the aid of 2D-COSY, NOESY, HMQC and HMBC experiments. Mass spectra were recorded on a Bruker micrOTOF using electrospray ionisation.

HC≡CPh was supplied by Acros Organics and HC≡CC_6H_4-4-CF_3 was supplied by Sigma-Aldrich. Both were used as supplied. NMR experiments were performed in 5 mm NMR tubes fitted with PTFE J Young's taps typically using *ca*. 20 mg of the appropriate organometallic complex and 0.55 ml of the appropriate solvent.

Synthesis of $[Ru(\eta^5\text{-}C_5H_5)(6\text{-DPPAP})(3\text{-DPICon})(MeCN)]PF_6$, 1

To an oven dried Schlenk tube was added $[Ru(\eta^5\text{-}C_5H_5)(NCMe)_3]PF_6$ (100 mg, 230 µM) and 3-DPICon (76 mg, 230 µM, 1 equivalent) in dichloromethane (10 ml). The reaction mixture was allowed to stir for 4 hours before the addition of 6-DPPAP (83 mg, 230 µM, 1 equivalent). The reaction was stirred for a further 4 hours before removal of the solvent under vacuum to yield a yellow powdered solid.

^{1}H NMR (CD_2Cl_2, 400 MHz, 295 K): δ 1.10 (s, 9H, ^{t}Bu), 1.47 (s, 3H, MeCN), 4.52 (s, 5H, η^5-C_5H_5), 6.24 (dd, 1H, J = 7.3 Hz, 1.3 Hz), 6.89 (t, 1H, J = 2.3 Hz), 7.06 (dd, 1H, J = 7.6 Hz, 3.6 Hz), 7.15 (td, 2H, J = 8.0 Hz, 1.8 Hz), 7.22 – 7.38 (m, 10H), 7.42 – 7.57 (m, 11H), 7.63 – 7.76 (m, 2H), 7.82 (dd, 1H, J = 8.4 Hz, 1.8 Hz), 8.14 (d, 1H, J = 8.1 Hz), 10.53 (s, 1H), 12.67 (d, 1H, J = 4.6 Hz).

^{31}P NMR (CD_2Cl_2, 162 MHz, 295 K): δ -143.0 (sept, $^1J_{PF}$ = 711 Hz, PF_6^-), 54.2 (d, $^2J_{PP}$ = 36.1 Hz), 46 (d, $^2J_{PP}$ = 36.1 Hz)

MS (ESI+): Measured m/z =899.2178, $C_{50}H_{47}N_4O_2P_2Ru^+$
Calculated m/z = 899.2226
Difference = 3.4 mDa

Synthesis of $[Ru(\eta^5\text{-}C_5H_5)(6\text{-DPPAP})_2]PF_6$, 13

To an oven dried Schlenk tube was added $[Ru(\eta^5\text{-}C_5H_5)(NCMe)_3]PF_6$ (100 mg, 230 µM) and 6-DPPAP (167 mg, 460 µM, 2 equivalents) in dichloromethane (10 ml). The reaction mixture was allowed to stir for 4 hours before removal of the solvent under vacuum to yield a yellow solid, which was washed in ether to remove traces of free phosphine.

^{1}H NMR (CD_2Cl_2, 400 MHz, 295 K): δ 1.07 (s, 9H, ^{t}Bu), 1.31 (s, 9H, ^{t}Bu), 4.80 (s, 5H, η^5-C_5H_5), 6.82 (ddd, 1H, J = 7.5 Hz, 4.3 Hz, 0.8 Hz), 7.12 (td, 3H, J = 7.8 Hz, 2.3 Hz), 7.16 – 7.29 (m, 4H), 7.30 – 7.51 (m, 13H), 7.66 (s, 1H), 7.78 (s, 1H), 7.88 (m, 1H), 7.99 (d, 1H, J = 7.8 Hz).

^{31}P NMR (CD_2Cl_2, 162 MHz, 295 K): δ -143.0 (sept, $^1J_{PF}$ = 711 Hz, PF_6^-), -16.6 (d, J = 36.6 Hz), 48.8 (br)

MS (ESI+): Measured m/z = 891.2434, $C_{59}H_{51}N_4O_2P_2Ru^+$
Calculated m/z = 891.2531
Difference = 9.7 mDa

Synthesis of $[Ru(\eta^5\text{-}C_5H_5)(3\text{-DPICon})_2(NCMe)]PF_6$, 14

To an oven dried Schlenk tube was added $[Ru(\eta^5\text{-}C_5H_5)(NCMe)_3]PF_6$ (100 mg, 230 µM) and 3-DPICon (152 mg, 460 µM, 2 equivalents) in dichloromethane (10 ml). The reaction mixture was allowed to stir for 4 hours before removal of the solvent under vacuum to yield a yellow solid, which was washed in ether to remove traces of free phosphine.

^{1}H NMR (CD_2Cl_2, 400 MHz, 295 K): δ 1.59 (s, 3H, MeCN), 4.56 (s, 5H, η^5-C_5H_5), 6.63 (t, 2H, J = 2.9 Hz), 7.11 – 7.35 (15H, m), 7.38 – 7.51 (10H, m), 7.59 – 7.77 (5H, m), 8.29 (d, 2H, J = 8.0 Hz).

^{31}P NMR (CD_2Cl_2, 162 MHz, 295 K): δ -143.0 (sept, $^1J_{PF}$ = 711 Hz, PF_6^-), 50.4 (s)

MS (ESI+): Measured m/z =866.1600, $C_{49}H_{40}N_3O_2P_2Ru^+$
Calculated m/z = 866.1647
Difference = 4.7 mDa

Synthesis of 15

To a Young's NMR tube was added $[Ru(\eta^5\text{-}C_5H_5)(NCMe)_3]PF_6$ (20 mg, 46 µmol) and 3-DPICon (15 mg, 46 µmol, 1 equivalent) in deuterated dichloromethane (0.5 ml). After two hours, 6-DPPAP was added (16 mg, 46 µmol, 1 equivalent) and the reaction heated at 50 °C for 20 hours (until $[Ru(\eta^5\text{-}C_5H_5)(6\text{-DPPAP})(3\text{-DPICon})(NCMe)]PF_6$, **15**, was the only product in the ^{31}P NMR spectrum). Phenylacetylene was added (6.3 µl, 138 µmol, 3 equivalents) and the reaction heated at 50 °C for 1 week.

^{1}H NMR (CD_2Cl_2, 400 MHz, 295 K): δ 1.20 (s, 9H, H_{24}), 5.00 (s, 5H, H_1), 6.00 (br, 1H), 6.32 (br, 2H), 6.48 (d, J = 6.7 Hz, 1H), 6.53 (dd, J = 7.4, 3.5 Hz, 1H), 6.65 (br, 2H), 6.97 (dd, J = 9.9, 3.2 Hz, 1H, H_{12}), 7.00 – 7.10 (m, 4H), 7.21 (m, 4H), 7.27 – 7.40 (m, 4H), 7.43 – 7.46 (d, J = 7.9 Hz, 1H), 7.46 – 7.50 (m, 3H), 7.50 – 7.55 (m, 2H), 7.55 – 7.61 (m, 3H), 7.64 – 7.80 (m, 6H), 8.31 (d, J = 7.8 Hz, 1H), 8.39 (d, J = 7.1 Hz, 1H).

^{13}C NMR (CD_2Cl_2, 100 MHz, 295 K): δ 27.4 (s, C_{24}), 40.0 (s, C_{23}), 62.3 (s, C_{11}), 76.4 (d, J = 6.7 Hz, C_{12}), 93.2 (s, C_1), 110.9 (d, J = 2.9 Hz), 116.1 (s), 124.6 (d, J = 14.5 Hz), 126.0 (s), 127.5 (s), 128.1 (d, J = 8.0 Hz), 128.8 (d, J = 9.2 Hz), 129.1 (d, J = 10.2 Hz), 129.2 (d, J = 6.8 Hz), 130.1 (d, J = 10.9 Hz), 130.3 (d, J = 10.9 Hz), 131.3 (d, J = 2.2 Hz), 131.9 (d, J = 2.6 Hz), 132.3 (d, J = 2.3 Hz), 132.5 (s), 132.6 (d, J = 10.6 Hz), 133.2 (d, J = 11.5 Hz). 133.6 (d, J = 9.2 Hz), 133.7 (s), 134.4 (d, J = 19.6 Hz), 137.0 (d, J = 9.1 Hz), 139.7 (d, J = 5.9 Hz), 141.3 (s), 143.8 (d, J = 66.3 Hz), 153.5 (d, J = 18.9 Hz), 156.1 (d, J = 72.3 Hz, $C_{2/17}$), 163.9 (d, J = 9.9 Hz, C_{10}), 177.1 (s, C_{22}). Residual resonances for free phenylacetylene and acetonitrile have been omitted.

^{31}P NMR (CD_2Cl_2, 162 MHz, 295 K): δ -143.0 (sept, $^1J_{PF}$ = 711 Hz, PF_6^-), 40.3 (br), 65.5 (d,^{2} J_{PP} = 32.4 Hz)

MS (ESI+): Measured m/z = 960.2372, $C_{56}H_{50}N_3O_2P_2Ru^+$
Calculated m/z = 960.2431
Difference = 4.4 mDa

Synthesis of 15^{CF3}

To a Young's NMR tube was added [Ru(η^5-C_5H_5) $(NCMe)_3$][PF_6] (20 mg, 46 µmol) and 3-DPICon (15 mg, 46 µmol, 1 equivalent) in deuterated dichloromethane (0.5 ml). After two hours, 6-DPPAP was added (16 mg, 46 µmol, 1 equivalent) and the reaction heated at 50 °C for 20 hours (until [CpRu(6-DPPAP)(3-DPICon)][PF_6]was the only product in the ^{31}P NMR). 4-ethynyl-α,α,α-trifluorotoluene was added (9.3 µl, 138 µmol, 3 equivalents) and the reaction heated at 50 °C for 1 week.

^{1}H NMR (CD_2Cl_2, 700 MHz, 290 K): δ 1.17 (s, 9H, H_{25}), 4.73 (br, 1H, H_{11}), 5.05 (s, 5H, H_1), 5.96 (br, 1H), 6.25 (br, 2H), 6.47 (d, J = 6.7 Hz, 1H), 6.52 (br, 1H), 6.56 – 6.71 (br, 2H), 6.93 (br, d, J = 8.4 Hz, 1H, H_{12}), 6.96 – 7.12 (m, 4H), 7.18 – 7.32 (m, 3H), 7.44 (d, J = 7.7 Hz, 2H), 7.48 – 7.53 (br, 3H), 7.57 – 7.58 (m, 1H), 7.59 – 7.64 (m, 10H), 7.66 (br, 1H), 7.69 – 7.78 (m, 5H), 8.29 (d, J = 7.8 Hz, 1H), 8.38 (d, J = 6.6 Hz, 1H).

^{13}C NMR (176 MHz, 290 K): δ 26.9 (s, C_{25}), 39.6 (s, C_{24}), 58.5 (s, C_{11}), 76.4 (d, 5.9 Hz, C_{12}), 87.6 (s), 93.0 (s, C_1), 110.8 (s), 116.0 (s), 123.9 (q, $^1J_{CF}$ = 271 Hz, C_{17}), 124.4 (d, J = 14.4 Hz), 125.2 (q, $^3J_{CF}$ = 3.8 Hz, C_{15}), 125.5 (s, quat.), 125.9 (br, quat.), 127.2 (s), 127.7 (s), 128.5 (d, J = 9.2 Hz), 128.8 (d, J = 10.8 Hz), 129.2 (s), 129.8 (d, J = 11.2 Hz), 130.0 (d, J = 10.7 Hz), 130.3 (q, $^2J_{CF}$ = 32.6 Hz, C_{16}), 131.1 (s), 131.7 (s), 131.9 (br, quat.), 132.0 (br), 132.3 (d, J = 10.2 Hz), 132.5 (s), 132.8 (br), 133.2 (br), 133.5 (s), 136.6 (d, J = 8.6 Hz, quat.), 139.4 (br), 143.3 (d, J = 67.6 Hz, $C_{2/18}$), 145.8 (s, C_{22}), 155.9 (d, J = 71.2 Hz, $C_{2/18}$), 163.4 (d, J = 9.8 Hz, C_{10}), 176.8 (s, C_{23}). Residual resonances for free alkyne and acetonitrile have been omitted.

^{31}P NMR (CD_2Cl_2, 162 MHz, 295 K): δ -143.0 (sept, $^1J_{PF}$ = 711 Hz, PF_6^-), 39.5 (br), 65.1 (d, $^2J_{PP}$ = 31.4 Hz).

^{19}F NMR (CD_2Cl_2, 376 MHz, 295 K): δ -72.7 (PF_6^-), -63.2 (CF_3).

MS (ESI+): Measured m/z = 1028.2245, $C_{57}H_{49}F_3N_3O_2P_2Ru^+$
Calculated m/z = 1028.2305
Difference = 4.5 mDa

Catalytic anti-Markovnikov hydration of phenylacetylene[1]

To a Young's ampoule was added [Ru(η^5-C_5H_5)(6-DPPAP)(3-DPICon)(MeCN)][PF_6] (21 mg, 2 mol %), water (90 mg, 5 mmol), phenylacetylene (109.8 µl, 1 mmol) and deoxygenated acetone (1.6 ml). The ampoule was then sealed under nitrogen and heated under nitrogen for 26 hours at 120 °C. The solvent was removed under vacuum, and NMR spectra recorded.

The ^{1}H and ^{31}P{^{1}H} NMR spectra showed both the deactivation product and the aldehyde after the reaction.

Catalytic testing of 15

To a Young's NMR tube was added [Ru(η^5-C_5H_5)(6-DPPAP)(3-DPICon)(MeCN)]PF_6 (20 mg, 19 µmol) and phenylacetylene (2 µl, 19 µmol, 1 equivalent) in degassed acetone (1 ml). The reaction was heated at 120 °C for 6 hours until complete conversion to isoq5 (9) was observed. A stoichiometric volume of water was added (0.3 µl, 19 µmol, 1 equivalent) and the reaction mixture heated at 120 °C for 20 hours, with monitoring by high resolution mass spectrometry.

After reaction, the MS showed no trace of aldehyde.

Crystallographic Details

Diffraction data for crystals of 15^{CF3} were collected at 109.95(10) K on an Oxford Diffraction SuperNova diffractometer with Mo-K_a radiation (0.71073 Å) using an EOS CCD camera. The crystal was cooled with an Oxford Instruments Cryojet. Diffractometer control, data collection, initial unit cell determination, frame integration and unit-cell refinement was carried out with "CrysalisPro".[2]

Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid.[3] implemented within "CrysalisPro".[2] OLEX2[4] was used for overall structure solution, refinement and preparation of computer graphics and publication data. Using Olex2,[4] the structure was solved with the ShelXS structure solution program using Direct Methods and refined with the ShelXL refinement package using Least Squares minimisation.[5] All non-hydrogen atoms were refined anisotropically.

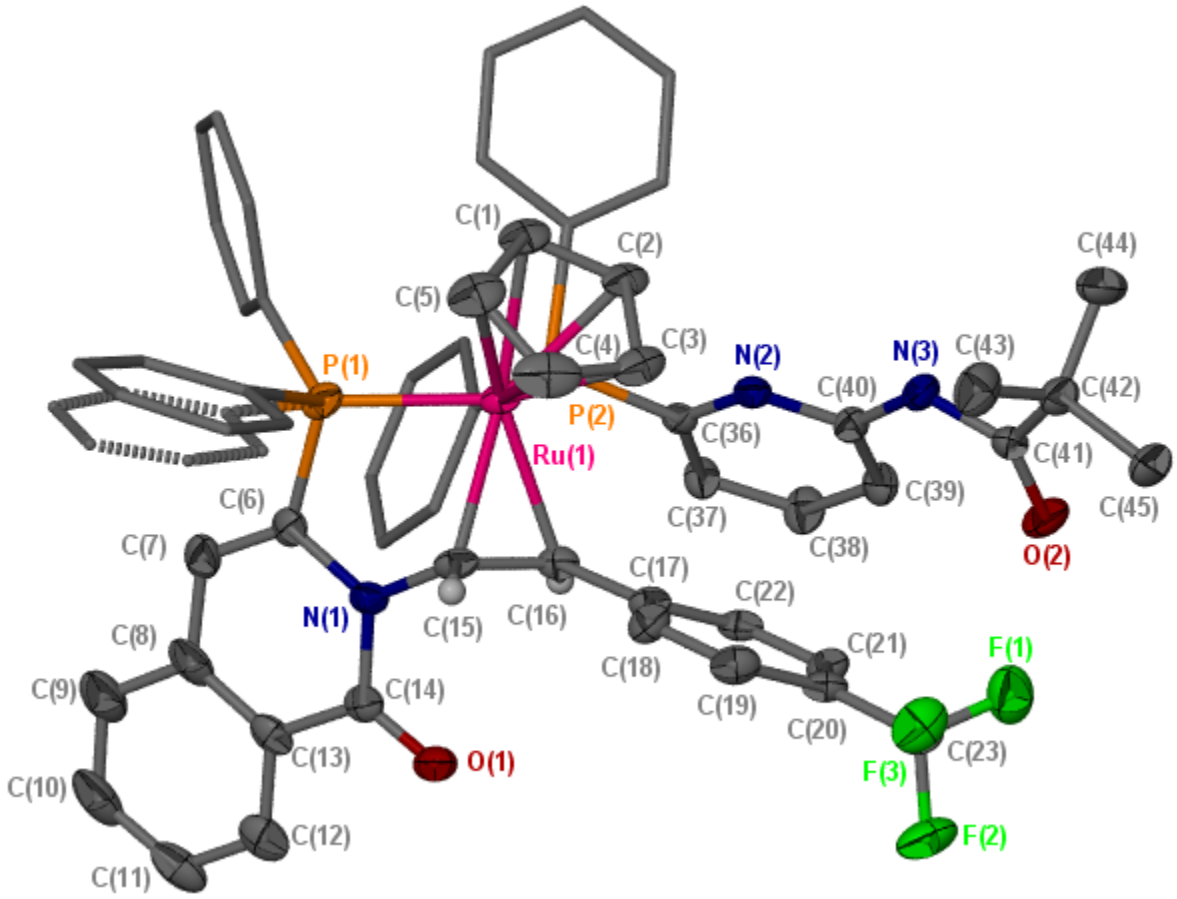
One phenyl group exhibited disorder and was modelled in two positions of equal occupancy. Equivalent pairs of carbon atoms were constrained to have the same ADP e.g. C30A & C30B. The ADP of 6 carbons in the rings were restrained to be approximately isotropic, namely C30A, C30B, C33A, C33B, C34A, C34B, C35A & C35B.

A dichloromethane was present with occupancy of 0.5 per asymmetric unit; this was also disordered and modelled in two positions with refined occupancies of 0.405:0.095(3). The C-Cl bond lengths were restrained to 1.745 angstroms.
A diethyl ether of crystallisation was also present. This was partially occupied and modelled at 40% occupancy disordered about a centre of inversion. The C-C and C-O bond lengths in this ether were restrained to 1.51 and 1.43 angstroms, respectively. The ADP were restrained to be approximately isotropic (ISOR).

Non-acidic hydrogen atoms were placed using a "riding model" and included in the refinement at calculated positions. The N-H hydrogen was located by difference map after all other atoms had been located and refined.

X-Ray Structure of 15^{CF3}

Empirical formula	$C_{58.3}H_{52}ClF_9N_3O_{2.2}P_3Ru$
Formula weight	1230.26
Temperature	109.95(10) K
Crystal system	monoclinic
Space group	C2/c
a	23.0193(7) Å
b	15.7635(7) Å
c	31.3450(14) Å
α	90 °
β	101.205(3) °
γ	90 °
Volume	11157.1(8) $Å^3$
Z	8
Calculated density	1.465 mg mm^{-3}
Absorption Coefficient	0.491 mm^{-1}
F(000)	5019.2
Crystal size	0.181 × 0.1127 × 0.0908 mm^3
Radiation	MoKα (λ = 0.71073)
2Theta range for data collection	5.804 to 56.156°
Index ranges	$-26 \leq h \leq 28$, $-9 \leq k \leq 20$, $-37 \leq l \leq 40$
Reflections collected	23119
Independent reflections	11380 [R_{int} = 0.0345, R_{sigma} = 0.0722]
Data/restraints/parameters	11380/92/775
Goodness-of-fit on F^2	1.090
Final R indices [I>=2σ (I)]	R_1 = 0.0639, wR_2 = 0.1192
R indices (all data)	R_1 = 0.0996, wR_2 = 0.1336
Largest diff. peak and hole	0.72 and -0.69 e.$Å^{-3}$



Solid state structure of the cation 15^{CF3}, thermal ellipsoids shown at the 50 % probablility level, most hydrogen atoms omitted for clarity. Two molecules of dichloromethane, one molecule of ether and one BF_4 counter-ion also omitted. Selected bond lengths / Å Ru(1)-C(15) 2.181(4), Ru(1)-C(16) 2.248(4), Ru(1)-P(1) 2.2966(14), C(15)-C(16) 1.405(6). Selected bond angles / °P(1)-Ru(1)-C(15) 74.91(13), P(1)-Ru(1)-C(16) 106.82(12), N(1)-C(15)-C(16) 74.1(3), C(15)-C(16)-C(17) 123.0(4), C(15)-Ru(1)-C(16) 36.95(16), P(1)-C(6)-N(1) 109.1(3).

Computational details

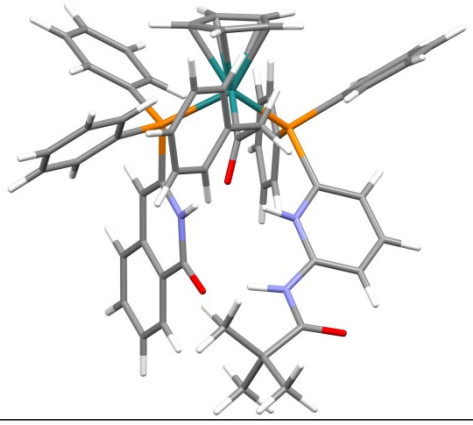
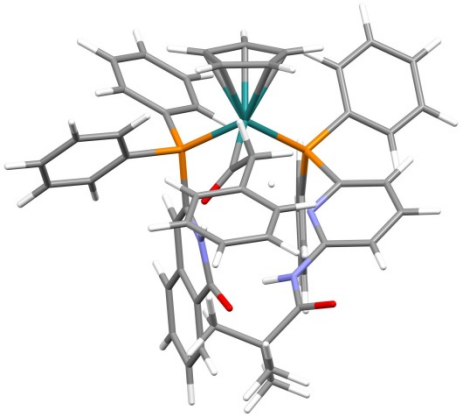
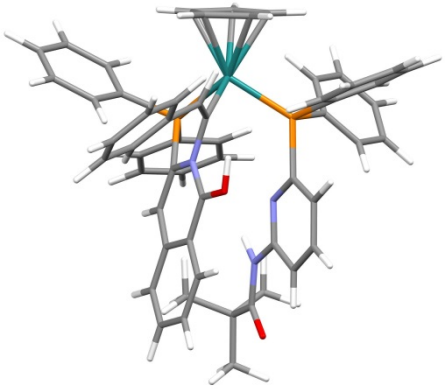
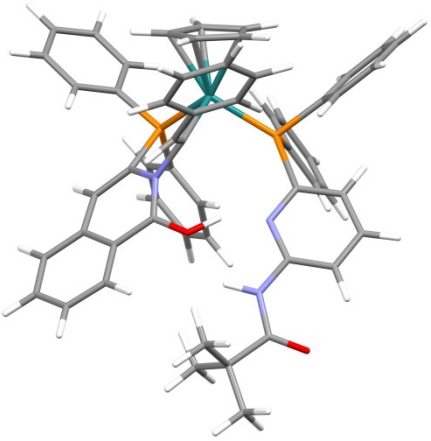
General Considerations

Initial optimisations were performed at the (RI-)BP86/SV(P) level, followed by frequency calculations at the same level. Transition states were located by initially performing a constrained minimisation (by freezing internal coordinates that change most during the reaction) of a structure close to the anticipated transition state. This was followed by a frequency calculation to identify the transition vector to follow during a subsequent transition state optimisation. A final frequency calculation was then performed on the optimised transition-state structure. All minima were confirmed as such by the absence of imaginary frequencies and all transition states were identified by the presence of only one imaginary frequency. All transition states were verified as connecting to the expected adjacent minima using the DRC module of TURBOMOLE (using an initial distortion length of 100, 50 cycles and a damping factor of 1). Dynamic reaction coordinate (DRC) calculations aim to follow a classical trajectory from a transition state to the minima on either side of it by moving along its imaginary vibrational mode.[4, 5] DRC calculations are similar to, but computationally less expensive than, intrinsic reaction coordinate (IRC) calculations, which attempt to find the minimum energy path (MEP) from the transition state to connecting minima.

Single-point calculations on the (RI-)BP86/SV(P) optimised geometries were performed using the hybrid PBE0 functional and the flexible def2-TZVPP basis set. The (RI-)PBE0/def2-TZVPP SCF energies were corrected for their zero point energies, thermal energies and entropies (obtained from the (RI-)BP86/SV(P)-level frequency calculations). In all calculations, a 28 electron quasi-relativistic ECP replaced the core electrons of Ru. No symmetry constraints were applied during optimisations. All calculations were performed using the TURBOMOLE V6.40 package using the resolution of identity (RI) approximation.[6-14] Solvation effects were modelled using the COSMO module of TURBOMOLE. The pre-optimised gas phase structures were computed in a single-point calculation at the (RI)PBE0/def2-TZVPP level with solvent corrected SCF energies. The dielectric constants used were dichloromethane (8.93 at 298 K) and acetone (13.26 at 298 K).[15]

Single-point DFT-D3 corrections (on the (RI)-BP86/SV(P) geometries) have been applied at the PBE0-D3 level using Grimme's DFT-D3 V3.0 Rev 2 program (with BJ-damping)[14, 15] and data presented in the main section of the paper includes this correction. Both DFT-D3 and DFT data are presented in the tables and PES given below. We made the decision, following suggestions from one referee, to include DFT-D3 corrected data here, as dispersion corrections resulted in changes to the difference between the energetic spans for the productive and deactivation pathways, which fit better with the experimental observations. Without DFT-D3 corrections the difference in energetic spans (with acetone solvation) is 51 kJ mol^{-1} (in favour of the deactivation pathway), which suggests that rapid catalyst deactivation should be observed in this system rather than productive catalysis. This is inconsistent with the experimental observation of productive catalysis (albeit with significant catalyst decomposition) being observed. The difference in energetic spans is significantly smaller with the DFT-D3 corrections (22 kJ mol^{-1}, still in favour of the deactivation pathway). This is more consistent with the experimental observation of productive catalysis, but it could also be coincidence and there may be other effects (such as explicit solvation) that we have been unable to model that explain the difference between experiment and theory in this case. Unfortunately, we don't have quantitative experimental data in this system that would allow us to determine whether or not DFT-D3 is an appropriate correction here. However, inspection of the structures of **9**, $\mathbf{TS_{911}}$, **17** and **TS1718** (see figure below) suggest that the changes in the energetic spans for the catalytic and deactivation

pathways are consistent with potentially different C-H to π and π-π interactions between the TDIs and TDTSs that may not be well described by DFT. Although we cannot be sure that the magnitudes of the DFT-D3 corrections are appropriate, there seems to be qualitative evidence that they may be modelling the system better.

	
9	**TS_{911}**
	
17	**TS_{1718}**

Energies, geometries and vibrational frequencies for each state are presented below. Energies reported are relative to structure **2** + **water** + **MeCN.** In the tabulated eneriges, the isomers marked "*****" are those used in the discussion in the manuscript.

Consideration of Conformational Isomers

Conformational (and where appropriate stereo-) isomers were chosen based on their relative energies (generally the lowest energy isomer has been shown on the PES). Where appropriate, a higher energy (but still accessible under the experimental conditions) isomer is presented on the PES in order to ensure that no significant structural changes (e.g. large bond rotations) were made between the preceding isomer and the outcome generated after passing through the transition state. The naming system used is identical to that found in the manuscript in terms of discrete ground state and transition state points on the potential energy surface. Where more than one isomer has been found, this is designated with a slash (/) and then the following symbols:

a = Phenyl ring of vinylidene points towards Cp or is next to 3-DPICon ligand

b = Phenyl ring of vinylidene points away from Cp or is next to 6-DPPAP ligand

For structures **8** and **9**, three isomers have been calculated, corresponding to the orientation of the acyl moiety with respect to the cyclopentadienyl ring. These are labelled as:

a = Phenyl ring points towards Cp and 3-DPICon

b = Phenyl ring points away from Cp

c = Phenyl ring points towards Cp and 6-DPPAP

For structures **11** and **12**, three isomers have been calculated, corresponding to the orientation of the acyl moiety with respect to the cyclopentadienyl ring. These are labelled as:

a = Phenyl ring points away from Cp and towards 6-DPPAP ligand

b = Phenyl ring points away from Cp and towards 3-DPICon ligand

c = Phenyl ring points upwards towards Cp

Isomers of **6** can be ‘open’, which refers to the lack of hydrogen bonding between the amide of 6-DPPAP and the carbonyl group of 3-DPICon. The NH of the 6-DPPAP amide moiety is engaged in hydrogen bonding to water in these structures.

Isomers of **3** can be ‘hbond’, which refers to the orientation of the ligands with respect to the coordinated alkyne group.

Table 1 – Summary of energetic data (no dispersion corrections applied).

Structures	BP86/SV(P) SCF energy (a.u.)	BP86/SV(P) Zero Point Energy (a.u.)	BP86/SV(P) Chem Pot (kJ mol^{-1})	pbe0/def2-TZVVP Single Point SCF energy (a.u.)	Relative PBE0/def2-TZVPP $E_{SCF+ZPE}$ (kJ mol^{-1})	Relative PBE0/def2-TZVP G (kJ mol^{-1})	PBE0/def2-TZVVP Single Point DCM COSMO SCF energy (a.u.)	Relative PBE0/def2-TZVVP DCM COSMO $E_{SCF+ZPE}$ (kJ mol^{-1})	Relative PBE0/def2-TZVVP DCM COSMO G (kJ mol^{-1})	PBE0/def2-TZVVP Single Point Acetone COSMO SCF energy (a.u.)	Relative PBE0/def2-TZVVP Acetone COSMO $E_{SCF+ZPE}$ (kJ mol^{-1})	Relative PBE0/def2-TZVVP Acetone COSMO G (kJ mol^{-1})
2b + water + MeCN	-3463.506039	0.954199	2135.67	-3463.029759			-3463.096868			-3463.110238		
3a	-3254.498091	0.888630	2074.51	-3253.995934	31	30	-3254.044310	33	32	-3254.049782	48	47
3b *****	-3254.501301	0.888487	2067.63	-3253.997157	27	20	-3254.046728	26	19	-3254.052300	41	34
3a hbond	-3254.501322	0.888830	2068.54	-3253.997230	28	21	-3254.046431	28	21	-3254.051948	43	36
3b hbond	-3254.492694	0.889683	2079.79	-3253.990595	47	49	-3254.046728	29	31	-3254.043300	68	69
2a	-3254.501135	0.890573	2085.35	-3254.000923	23	28	-3254.051456	19	25	-3254.057223	33	39
2b *****	-3254.508307	0.890358	2079.64	-3254.009299	0	0	-3254.058618	0	0	-3254.069713	0	0
4 *****	-3254.511154	0.890680	2078.67	-3254.017893	-22	-24	-3254.066621	-20	-22	-3254.072066	-5	-7
5a	-3254.524218	0.890779	2079.11	-3254.021085	-30	-31	-3254.072195	-35	-36	-3254.078013	-21	-22
5b *****	-3254.528707	0.890236	2073.64	-3254.025901	-44	-50	-3254.075709	-45	-51	-3254.081333	-31	-37
6a open	-3330.874593	0.914309	2133.53	-3330.391004	6	45	-3330.446713	11	51	-3330.453162	26	65
6b open	-3330.879826	0.914720	2132.85	-3330.395188	-4	34	-3330.447997	9	46	-3330.454065	25	62
6a *****	-3330.888017	0.914790	2141.79	-3330.406500	-34	13	-3330.456730	-14	32	-3330.462422	3	49
6b	-3330.885698	0.914204	2138.12	-3330.403068	-26	18	-3330.453868	-8	36	-3330.459638	9	53
7a	-3330.896329	0.917913	2154.11	-3330.412125	-40	10	-3330.461226	-17	33	-3330.466708	0	50
7b *****	-3330.908858	0.918663	2152.70	-3330.423917	-69	-22	-3330.471820	-43	4	-3330.477160	-25	22
8a	-3330.911092	0.918085	2144.80	-3330.426937	-79	-38	-3330.479829	-66	-25	-3330.485859	-50	-9
8b *****	-3330.920124	0.917880	2143.16	-3330.436054	-103	-63	-3330.479829	-66	-27	-3330.494150	-72	-33
8c	-3330.908343	0.917867	2144.36	-3330.425014	-74	-33	-3330.479716	-66	-25	-3330.485974	-51	-10
9a *****	-3330.941397	0.918341	2147.20	-3330.448736	-135	-93	-3330.497944	-113	-70	-3330.503466	-95	-53
9b	-3330.938091	0.918190	2149.14	-3330.445836	-128	-83	-3330.495225	-106	-61	-3330.500756	-89	-44
9c	-3330.938841	0.918774	2148.63	-3330.445161	-125	-82	-3330.493651	-100	-58	-3330.499059	-83	-40
11a	-3330.915154	0.915427	2144.92	-3330.422875	-75	-27	-3330.474902	-60	-12	-3330.480918	-44	4
11b *****	-3330.910524	0.915538	2135.42	-3330.418580	-63	-25	-3330.471343	-50	-12	-3330.477403	-34	4
11c	-3330.913002	0.916014	2143.85	-3330.418484	-62	-17	-3330.469755	-45	0	-3330.475597	-28	17
12a	-3330.941483	0.918083	2146.19	-3330.450720	-141	-99	-3330.498520	-115	-73	-3330.503880	-97	-55
12b	-3330.937950	0.917211	2142.23	-3330.448040	-136	-96	-3330.496987	-113	-73	-3330.502488	-96	-55
12c *****	-3330.943612	0.917369	2137.27	-3330.453178	-149	-114	-3330.501634	-125	-90	-3330.507035	-107	-72
10a *****	-3330.922446	0.914870	2135.62	-3330.425246	-83	-43	-3330.484331	-86	-46	-3330.491254	-72	-33
10b	-3330.922379	0.914895	2134.98	-3330.425282	-83	-43	-3330.483907	-85	-46	-3330.490760	-71	-32
10c	-3330.923960	0.915394	2140.69	-3330.426733	-85	-41	-3330.483810	-83	-40	-3330.490436	-69	-25
TS34	-3254.497737	0.883729	2069.06	-3253.995627	18	25	-3254.042945	24	31	-3254.048194	39	46
TS35	-3254.489750	0.886713	2071.94	-3253.992168	35	37	-3254.039565	40	42	-3254.044878	56	58
TS45	-3254.498897	0.886877	2073.71	-3253.996019	26	29	-3254.044331	28	32	-3254.049726	43	47

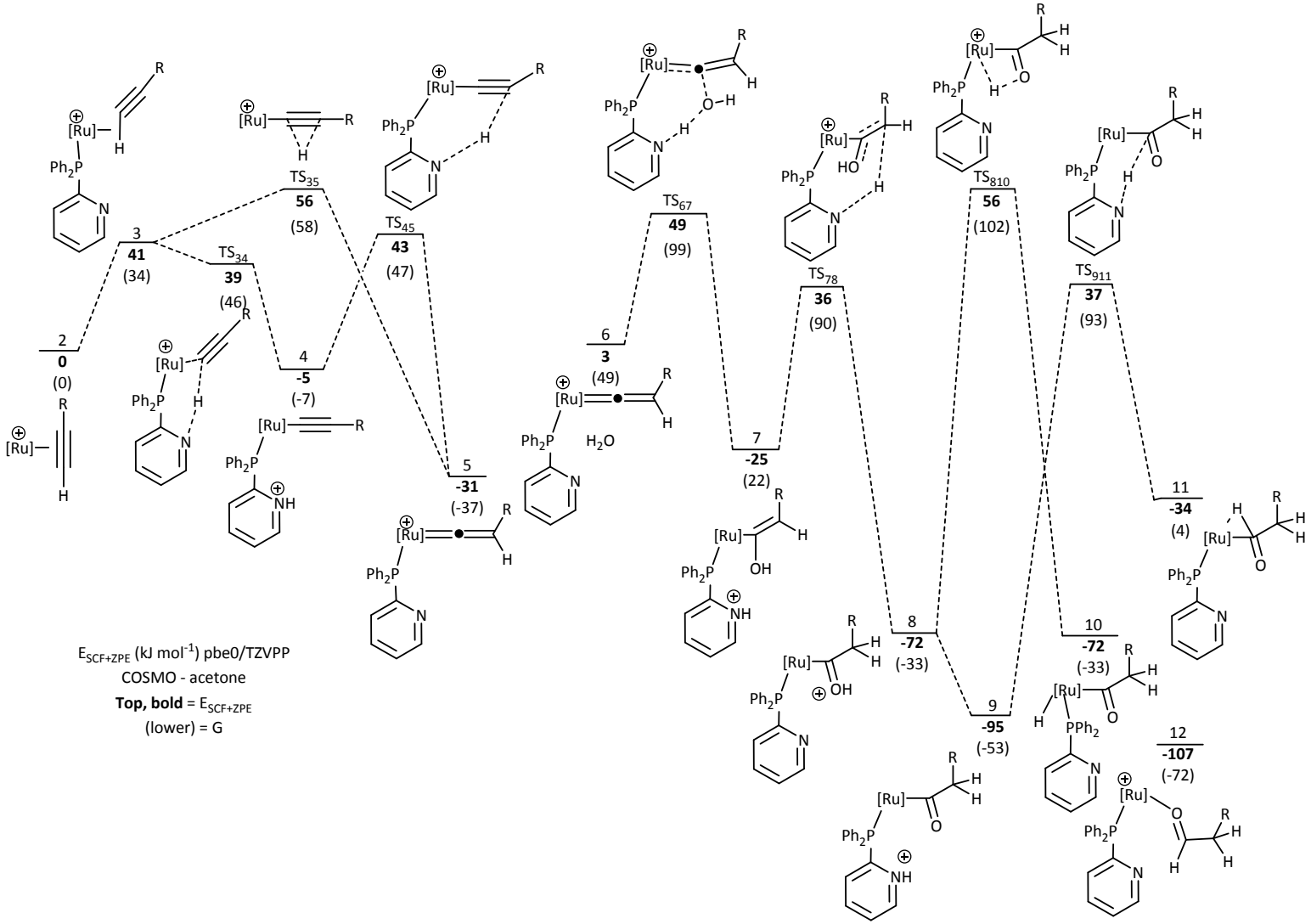
TS67	-3330.880889	0.912646	2139.54	-3330.388551	8	58	-3330.437153	32	82	-3330.442603	49	99
TS78	-3330.880216	0.913265	2145.41	-3330.393146	-2	51	-3330.442923	18	72	-3330.448488	36	90
TS911	-3330.888679	0.912183	2144.84	-3330.389896	3	59	-3330.441092	20	77	-3330.446929	37	93
TS810	-3330.873118	0.911274	2132.32	-3330.378632	30	76	-3330.432399	41	87	-3330.438624	56	102
Water	-76.345198	0.019981	4.17	-76.379977			-76.388403			-76.389417		
MeCN	-132.652534	0.043860	51.86	-132.640483			-132.649847			-132.651108		
Phenylacetylene	-308.169905	0.106497	199.28	-308.123227			-308.129314			-308.130055		
Phenylacetaldehyde	-384.602070	0.133542	260.28	-384.569210			-384.576947			-384.577910		
Deactivation Mechanism												
5a	-3254.524218	0.890779	2079.11	-3254.021085	-30	-31	-3254.072195	-35	-36	-3254.078013	-21	-22
5b *****	-3254.528707	0.890236	2073.64	-3254.025901	-44	-50	-3254.075709	-45	-51	-3254.081333	-31	-37
16a	-3254.488272	0.888888	2070.04	-3253.994804	34	28	-3254.050826	17	11	-3254.057127	29	23
16b *****	-3254.489752	0.889086	2069.93	-3253.996991	29	23	-3254.053202	11	5	-3254.059528	23	17
17a	-3254.516813	0.891462	2085.89	-3254.024608	-37	-34	-3254.077110	-46	-42	-3254.082977	-32	-29
17b *****	-3254.521601	0.891652	2087.13	-3254.028476	-47	-43	-3254.080965	-55	-51	-3254.086818	-42	-37
18a	-3254.523080	0.893265	2101.24	-3254.021094	-23	-9	-3254.073053	-30	-16	-3254.078891	-16	-2
18b *****	-3254.515705	0.892163	2089.78	-3254.017885	-18	-12	-3254.076397	-42	-37	-3254.083167	-31	-25
TS1617	-3254.485957	0.889309	2080.78	-3253.992068	42	46	-3254.048472	24	28	-3254.054833	36	40
TS1718	-3254.498417	0.890664	2093.55	-3253.997116	33	46	-3254.049431	25	38	-3254.055321	39	52
TS1815	-3254.512677	0.887897	2085.40	-3254.004646	6	18	-3254.056819	-2	10	-3254.062663	12	24
15 *****	-3254.555775	0.893460	2093.57	-3254.058835	-122	-116	-3254.117098	-145	-140	-3254.123844	-134	-128

Table 2 – Summary of energetic data (PBE0-D3 dispersion corrections applied).

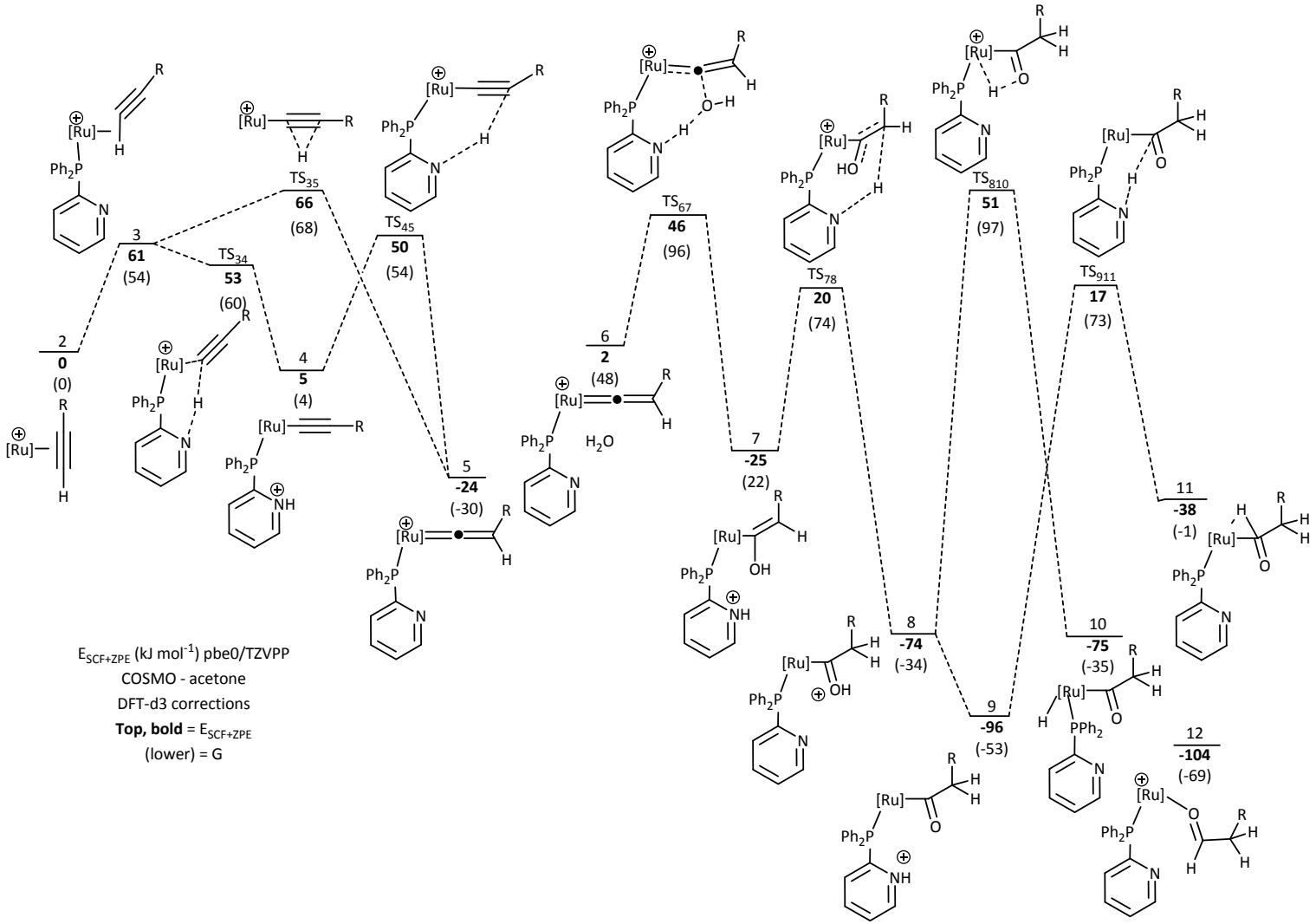
Structures	PBE0/def2-TZVVP Single Point DCM COSMO SCF energy (a.u.)	DFT-d3 correction (A.U.)	PBE0/def2-TZVVP Single Point DCM COSMO SCF energy + DFT-d3 correction (a.u.)	Relative PBE0/def2-TZVVP DCM COSMO ESCF+ZPE (kJ mol^{-1}) + DFT-d3 correction	Relative PBE0/def2-TZVVP DCM COSMO G (kJ mol^{-1}) + DFT-d3 correction	PBE0/def2-TZVVP Single Point Acetone COSMO SCF energy (a.u.)	DFT-d3 correction (A.U.)	PBE0/def2-TZVVP Single Point Acetone COSMO SCF energy + DFT-d3 correction (a.u.)	Relative PBE0/def2-TZVVP Acetone COSMO ESCF+ZPE (kJ mol^{-1}) + DFT-d3 correction	Relative PBE0/def2-TZVVP Acetone COSMO G (kJ mol^{-1}) + DFT-d3 correction
2b + water + MeCN	-3463.096868	-0.209278	-3463.306146			-3463.110238	-0.209278	-3463.319516		
3a	-3254.044310	-0.202806	-3254.247116	43	43	-3254.049782	-0.202806	-3254.252588	58	57
3b *****	-3254.046728	-0.198848	-3254.245575	47	40	-3254.052300	-0.198848	-3254.251147	61	54
3a hbond	-3254.046431	-0.198634	-3254.245065	49	42	-3254.051948	-0.198634	-3254.250582	64	57
3b hbond	-3254.046728	-0.207522	-3254.254249	27	29	-3254.043300	-0.207522	-3254.250821	65	67
2a	-3254.051456	-0.210500	-3254.261956	9	15	-3254.057223	-0.210500	-3254.267723	23	28
2b *****	-3254.058618	-0.206690	-3254.265308	0	0	-3254.069713	-0.206690	-3254.276403	0	0
4 *****	-3254.066621	-0.202607	-3254.269228	-9	-11	-3254.072066	-0.202607	-3254.274673	5	4
5a	-3254.072195	-0.204217	-3254.276412	-28	-30	-3254.078013	-0.204217	-3254.282230	-14	-16
5b *****	-3254.075709	-0.204231	-3254.279940	-39	-44	-3254.081333	-0.204231	-3254.285564	-24	-30
6a open	-3330.446713	-0.206812	-3330.653525	12	51	-3330.453162	-0.206812	-3330.659974	26	66
6b open	-3330.447997	-0.206707	-3330.654704	10	47	-3330.454065	-0.206707	-3330.660771	25	63
6a *****	-3330.456730	-0.207503	-3330.664233	-15	31	-3330.462422	-0.207503	-3330.669925	2	48
6b	-3330.453868	-0.208865	-3330.662733	-13	31	-3330.459638	-0.208865	-3330.668502	4	48
7a	-3330.461226	-0.208430	-3330.669656	-21	29	-3330.466708	-0.208430	-3330.675138	-4	47
7b *****	-3330.471820	-0.206880	-3330.678700	-43	4	-3330.477160	-0.206880	-3330.684040	-25	22
8a	-3330.479829	-0.207692	-3330.687521	-68	-27	-3330.485859	-0.207692	-3330.693552	-52	-11
8b *****	-3330.479829	-0.207584	-3330.687412	-68	-28	-3330.494150	-0.207584	-3330.701734	-74	-34
8c	-3330.479716	-0.210510	-3330.690226	-75	-35	-3330.485974	-0.210510	-3330.696484	-60	-19
9a *****	-3330.497944	-0.207125	-3330.705070	-113	-71	-3330.503466	-0.207125	-3330.710591	-96	-53
9b	-3330.495225	-0.208050	-3330.703275	-109	-64	-3330.500756	-0.208050	-3330.708806	-92	-47
9c	-3330.493651	-0.207514	-3330.701165	-102	-59	-3330.499059	-0.207514	-3330.706573	-84	-41
11a	-3330.474902	-0.210580	-3330.685481	-69	-22	-3330.480918	-0.210580	-3330.691498	-53	-6
11b *****	-3330.471343	-0.208542	-3330.679885	-54	-16	-3330.477403	-0.208542	-3330.685946	-38	-1
11c	-3330.469755	-0.207036	-3330.676791	-45	0	-3330.475597	-0.207036	-3330.682633	-29	17
12a	-3330.498520	-0.207087	-3330.705607	-115	-73	-3330.503880	-0.207087	-3330.710968	-97	-55
12b	-3330.496987	-0.203512	-3330.700499	-104	-64	-3330.502488	-0.203512	-3330.706000	-87	-46
12c *****	-3330.501634	-0.205590	-3330.707224	-121	-86	-3330.507035	-0.205590	-3330.712625	-104	-69
10a *****	-3330.484331	-0.207755	-3330.692086	-88	-48	-3330.491254	-0.207755	-3330.699009	-75	-35
10b	-3330.483907	-0.207715	-3330.691622	-87	-48	-3330.490760	-0.207715	-3330.698475	-73	-34
10c	-3330.483810	-0.207898	-3330.691708	-86	-42	-3330.490436	-0.207898	-3330.698334	-71	-28
TS34	-3254.042945	-0.201387	-3254.244332	38	44	-3254.048194	-0.201387	-3254.249581	53	60
TS35	-3254.039565	-0.202709	-3254.242274	51	53	-3254.044878	-0.202709	-3254.247587	66	68

TS45	-3254.044331	-0.204038	-3254.248368	35	39	-3254.049726	-0.204038	-3254.253763	50	54
TS67	-3330.437153	-0.208102	-3330.645255	29	79	-3330.442603	-0.208102	-3330.650705	46	96
TS78	-3330.442923	-0.212727	-3330.655650	3	57	-3330.448488	-0.212727	-3330.661215	20	74
TS911	-3330.441092	-0.214684	-3330.655775	0	56	-3330.446929	-0.214684	-3330.661613	17	73
TS810	-3330.432399	-0.208922	-3330.641322	36	82	-3330.438624	-0.208922	-3330.647546	51	97
Water	-76.388403	-0.000277	-76.388680			-76.389417	-0.000277	-76.389694		
MeCN	-132.649847	-0.002311	-132.652158			-132.651108	-0.002311	-132.653419		
Phenylacetylene	-308.129314	-0.012246	-308.141560			-308.130055	-0.012246	-308.142301		
Phenylacetaldehyde	-384.576947	-0.015168	-384.592116			-384.577910	-0.015168	-384.593078		
Deactivation Mechanism										
5a	-3254.072195	-0.204217	-3254.276412	-28	-30	-3254.078013	-0.204217	-3254.282230	-14	-16
5b *****	-3254.075709	-0.204231	-3254.279940	-39	-44	-3254.081333	-0.204231	-3254.285564	-24	-30
16a	-3254.050826	-0.202428	-3254.253254	28	22	-3254.057127	-0.202428	-3254.259554	40	35
16b *****	-3254.053202	-0.202444	-3254.255646	22	16	-3254.059528	-0.202444	-3254.261972	35	28
17a	-3254.077110	-0.209755	-3254.286865	-54	-50	-3254.082977	-0.209755	-3254.292732	-40	-37
17b *****	-3254.080965	-0.208785	-3254.289750	-61	-57	-3254.086818	-0.208785	-3254.295603	-47	-43
18a	-3254.073053	-0.208209	-3254.281262	-34	-20	-3254.078891	-0.208209	-3254.287099	-20	-6
18b *****	-3254.076397	-0.210105	-3254.286502	-51	-46	-3254.083167	-0.210105	-3254.293272	-40	-34
TS1617	-3254.048472	-0.206542	-3254.255014	24	28	-3254.054833	-0.206542	-3254.261375	37	41
TS1718	-3254.049431	-0.204656	-3254.254087	30	43	-3254.055321	-0.204656	-3254.259976	44	57
TS1815	-3254.056819	-0.209072	-3254.265891	-8	4	-3254.062663	-0.209072	-3254.271735	6	18
15 *****	-3254.117098	-0.206717	-3254.323815	-145	-140	-3254.123844	-0.206717	-3254.330561	-134	-128

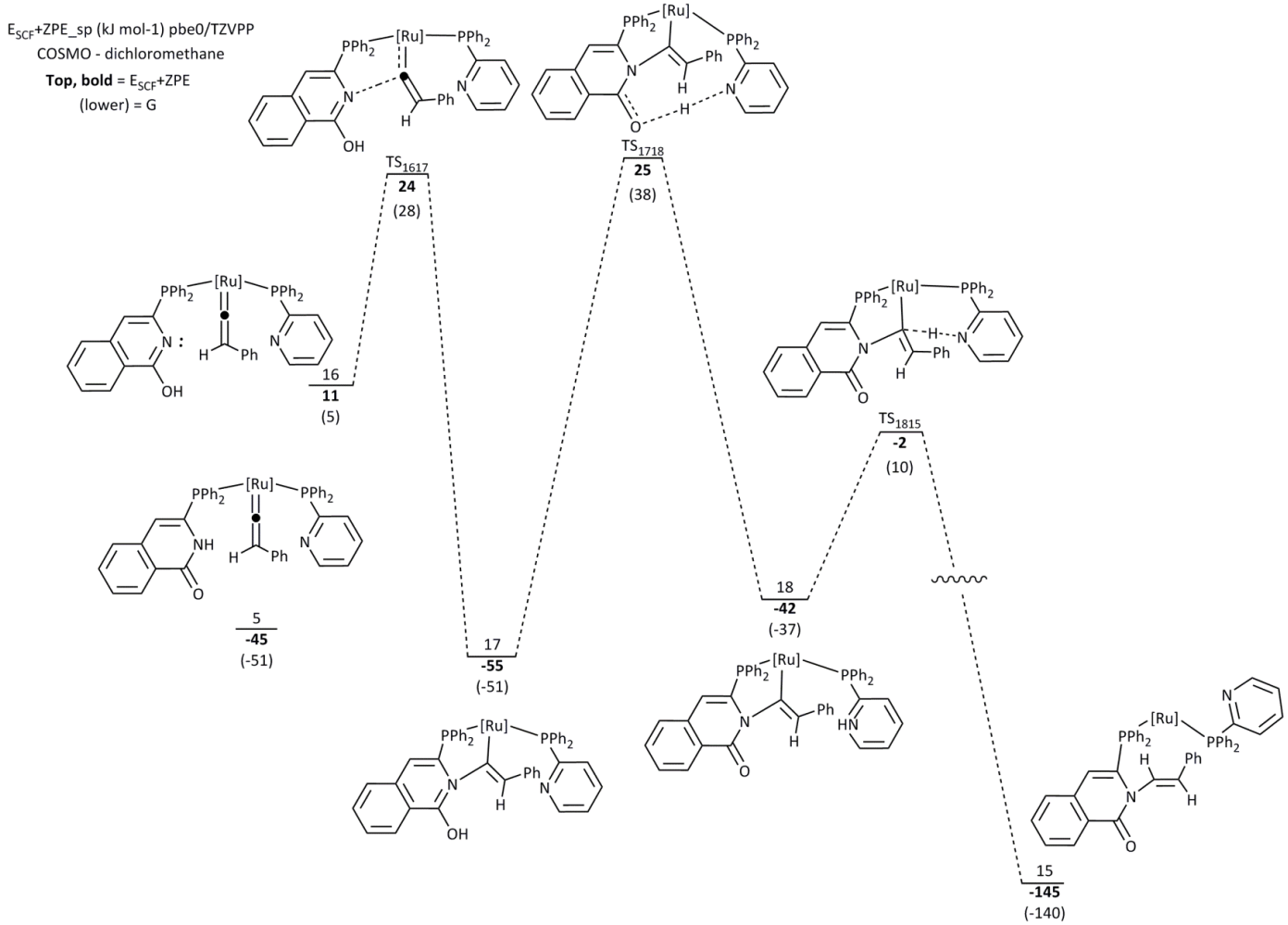
PES for the catalytic reaction at the (RI-)PBE0/def2-TZVPP//BP86/SV(P) level (acetone solvation, no dispersion corrections)



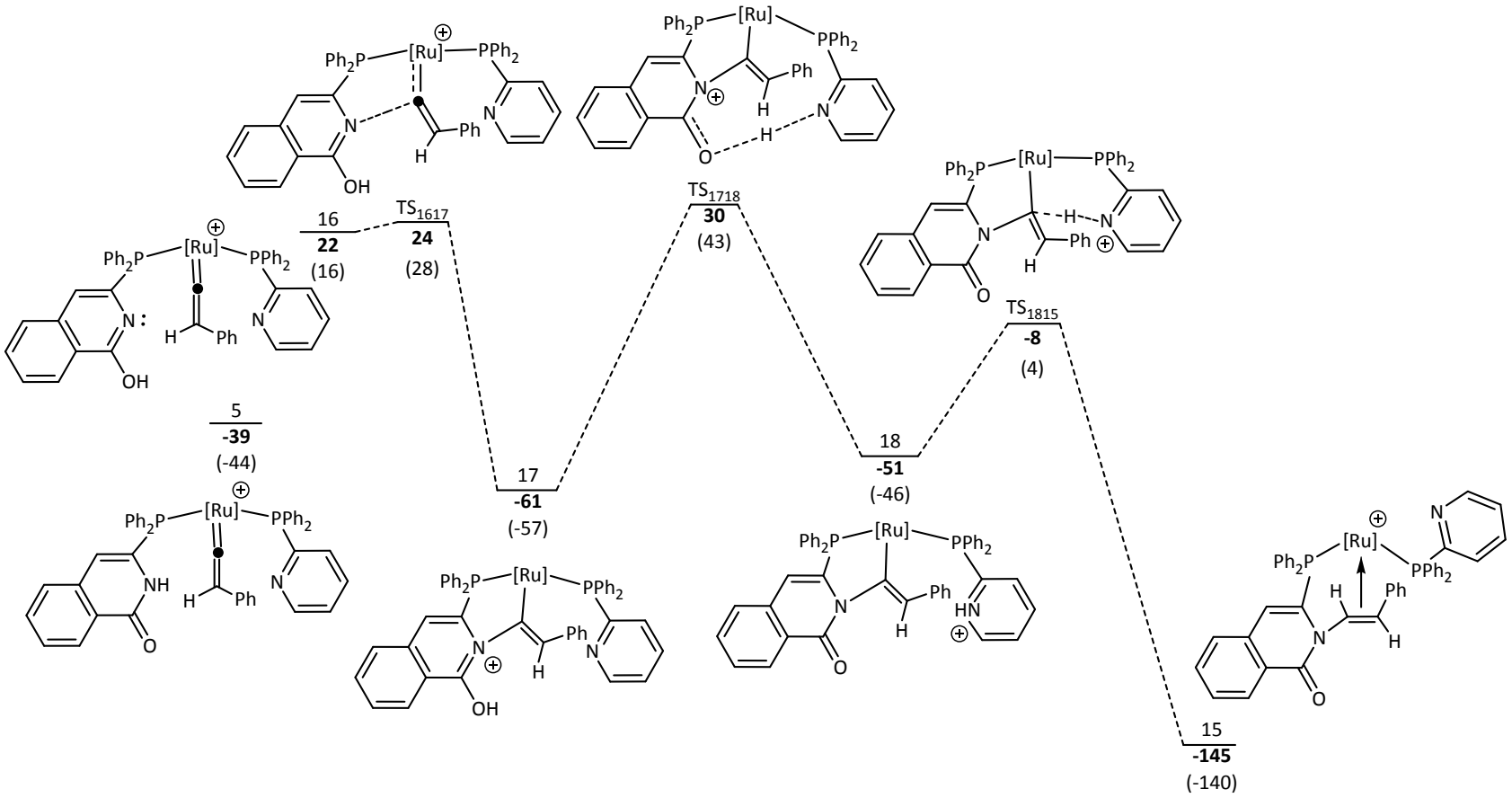
PES for the catalytic reaction at the (RI-)PBE0-D3/def2-TZVPP//BP86/SV(P) level (acetone solvation, with dispersion correction)



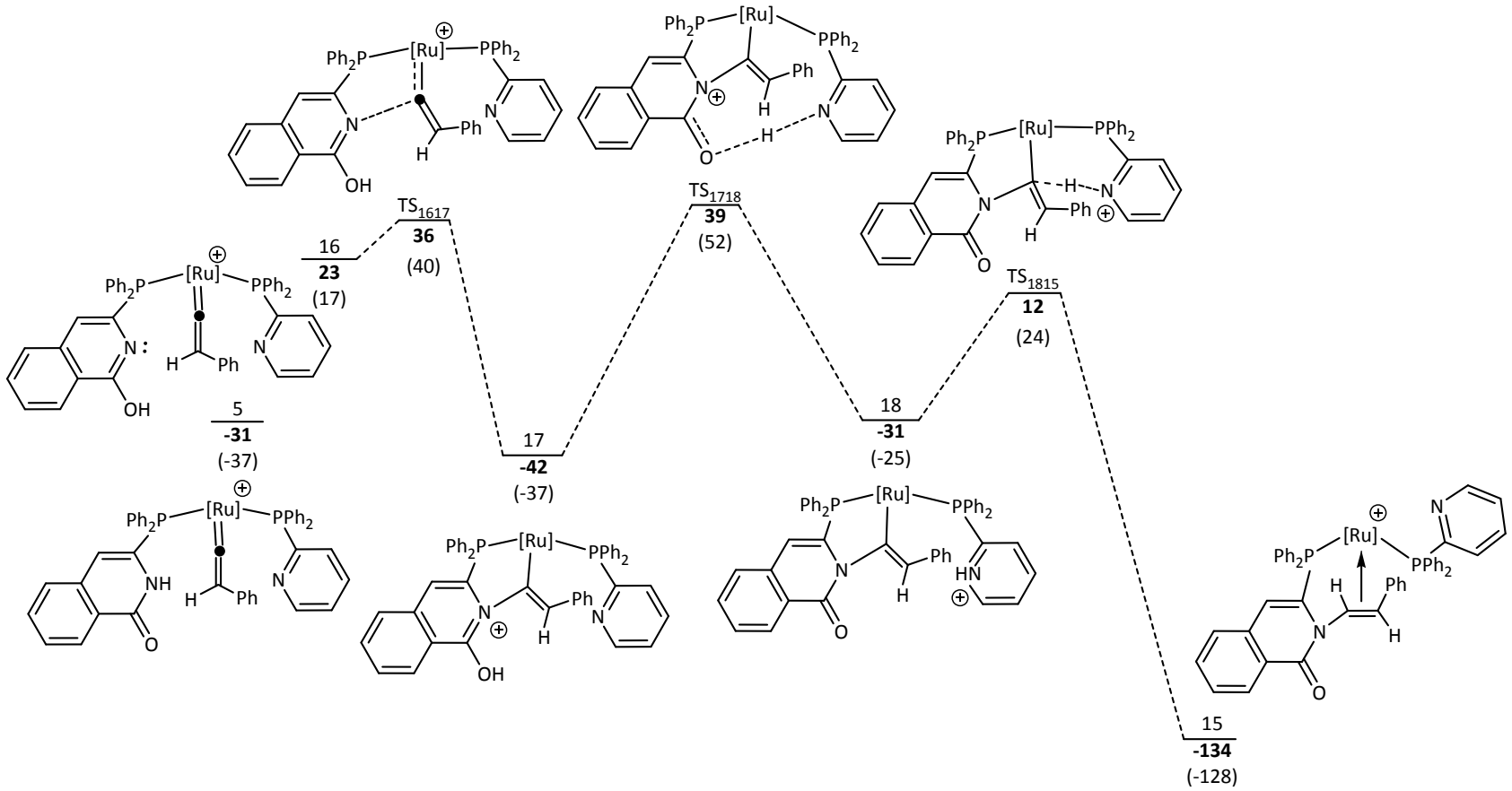
PES for the deactivation pathway at the (RI-)PBE0/def2-TZVPP//BP86/SV(P) level (CH_2Cl_2 solvation, no dispersion corrections)



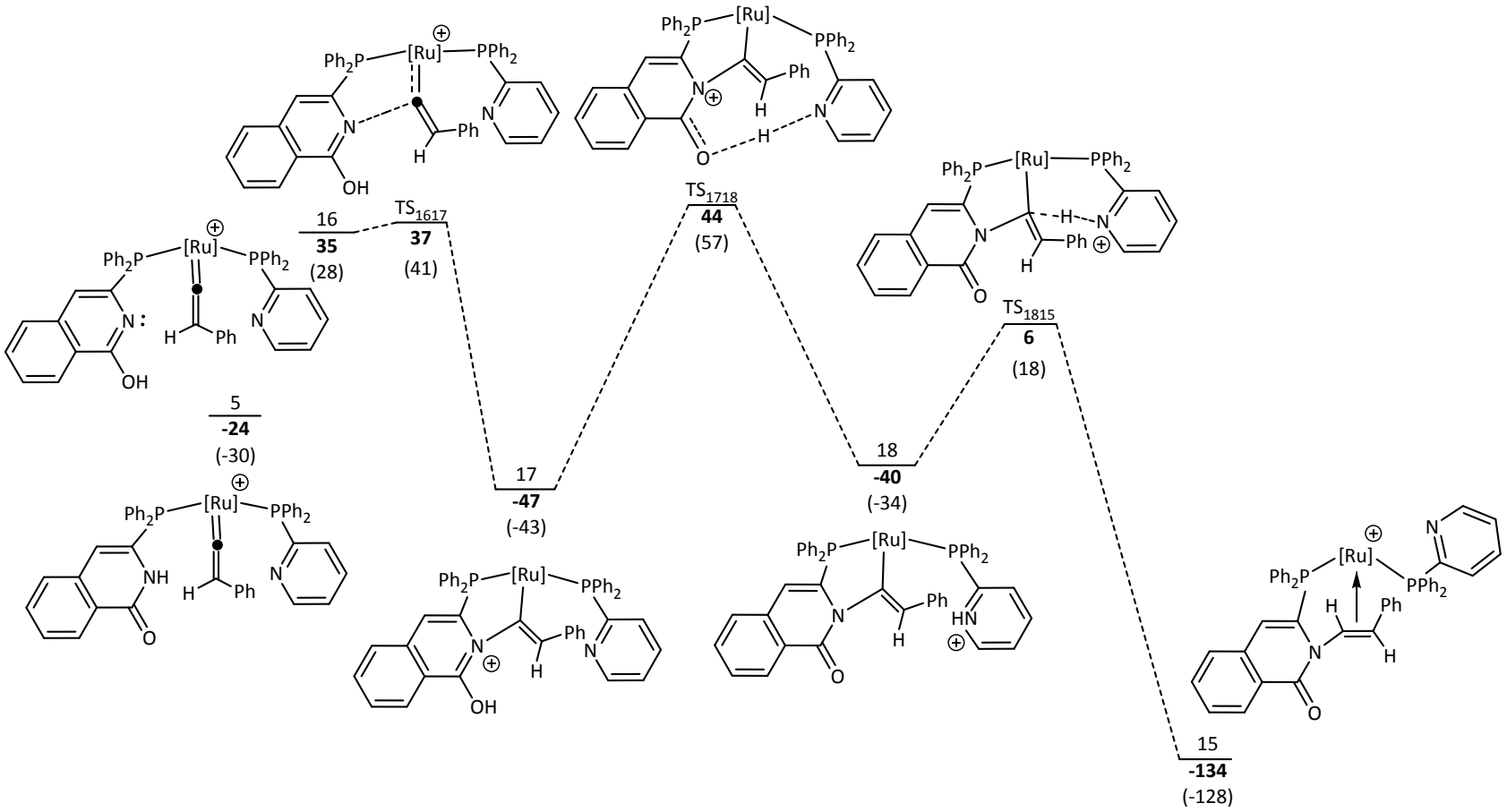
PES for the deactivation pathway at the (RI-)PBE0-D3/def2-TZVPP//BP86/SV(P) level (CH_2Cl_2 solvation, with dispersion corrections)



PES for the deactivation pathway at the (RI-)PBE0/def2-TZVPP//BP86/SV(P) level (acetone solvation, no dispersion corrections)



PES for the deactivation pathway at the (RI-)PBE0-D3/def2-TZVPP//BP86/SV(P) level (acetone solvation, with dispersion correction)



SCF energies, ZPEs, XYZ coordinates and vibrational frequencies

./3/a

BP86/SV(P) energy (au): -3254.4980909560

PBE0/def2-TZVPP energy (au): -3253.995934192
cosmo_dcm Total energy + OC corr. = -3254.0443098511
cosmo_acetone Total energy + OC corr. = -3254.0497818941

Zero point energy (au): 0.8886301
Entropy (kJ mol^-1): 1.40132
Chemical potential (kJ mol^-1): 2074.51

XYZ coordinates:

114

C	-2.18296	2.46065	3.02189
C	-0.87307	2.96188	3.36459
C	-2.54854	2.98661	1.74788
C	-0.43038	3.79588	2.28048
C	-1.45076	3.80825	1.27072
H	-2.79286	1.79159	3.64388
H	-0.34593	2.78601	4.31064
H	-3.50395	2.83119	1.23086
H	0.51594	4.35137	2.24562
H	-1.45648	4.41805	0.36054
Ru	-0.69753	1.71032	1.47867
C	-1.24522	-1.37911	2.65601
C	-0.89352	-0.24753	2.24061
C	-2.69583	2.21789	-1.38716
P	-1.61781	0.91637	-0.58998
C	-2.80097	-0.50922	-0.42130
C	-0.62434	0.37613	-2.08038
C	-0.95275	0.76032	-3.36270
N	0.37587	-0.55955	-1.88157
C	-0.25025	0.21283	-4.49524
C	0.76762	-0.76326	-4.27409
C	1.08205	-1.19042	-2.90434
O	1.92789	-2.06880	-2.63346
C	2.25554	1.91715	-0.70983
P	1.62829	1.50431	0.97644
C	2.68073	2.59992	2.05841
C	2.30967	-0.20489	1.34511
C	3.12237	-0.45804	2.46163
N	1.87239	-1.18736	0.52868
C	3.43632	-1.79967	2.75818
C	2.98052	-2.82338	1.93184
C	2.23150	-2.47044	0.77611
N	1.86494	-3.39935	-0.19649
C	1.71567	-4.77377	0.00236
C	1.51612	-5.61947	-1.27938
O	1.73693	-5.26827	1.12940
H	-1.77180	1.46767	-3.54220
H	0.74410	-0.79151	-0.91573

H	3.50862	0.35634	3.08804
H	4.05842	-2.03860	3.63641
H	3.20310	-3.87837	2.13245
H	1.79345	-2.98569	-1.16005
C	1.46546	-1.32884	-5.36570
C	-0.54677	0.59714	-5.83141
H	-0.01349	0.35977	2.68869
C	4.25911	4.23943	3.74822
C	4.44171	4.27212	2.35703
C	3.66375	3.45558	1.51593
C	2.50363	2.57668	3.46254
C	3.29018	3.38251	4.30048
H	4.87194	4.87889	4.40409
H	5.20187	4.93594	1.91384
H	3.83182	3.49041	0.42929
H	1.75111	1.90958	3.91293
H	3.14357	3.34258	5.39237
C	3.27965	2.76101	-3.20127
C	2.26562	3.50345	-2.57041
C	1.75139	3.07827	-1.33502
C	3.28274	1.18331	-1.34082
C	3.78355	1.60250	-2.58582
H	3.67819	3.08744	-4.17552
H	1.87162	4.41728	-3.04449
H	0.96225	3.66399	-0.83483
H	3.69227	0.27547	-0.87260
H	4.57668	1.01545	-3.07631
C	-4.28450	4.23559	-2.58552
C	-4.88327	3.07587	-2.06963
C	-4.09605	2.06881	-1.48023
C	-2.10107	3.38834	-1.91416
C	-2.88767	4.38541	-2.51260
H	-4.90285	5.02007	-3.05122
H	-5.97555	2.94165	-2.13180
H	-4.58467	1.15882	-1.09960
H	-1.00681	3.50861	-1.88392
H	-2.40564	5.28540	-2.92882
C	-4.75606	-2.54084	-0.18901
C	-4.64366	-1.55261	0.80387
C	-3.66576	-0.55121	0.69479
C	-2.92417	-1.50223	-1.41688
C	-3.89141	-2.51504	-1.29480
H	-5.51701	-3.33297	-0.09820
H	-5.31703	-1.56532	1.67630
H	-3.57139	0.20562	1.48858
H	-2.27045	-1.49269	-2.30249
H	-3.97016	-3.28698	-2.07770
C	0.24415	-5.15004	-2.02952
C	1.35606	-7.09383	-0.86226
C	2.75825	-5.46235	-2.19409
H	2.87779	-4.42073	-2.56097
H	2.65180	-6.12316	-3.08302
H	3.68907	-5.76101	-1.66277
H	1.22479	-7.72744	-1.76656
H	0.47301	-7.23615	-0.20376
H	2.24617	-7.45586	-0.30622
H	0.06409	-5.81206	-2.90555
H	0.34560	-4.11268	-2.41416

H	-0.65396	-5.20118	-1.37480
C	1.16238	-0.93176	-6.66955
H	2.24196	-2.08086	-5.15816
C	0.15137	0.03276	-6.89969
H	-1.33553	1.34551	-6.01436
H	1.70544	-1.37101	-7.52190
H	-0.08754	0.33834	-7.93159
C	-1.64312	-2.64604	3.15301
C	-2.41618	-5.16444	4.18092
C	-3.13638	-4.00808	4.53925
C	-2.75553	-2.75882	4.03777
C	-0.92414	-3.82450	2.80241
C	-1.30977	-5.06753	3.31665
H	-2.71717	-6.14544	4.58382
H	-3.99862	-4.08471	5.22167
H	-3.30988	-1.85072	4.32336
H	-0.04800	-3.75995	2.13978
H	-0.73216	-5.96372	3.03915

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	11.43	0.22865	YES	YES
8	a	15.97	0.25110	YES	YES
9	a	20.14	0.06514	YES	YES
10	a	20.38	0.25104	YES	YES
11	a	23.19	0.13992	YES	YES
12	a	26.32	0.16039	YES	YES
13	a	29.47	0.33267	YES	YES
14	a	32.82	0.17819	YES	YES
15	a	38.02	0.16689	YES	YES
16	a	41.82	0.01398	YES	YES
17	a	44.79	0.08803	YES	YES
18	a	49.30	0.04775	YES	YES
19	a	50.02	0.19156	YES	YES
20	a	53.47	0.30239	YES	YES
21	a	59.80	2.91952	YES	YES
22	a	62.10	0.11512	YES	YES
23	a	62.66	0.31463	YES	YES
24	a	65.74	0.22937	YES	YES
25	a	69.46	0.98148	YES	YES
26	a	75.52	0.20481	YES	YES
27	a	81.31	0.16458	YES	YES
28	a	84.32	0.21000	YES	YES
29	a	88.45	2.80838	YES	YES
30	a	91.29	0.12068	YES	YES
31	a	96.16	0.10822	YES	YES
32	a	97.51	0.35549	YES	YES

33	a	104.10	0.87511	YES	YES
34	a	111.81	1.21597	YES	YES
35	a	115.26	0.25799	YES	YES
36	a	124.36	0.80640	YES	YES
37	a	126.41	3.88154	YES	YES
38	a	140.42	2.16520	YES	YES
39	a	163.60	0.86691	YES	YES
40	a	167.69	0.78490	YES	YES
41	a	171.28	1.74950	YES	YES
42	a	181.84	2.19403	YES	YES
43	a	184.55	3.23110	YES	YES
44	a	192.86	0.12801	YES	YES
45	a	198.89	0.32528	YES	YES
46	a	208.90	0.59017	YES	YES
47	a	211.79	0.87734	YES	YES
48	a	216.57	4.16039	YES	YES
49	a	224.20	2.66894	YES	YES
50	a	228.66	0.73704	YES	YES

./3/b

BP86/SV(P) energy (au): -3254.5013010180

PBE0/def2-TZVPP energy (au): -3253.997156759
cosmo_dcm Total energy + OC corr. = -3254.0467275606
cosmo_acetone Total energy + OC corr. = -3254.0522996377

Zero point energy (au): 0.8884867
Entropy (kJ mol^-1): 1.42718
Chemical potential (kJ mol^-1): 2067.63

XYZ coordinates:

114

C	-1.83421	2.39561	2.89983
C	-0.45737	2.63924	3.26849
C	-2.12134	3.11559	1.70292
C	0.10159	3.51258	2.27655
C	-0.91328	3.80550	1.30210
H	-2.54370	1.77361	3.46181
H	0.04213	2.27202	4.17212
H	-3.09079	3.16765	1.19123
H	1.12500	3.91072	2.27799
H	-0.82242	4.49943	0.45778
Ru	-0.49042	1.59893	1.26418
C	-1.11995	-0.87316	3.25184
C	-0.80441	-0.30524	2.16014
C	-2.35680	2.60282	-1.54148
P	-1.47947	1.11858	-0.83173
C	-2.84401	-0.15128	-0.75263
C	-0.56074	0.51158	-2.33693
C	-0.71072	1.03932	-3.59952
N	0.18393	-0.64217	-2.16085
C	-0.08608	0.40334	-4.73372
C	0.63744	-0.81392	-4.53966
C	0.74995	-1.39028	-3.19158
O	1.30564	-2.47716	-2.93740
C	2.52939	1.43583	-0.77897
P	1.75601	1.00541	0.84505
C	2.91451	1.81184	2.06024
C	2.17635	-0.81475	1.06507
C	3.12078	-1.25260	2.00563
N	1.45701	-1.67400	0.30675
C	3.26967	-2.64164	2.19755
C	2.52797	-3.53679	1.43271
C	1.65937	-3.01115	0.43726
N	1.00153	-3.81689	-0.48752
C	0.71358	-5.17990	-0.32926
C	0.13347	-5.88419	-1.58160
O	0.91303	-5.76528	0.73065
H	-1.33364	1.92845	-3.76135
H	0.43623	-0.99268	-1.20025

H	3.72850	-0.54157	2.58051
H	3.98900	-3.02024	2.94279
H	2.60796	-4.62367	1.55446
H	0.89796	-3.36533	-1.42678
C	1.23626	-1.47232	-5.63740
C	-0.18871	0.92992	-6.04971
H	-0.51009	-0.86947	1.24466
C	4.60092	3.04366	3.97297
C	4.80685	3.26342	2.60213
C	3.97352	2.64836	1.64900
C	2.71355	1.59718	3.44492
C	3.55383	2.20201	4.39226
H	5.25667	3.52455	4.71690
H	5.62798	3.91621	2.26327
H	4.15996	2.82377	0.57838
H	1.90030	0.93359	3.78118
H	3.39087	2.01654	5.46676
C	3.77577	2.25991	-3.17426
C	2.82845	3.09194	-2.55229
C	2.20187	2.67668	-1.36623
C	3.48869	0.60948	-1.40279
C	4.10117	1.01956	-2.59946
H	4.26155	2.57981	-4.11043
H	2.57258	4.06791	-2.99646
H	1.45711	3.32527	-0.87535
H	3.76329	-0.36111	-0.96065
H	4.84206	0.36298	-3.08381
C	-3.64529	4.90263	-2.57445
C	-4.40110	3.79560	-2.15754
C	-3.76307	2.64876	-1.64941
C	-1.60307	3.72209	-1.96470
C	-2.24229	4.86013	-2.48276
H	-4.14700	5.79796	-2.97626
H	-5.50054	3.81538	-2.23297
H	-4.37198	1.78521	-1.33995
H	-0.50326	3.69593	-1.91097
H	-1.63984	5.72022	-2.81877
C	-5.02061	-1.95367	-0.60710
C	-4.69430	-1.15042	0.49849
C	-3.60804	-0.26188	0.43012
C	-3.18473	-0.95645	-1.86272
C	-4.26165	-1.85558	-1.78565
H	-5.86741	-2.65695	-0.55046
H	-5.28903	-1.21747	1.42445
H	-3.34729	0.35523	1.30385
H	-2.61609	-0.87955	-2.80279
H	-4.51153	-2.48028	-2.65862
C	-1.10361	-5.12081	-2.11467
C	-0.27260	-7.31459	-1.17873
C	1.23407	-5.93771	-2.67364
H	1.52892	-4.92408	-3.02012
H	0.85529	-6.50144	-3.55543
H	2.14095	-6.46323	-2.30089
H	-0.67315	-7.85595	-2.06381
H	-1.05423	-7.30737	-0.38886
H	0.59379	-7.88218	-0.77956
H	-1.54994	-5.68304	-2.96483
H	-0.84316	-4.10831	-2.49137

H	-1.88468	-5.01358	-1.32950
C	1.12818	-0.93227	-6.92068
H	1.78270	-2.40986	-5.45174
C	0.41212	0.27191	-7.12394
H	-0.75051	1.86444	-6.21280
H	1.59611	-1.44401	-7.77714
H	0.32546	0.69153	-8.13971
C	-1.48349	-1.47357	4.47303
C	-2.20929	-2.68572	6.92082
C	-0.85504	-2.40157	6.65446
C	-0.48925	-1.80327	5.44571
C	-2.85082	-1.77633	4.75875
C	-3.20327	-2.37365	5.97196
H	-2.49257	-3.15828	7.87551
H	-0.08302	-2.65505	7.39873
H	0.56708	-1.58549	5.22335
H	-3.61841	-1.53781	4.00600
H	-4.25955	-2.60464	6.18476

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	7.37	0.26118	YES	YES
8	a	10.89	0.43551	YES	YES
9	a	17.27	0.19290	YES	YES
10	a	18.61	0.25228	YES	YES
11	a	22.24	0.02137	YES	YES
12	a	26.36	0.13515	YES	YES
13	a	29.07	0.08701	YES	YES
14	a	30.28	0.05606	YES	YES
15	a	33.10	0.58418	YES	YES
16	a	38.23	0.12883	YES	YES
17	a	43.41	0.03075	YES	YES
18	a	45.02	0.10669	YES	YES
19	a	49.06	0.34711	YES	YES
20	a	49.56	0.61765	YES	YES
21	a	53.63	1.29514	YES	YES
22	a	57.32	0.34958	YES	YES
23	a	58.03	0.12884	YES	YES
24	a	63.28	0.50755	YES	YES
25	a	65.78	0.34082	YES	YES
26	a	66.21	0.66902	YES	YES
27	a	77.93	2.10702	YES	YES
28	a	80.53	0.37520	YES	YES
29	a	85.48	1.78608	YES	YES
30	a	87.35	1.55432	YES	YES
31	a	89.71	2.69352	YES	YES
32	a	94.19	7.61261	YES	YES

33	a	97.32	1.82798	YES	YES
34	a	104.82	0.86451	YES	YES
35	a	112.91	0.90808	YES	YES
36	a	119.86	1.69081	YES	YES
37	a	125.81	1.28715	YES	YES
38	a	134.67	1.54635	YES	YES
39	a	155.13	1.43107	YES	YES
40	a	164.87	1.55689	YES	YES
41	a	168.84	0.65935	YES	YES
42	a	178.20	4.01942	YES	YES
43	a	189.07	0.63236	YES	YES
44	a	193.62	7.74911	YES	YES
45	a	198.41	0.88086	YES	YES
46	a	205.33	6.12369	YES	YES
47	a	210.21	1.32843	YES	YES
48	a	212.63	3.55284	YES	YES
49	a	218.69	0.53425	YES	YES
50	a	224.79	1.69106	YES	YES

./3/hbond/a

BP86/SV(P) energy (au): -3254.5013223690

PBE0/def2-TZVPP energy (au): -3253.997229563
cosmo_dcm Total energy + OC corr. = -3254.0464305370
cosmo_acetone Total energy + OC corr. = -3254.0519479873

Zero point energy (au): 0.8888298
Entropy (kJ mol^-1): 1.42639
Chemical potential (kJ mol^-1): 2068.54

XYZ coordinates:

114

C	-1.92255	2.70006	2.49917
C	-0.56982	3.13643	2.76182
C	-2.31365	3.17066	1.20964
C	-0.12847	3.87232	1.61044
C	-1.19317	3.89283	0.64445
H	-2.54967	2.12026	3.18959
H	-0.01230	2.98401	3.69291
H	-3.29765	3.04347	0.74010
H	0.84820	4.36215	1.49974
H	-1.19426	4.42910	-0.31254
Ru	-0.54930	1.76636	0.96569
C	-1.08568	-0.44672	3.25609
C	-0.70292	-0.00339	2.12786
C	-2.46433	2.15358	-1.95546
P	-1.53824	0.86467	-0.98001
C	-2.86575	-0.40736	-0.65181
C	-0.61003	-0.00258	-2.34537
C	-0.81339	0.22572	-3.68738
N	0.19300	-1.05698	-1.94532
C	-0.18996	-0.62337	-4.67327
C	0.59046	-1.74008	-4.23931
C	0.76685	-1.99440	-2.80196
O	1.38184	-2.97106	-2.33015
C	2.40495	1.52162	-1.15865
P	1.73504	1.33486	0.55692
C	2.84080	2.46527	1.54341
C	2.36800	-0.35319	1.09430
C	3.44422	-0.49708	1.98283
N	1.66648	-1.41374	0.62988
C	3.75389	-1.79241	2.44518
C	3.02934	-2.88978	1.98828
C	2.01264	-2.66885	1.01954
N	1.34205	-3.70830	0.38178
C	1.19483	-5.01237	0.87505
C	0.56691	-6.02720	-0.11306
O	1.54522	-5.31788	2.01051
H	-1.48235	1.03065	-4.01875
H	0.48954	-1.16654	-0.94384

H	4.02854	0.36995	2.31713
H	4.57977	-1.93930	3.16084
H	3.23088	-3.91181	2.33118
H	1.11778	-3.50008	-0.61882
C	1.18649	-2.60612	-5.18409
C	-0.35202	-0.40970	-6.06897
H	-0.18851	-0.66785	1.38627
C	4.45593	4.16894	3.12765
C	4.59001	4.16420	1.73068
C	3.79283	3.31401	0.94101
C	2.71408	2.47532	2.95306
C	3.51872	3.31496	3.73835
H	5.08415	4.83295	3.74338
H	5.32761	4.82201	1.24266
H	3.92427	3.31475	-0.15158
H	1.99172	1.80035	3.44068
H	3.41549	3.30261	4.83599
C	3.46248	1.97377	-3.73851
C	2.56162	2.89534	-3.17608
C	2.02744	2.66410	-1.89834
C	3.31684	0.60627	-1.72515
C	3.83449	0.83011	-3.01299
H	3.87581	2.14888	-4.74509
H	2.27111	3.79828	-3.73820
H	1.32244	3.38840	-1.45615
H	3.62753	-0.29115	-1.16758
H	4.53849	0.10283	-3.44901
C	-3.82302	4.17429	-3.40046
C	-4.54584	3.15963	-2.75367
C	-3.87294	2.15063	-2.03975
C	-1.74373	3.18035	-2.60897
C	-2.41794	4.17814	-3.33110
H	-4.35205	4.96068	-3.96295
H	-5.64668	3.14310	-2.80790
H	-4.45672	1.35472	-1.55188
H	-0.64308	3.18773	-2.57021
H	-1.84141	4.96475	-3.84528
C	-4.99833	-2.20532	-0.16562
C	-4.68188	-1.21281	0.77771
C	-3.61521	-0.32819	0.54227
C	-3.19573	-1.40366	-1.59799
C	-4.24967	-2.29976	-1.35119
H	-5.82966	-2.90434	0.02174
H	-5.27118	-1.12494	1.70552
H	-3.35928	0.43374	1.29378
H	-2.63671	-1.47964	-2.54323
H	-4.49031	-3.07370	-2.09808
C	-0.76181	-5.48345	-0.69244
C	0.30180	-7.33704	0.65309
C	1.57876	-6.28335	-1.26115
H	1.77287	-5.36664	-1.85862
H	1.17289	-7.05846	-1.94932
H	2.54666	-6.65954	-0.86313
H	-0.12518	-8.09739	-0.03716
H	-0.41424	-7.17986	1.48819
H	1.23647	-7.74312	1.09206
H	-1.23051	-6.25946	-1.33768
H	-0.61030	-4.58172	-1.32448

H	-1.48508	-5.23202	0.11456
C	1.01889	-2.37202	-6.55056
H	1.77805	-3.45788	-4.81434
C	0.24552	-1.27091	-6.99049
H	-0.95792	0.44368	-6.41563
H	1.48446	-3.04547	-7.28809
H	0.11184	-1.09400	-8.07039
C	-1.52027	-0.92705	4.50684
C	-2.38888	-1.90618	7.01102
C	-1.09975	-1.35096	6.88504
C	-0.66294	-0.86727	5.64896
C	-2.82245	-1.49786	4.65357
C	-3.24602	-1.98015	5.89486
H	-2.72706	-2.28925	7.98769
H	-0.43320	-1.30326	7.76113
H	0.34565	-0.43952	5.53752
H	-3.47770	-1.56043	3.77081
H	-4.24965	-2.42277	5.99982

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	5.83	0.29005	YES	YES
8	a	11.89	0.15546	YES	YES
9	a	16.82	0.33284	YES	YES
10	a	17.77	0.05805	YES	YES
11	a	20.72	0.10427	YES	YES
12	a	25.53	0.10152	YES	YES
13	a	30.92	0.30415	YES	YES
14	a	34.72	0.41198	YES	YES
15	a	35.97	0.57603	YES	YES
16	a	38.05	0.05078	YES	YES
17	a	40.43	0.47511	YES	YES
18	a	44.05	0.18617	YES	YES
19	a	48.83	0.19299	YES	YES
20	a	53.34	0.65743	YES	YES
21	a	55.31	0.17482	YES	YES
22	a	57.82	0.59288	YES	YES
23	a	60.84	0.33527	YES	YES
24	a	63.04	0.14124	YES	YES
25	a	64.71	0.02334	YES	YES
26	a	67.85	0.54868	YES	YES
27	a	77.71	0.15613	YES	YES
28	a	78.89	1.66036	YES	YES
29	a	82.62	0.99264	YES	YES
30	a	87.41	1.72843	YES	YES
31	a	89.46	0.62751	YES	YES
32	a	95.22	6.98990	YES	YES

33	a	97.15	2.03764	YES	YES
34	a	104.86	0.82654	YES	YES
35	a	112.74	0.96447	YES	YES
36	a	121.76	0.72738	YES	YES
37	a	125.92	1.20908	YES	YES
38	a	135.55	1.01113	YES	YES
39	a	155.21	1.16637	YES	YES
40	a	164.70	0.97843	YES	YES
41	a	169.19	0.55811	YES	YES
42	a	176.65	3.17113	YES	YES
43	a	188.39	2.62634	YES	YES
44	a	195.96	2.53008	YES	YES
45	a	199.31	6.97868	YES	YES
46	a	207.80	2.92838	YES	YES
47	a	208.00	1.19469	YES	YES
48	a	212.01	4.32320	YES	YES
49	a	218.79	0.42452	YES	YES
50	a	223.13	2.17033	YES	YES

./3/hbond/b

BP86/SV(P) energy (au): -3254.4926937690

PBE0/def2-TZVPP energy (au): -3253.990594902
cosmo_dcm
cosmo_acetone Total energy + OC corr. = -3254.0432995137 Total energy + OC corr. = -3254.0432995137

Zero point energy (au): 0.8896829
Entropy (kJ mol^-1): 1.39334
Chemical potential (kJ mol^-1): 2079.79

XYZ coordinates:

114

C	-2.44113	3.87812	1.08663
C	-1.44572	3.91998	2.13512
C	-1.80276	4.14577	-0.15829
C	-0.18678	4.22108	1.51263
C	-0.39579	4.36074	0.09910
H	-3.51654	3.69757	1.22317
H	-1.62741	3.81943	3.21157
H	-2.29539	4.21961	-1.13581
H	0.76634	4.36409	2.03787
H	0.35041	4.67105	-0.64107
Ru	-0.89858	2.24492	0.72220
C	-2.54873	-0.26699	1.63751
C	-2.34897	0.99463	1.70351
C	-0.82704	2.59390	-2.75324
P	-0.87172	1.25891	-1.43631
C	-2.42866	0.35003	-1.91846
C	0.44666	0.12347	-2.14123
C	0.91729	0.27441	-3.42854
N	0.88935	-0.94561	-1.37842
C	1.88470	-0.63924	-3.97731
C	2.33018	-1.73318	-3.17854
C	1.78525	-1.91774	-1.82735
O	2.08238	-2.88463	-1.09739
C	2.52794	1.07499	0.83445
P	0.92615	1.16526	1.76852
C	1.42556	2.11245	3.29796
C	0.80771	-0.58275	2.46613
C	0.95181	-0.83262	3.84194
N	0.64420	-1.57167	1.56062
C	0.91235	-2.16933	4.28375
C	0.75014	-3.19902	3.36256
C	0.63875	-2.86153	1.98627
N	0.57033	-3.83367	0.99024
C	0.16152	-5.15776	1.15987
C	0.36726	-6.08364	-0.06693
O	-0.32572	-5.56264	2.21480
H	0.55003	1.09103	-4.06234

H	0.61602	-1.06752	-0.36872
H	1.11554	-0.01831	4.55870
H	1.03347	-2.40023	5.35519
H	0.72391	-4.25362	3.66156
H	1.01156	-3.52642	0.08902
C	3.27898	-2.64967	-3.68694
C	2.40944	-0.49411	-5.29043
H	-3.02604	1.64119	2.29451
C	2.09659	3.56347	5.63652
C	3.05295	3.36298	4.62893
C	2.72429	2.63630	3.46886
C	0.46665	2.32298	4.31785
C	0.80164	3.03526	5.48045
H	2.35831	4.12881	6.54564
H	4.07143	3.76874	4.74352
H	3.49130	2.47949	2.69527
H	-0.54946	1.90892	4.20745
H	0.04665	3.17973	6.27086
C	5.00669	1.11159	-0.52509
C	4.06003	2.12386	-0.75942
C	2.82614	2.09937	-0.08878
C	3.48910	0.06801	1.07337
C	4.71722	0.08533	0.39036
H	5.97193	1.12252	-1.05710
H	4.28231	2.93437	-1.47270
H	2.07889	2.88749	-0.27300
H	3.28672	-0.73933	1.79306
H	5.45368	-0.71272	0.57847
C	-0.70848	4.67492	-4.67693
C	-1.88000	3.91799	-4.52298
C	-1.93891	2.87984	-3.57354
C	0.35146	3.35847	-2.92201
C	0.41178	4.38569	-3.87683
H	-0.66263	5.48356	-5.42436
H	-2.76032	4.12557	-5.15320
H	-2.86438	2.29040	-3.48483
H	1.24570	3.12652	-2.32205
H	1.34365	4.96187	-4.00033
C	-4.86703	-0.80164	-2.77894
C	-4.87621	0.27950	-1.87909
C	-3.66490	0.84146	-1.44156
C	-2.42843	-0.73813	-2.81747
C	-3.64117	-1.31373	-3.23745
H	-5.81627	-1.24581	-3.12089
H	-5.83253	0.68380	-1.50856
H	-3.67560	1.67693	-0.72295
H	-1.47929	-1.13711	-3.20824
H	-3.62427	-2.16365	-3.93926
C	-0.30355	-5.48236	-1.32624
C	-0.26509	-7.45164	0.25297
C	1.89017	-6.25382	-0.30832
H	2.37715	-5.29243	-0.57836
H	2.05713	-6.96733	-1.14597
H	2.39374	-6.66785	0.59303
H	-0.11036	-8.14645	-0.60142
H	-1.35720	-7.36144	0.43674
H	0.18639	-7.90266	1.16079
H	-0.21620	-6.19924	-2.17275

H	0.17909	-4.53473	-1.64670
H	-1.38603	-5.28916	-1.15529
C	3.78648	-2.48503	-4.97700
H	3.59968	-3.48398	-3.04444
C	3.34692	-1.40409	-5.77946
H	2.06806	0.34654	-5.91714
H	4.52760	-3.19729	-5.37440
H	3.74862	-1.28136	-6.79870
C	-2.83186	-1.64183	1.63970
C	-3.58972	-4.35376	1.79999
C	-3.90045	-3.60687	0.64558
C	-3.53652	-2.26133	0.56050
C	-2.51747	-2.41891	2.79944
C	-2.90470	-3.75744	2.87695
H	-3.88074	-5.41490	1.86244
H	-4.44144	-4.08130	-0.18881
H	-3.78968	-1.66457	-0.32732
H	-1.97991	-1.93894	3.63098
H	-2.65997	-4.35384	3.76869

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	8.24	0.47879	YES	YES
8	a	14.70	0.07464	YES	YES
9	a	19.34	0.01935	YES	YES
10	a	24.20	0.07445	YES	YES
11	a	30.24	0.84362	YES	YES
12	a	31.94	0.68943	YES	YES
13	a	35.01	0.86125	YES	YES
14	a	40.12	0.53106	YES	YES
15	a	43.24	0.10405	YES	YES
16	a	45.76	0.19836	YES	YES
17	a	49.15	0.53690	YES	YES
18	a	51.77	1.82112	YES	YES
19	a	55.82	0.71558	YES	YES
20	a	58.83	1.14301	YES	YES
21	a	62.98	0.54755	YES	YES
22	a	63.22	0.21831	YES	YES
23	a	66.53	0.42689	YES	YES
24	a	69.58	1.24680	YES	YES
25	a	75.39	2.75880	YES	YES
26	a	78.73	3.07453	YES	YES
27	a	85.55	1.48424	YES	YES
28	a	87.88	0.29498	YES	YES
29	a	91.44	1.70656	YES	YES
30	a	94.69	0.15428	YES	YES
31	a	97.08	0.75862	YES	YES

32	a	99.07	0.22426	YES	YES
33	a	104.09	8.88855	YES	YES
34	a	105.72	1.11109	YES	YES
35	a	113.62	1.03438	YES	YES
36	a	122.78	0.09252	YES	YES
37	a	125.15	2.01860	YES	YES
38	a	135.83	0.11034	YES	YES
39	a	153.77	4.50318	YES	YES
40	a	162.18	0.62640	YES	YES
41	a	165.64	0.36291	YES	YES
42	a	176.75	0.63840	YES	YES
43	a	180.75	1.43340	YES	YES
44	a	185.44	1.18892	YES	YES
45	a	193.14	0.01999	YES	YES
46	a	202.35	1.61411	YES	YES
47	a	208.51	0.90219	YES	YES
48	a	216.05	4.57405	YES	YES
49	a	216.47	1.07424	YES	YES
50	a	222.11	3.75611	YES	YES

./2/a

BP86/SV(P) energy (au): -3254.5011345750

PBE0/def2-TZVPP energy (au): -3254.000922851
cosmo_dcm Total energy + OC corr. = -3254.0514559894
cosmo_acetone Total energy + OC corr. = -3254.0572233415

Zero point energy (au): 0.8905734
Entropy (kJ mol^-1): 1.37979
Chemical potential (kJ mol^-1): 2085.35

XYZ coordinates:

114

C	-3.24622	-0.22968	-3.08133
C	-3.68942	-1.39721	-2.36415
C	-3.45760	0.90102	-2.23765
C	-4.19096	-0.97907	-1.08733
C	-4.03405	0.44117	-0.98881
H	-2.83010	-0.21960	-4.09726
H	-3.68414	-2.42184	-2.75887
H	-3.27455	1.94920	-2.50576
H	-4.63841	-1.63211	-0.32769
H	-4.38533	1.08098	-0.17122
Ru	-1.97292	-0.45504	-1.18835
C	-0.15891	-1.16414	-2.44441
C	-0.88007	-2.12253	-2.01415
C	-2.09259	2.95733	-0.24491
P	-0.85223	1.59843	-0.59024
C	0.16266	2.39140	-1.93612
C	0.27100	1.83715	0.88495
C	0.22855	2.98668	1.64403
N	1.28752	0.91821	1.09009
C	1.22594	3.24213	2.65213
C	2.27927	2.29766	2.83715
C	2.31911	1.07895	2.01702
O	3.20678	0.21010	2.12198
C	-1.41075	-0.78346	2.42854
P	-1.45831	-1.66785	0.80353
C	-2.69485	-3.02127	1.18748
C	0.13188	-2.67791	0.72671
C	0.06488	-4.08062	0.69913
N	1.29201	-1.99956	0.58717
C	1.25258	-4.79451	0.44690
C	2.45151	-4.11264	0.27520
C	2.44786	-2.69600	0.41282
N	3.61778	-1.94289	0.41162
C	4.88844	-2.37712	0.00081
C	6.05734	-1.40231	0.29959
O	5.06460	-3.46243	-0.54266
H	-0.54268	3.74469	1.46240
H	1.25302	-0.05170	0.67370

H	-0.88083	-4.61482	0.85427
H	1.23352	-5.89544	0.39105
H	3.39766	-4.62318	0.05959
H	3.52526	-1.03311	0.92097
C	3.28154	2.52673	3.80768
C	1.20951	4.41376	3.45654
H	-0.99974	-3.20740	-1.94291
C	-4.44617	-5.18023	1.76162
C	-3.89840	-4.41478	2.80317
C	-3.02636	-3.34780	2.52169
C	-3.24561	-3.80683	0.14862
C	-4.11085	-4.87636	0.43063
H	-5.12969	-6.01535	1.98492
H	-4.14561	-4.64846	3.85157
H	-2.60065	-2.77398	3.35805
H	-2.98859	-3.59100	-0.89846
H	-4.52480	-5.47633	-0.39619
C	-1.52357	0.47155	4.95794
C	-2.64529	0.49613	4.10934
C	-2.58700	-0.12128	2.85014
C	-0.29507	-0.81904	3.29075
C	-0.35325	-0.18645	4.54626
H	-1.56674	0.95833	5.94573
H	-3.57414	0.99347	4.43407
H	-3.47976	-0.12169	2.20253
H	0.62603	-1.34132	2.99195
H	0.52659	-0.21868	5.20873
C	-3.99444	4.98197	0.31443
C	-3.19917	5.05741	-0.83967
C	-2.24824	4.05675	-1.11640
C	-2.89595	2.89082	0.91662
C	-3.83470	3.89710	1.19608
H	-4.73376	5.76966	0.53229
H	-3.30756	5.90736	-1.53284
H	-1.62246	4.14646	-2.01726
H	-2.76603	2.05756	1.62436
H	-4.44349	3.83552	2.11303
C	1.52324	3.75776	-4.00648
C	0.45184	2.90186	-4.31147
C	-0.21520	2.21490	-3.28479
C	1.24203	3.25269	-1.63866
C	1.91973	3.92517	-2.66927
H	2.05326	4.29031	-4.81288
H	0.13997	2.75493	-5.35795
H	-1.03064	1.52147	-3.53849
H	1.55862	3.41277	-0.59689
H	2.76289	4.59003	-2.42009
C	5.76048	0.01120	-0.25575
C	7.32618	-1.96398	-0.37086
C	6.26205	-1.33789	1.83645
H	8.19036	-1.29834	-0.15533
H	7.20455	-2.03599	-1.47288
H	7.56233	-2.98211	0.00182
H	5.38379	-0.89853	2.35538
H	7.14661	-0.70294	2.06670
H	6.45484	-2.35025	2.25567
H	6.64250	0.66898	-0.09073
H	4.89530	0.49034	0.25024

H	5.56401	-0.02184	-1.35046
C	3.24400	3.68249	4.59066
H	4.08120	1.77928	3.92483
H	0.40207	5.15118	3.31692
C	2.20479	4.62754	4.41117
H	2.18273	5.53996	5.02928
H	4.02501	3.86326	5.34663
C	0.91804	-0.70214	-3.29642
C	3.02334	0.03909	-5.03667
C	3.14412	0.24249	-3.65033
C	2.10349	-0.12106	-2.78509
C	0.80559	-0.90400	-4.69755
C	1.85144	-0.53788	-5.55645
H	3.84597	0.32546	-5.71192
H	4.06297	0.68802	-3.23661
H	2.20971	0.03010	-1.70086
H	-0.10841	-1.36681	-5.10397
H	1.75342	-0.71235	-6.64055

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	11.31	0.01402	YES	YES
8	a	14.25	0.36210	YES	YES
9	a	21.72	0.27350	YES	YES
10	a	25.16	0.25553	YES	YES
11	a	30.41	0.53899	YES	YES
12	a	33.70	0.13412	YES	YES
13	a	37.50	0.00323	YES	YES
14	a	43.24	0.32627	YES	YES
15	a	44.27	0.47835	YES	YES
16	a	46.85	0.11835	YES	YES
17	a	50.79	0.17993	YES	YES
18	a	52.09	0.35960	YES	YES
19	a	55.11	0.42854	YES	YES
20	a	57.03	0.25078	YES	YES
21	a	62.02	0.20559	YES	YES
22	a	65.53	0.00380	YES	YES
23	a	67.81	0.67890	YES	YES
24	a	70.87	0.37515	YES	YES
25	a	72.07	0.22736	YES	YES
26	a	79.58	0.11588	YES	YES
27	a	85.53	0.58390	YES	YES
28	a	87.03	0.56421	YES	YES
29	a	90.95	0.76432	YES	YES
30	a	95.31	0.01758	YES	YES
31	a	96.56	0.61320	YES	YES
32	a	106.04	0.24098	YES	YES

33	a	108.90	0.84862	YES	YES
34	a	118.03	0.44682	YES	YES
35	a	122.94	1.46736	YES	YES
36	a	128.03	1.64388	YES	YES
37	a	139.30	0.18131	YES	YES
38	a	143.48	1.48147	YES	YES
39	a	161.24	2.32297	YES	YES
40	a	166.81	0.28994	YES	YES
41	a	172.52	1.66173	YES	YES
42	a	180.04	0.57451	YES	YES
43	a	181.08	2.88145	YES	YES
44	a	190.40	1.82337	YES	YES
45	a	198.44	3.64486	YES	YES
46	a	201.08	0.87669	YES	YES
47	a	210.96	2.33725	YES	YES
48	a	215.91	0.68327	YES	YES
49	a	218.83	2.65142	YES	YES
50	a	225.96	2.12051	YES	YES

./2/b

BP86/SV(P) energy (au): -3254.5083074330

PBE0/def2-TZVPP energy (au): -3254.009298856
cosmo_dcm Total energy + OC corr. = -3254.0586176636
cosmo_acetone Total energy + OC corr. = -3254.0697131657

Zero point energy (au): 0.8903583
Entropy (kJ mol^-1): 1.39862
Chemical potential (kJ mol^-1): 2079.64

XYZ coordinates:

114

C	-2.50613	-2.57181	-2.32655
C	-2.36309	-3.35116	-1.11232
C	-3.30513	-1.43615	-2.02624
C	-3.10906	-2.69753	-0.07787
C	-3.66290	-1.49785	-0.61910
H	-2.08266	-2.81929	-3.30944
H	-1.84232	-4.31145	-1.01712
H	-3.63753	-0.66916	-2.73713
H	-3.22911	-3.06114	0.95087
H	-4.32094	-0.79441	-0.09585
Ru	-1.40704	-1.32570	-0.75328
C	0.51308	-2.27195	-1.60209
C	0.49955	-1.00474	-1.72786
C	-3.30349	1.69042	-1.05458
P	-1.55329	1.05048	-1.05499
C	-0.94476	1.62599	-2.72491
C	-0.72298	2.30186	0.04978
C	-1.33296	3.47967	0.42106
N	0.62349	2.11092	0.31555
C	-0.58348	4.51609	1.08596
C	0.81430	4.32760	1.30511
C	1.46071	3.07691	0.87956
O	2.67863	2.85233	1.00492
C	-0.93521	-0.10313	2.62381
P	-0.41412	-1.38680	1.39475
C	-0.82671	-2.97912	2.27663
C	1.46343	-1.38949	1.52240
C	2.12693	-2.39470	2.24572
N	2.12143	-0.42119	0.84602
C	3.53450	-2.41661	2.21208
C	4.22600	-1.45931	1.47538
C	3.47953	-0.43715	0.82566
N	4.09201	0.61976	0.15757
C	5.39130	0.62133	-0.36433
C	5.87538	1.97999	-0.93187
O	6.09344	-0.38559	-0.36436
H	-2.38672	3.66269	0.17499
H	1.07740	1.16434	0.22907

H	1.57126	-3.15032	2.81554
H	4.08856	-3.19236	2.76596
H	5.31986	-1.45632	1.39564
H	3.55245	1.51190	0.21704
C	1.58205	5.33730	1.92799
C	-1.18090	5.73599	1.50344
H	1.02480	-0.13689	-2.13358
C	-1.38569	-5.45273	3.53961
C	-1.65434	-4.24412	4.20089
C	-1.37099	-3.01345	3.57871
C	-0.55035	-4.20308	1.62162
C	-0.82356	-5.42817	2.24986
H	-1.60610	-6.41484	4.03000
H	-2.08260	-4.25124	5.21652
H	-1.57193	-2.07951	4.12443
H	-0.09172	-4.20148	0.62018
H	-0.59211	-6.37114	1.72813
C	-1.82748	1.76183	4.55249
C	-2.75797	0.97163	3.85413
C	-2.31515	0.05431	2.88799
C	-0.00765	0.68432	3.33747
C	-0.45560	1.61724	4.28972
H	-2.17284	2.48663	5.30767
H	-3.83566	1.06835	4.06621
H	-3.05031	-0.56894	2.35152
H	1.07291	0.57563	3.15794
H	0.27974	2.23024	4.83596
C	-5.98316	2.60695	-1.02718
C	-5.26368	2.56097	-2.23154
C	-3.92998	2.11185	-2.24756
C	-4.03604	1.73878	0.15483
C	-5.36250	2.19937	0.16779
H	-7.02549	2.96457	-1.01685
H	-5.73697	2.88500	-3.17274
H	-3.37806	2.10080	-3.20010
H	-3.55805	1.43361	1.09951
H	-5.91560	2.24180	1.12050
C	-0.17112	2.51119	-5.30057
C	-0.59285	1.18489	-5.10746
C	-0.97081	0.74380	-3.82816
C	-0.51999	2.95773	-2.92933
C	-0.13267	3.39351	-4.20788
H	0.13334	2.85567	-6.30224
H	-0.62001	0.48252	-5.95636
H	-1.27276	-0.30471	-3.68205
H	-0.49253	3.66854	-2.08894
H	0.20206	4.43438	-4.34739
C	4.84040	2.57147	-1.91913
C	7.21201	1.74402	-1.66048
C	6.08882	2.95349	0.25748
H	7.60405	2.70875	-2.05099
H	7.08995	1.04425	-2.51494
H	7.96927	1.30407	-0.97912
H	5.13981	3.16757	0.79455
H	6.49277	3.91936	-0.11978
H	6.82263	2.54059	0.98454
H	5.24860	3.50208	-2.37208
H	3.88589	2.84580	-1.41947

H	4.61696	1.86220	-2.74685
C	0.97309	6.52599	2.33635
H	2.65824	5.16105	2.07850
H	-2.25850	5.89484	1.33194
C	-0.41193	6.72357	2.12097
H	-0.88583	7.66617	2.44063
H	1.57070	7.31382	2.82262
C	1.09716	-3.59368	-1.70167
C	2.38796	-6.10460	-1.97650
C	1.13795	-5.88277	-2.58173
C	0.49786	-4.64286	-2.44814
C	2.36453	-3.82955	-1.10467
C	2.99964	-5.07172	-1.24534
H	2.89080	-7.07923	-2.08620
H	0.66241	-6.67988	-3.17604
H	-0.46069	-4.47359	-2.96113
H	2.85532	-3.02088	-0.54336
H	3.98827	-5.22996	-0.78424

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	5.86	0.06578	YES	YES
8	a	15.93	0.13617	YES	YES
9	a	17.49	0.21172	YES	YES
10	a	20.71	0.50507	YES	YES
11	a	23.79	0.17907	YES	YES
12	a	31.73	0.03327	YES	YES
13	a	34.87	0.22541	YES	YES
14	a	36.28	0.04855	YES	YES
15	a	40.33	0.08822	YES	YES
16	a	41.43	0.15633	YES	YES
17	a	47.01	0.97648	YES	YES
18	a	48.00	0.49647	YES	YES
19	a	50.91	0.14778	YES	YES
20	a	53.92	0.00268	YES	YES
21	a	55.38	0.39507	YES	YES
22	a	60.23	0.08473	YES	YES
23	a	66.08	0.51678	YES	YES
24	a	71.78	0.22114	YES	YES
25	a	77.52	0.13744	YES	YES
26	a	78.40	0.90449	YES	YES
27	a	84.07	0.28283	YES	YES
28	a	89.37	1.00726	YES	YES
29	a	92.75	1.63593	YES	YES
30	a	95.94	0.23364	YES	YES
31	a	99.76	0.08981	YES	YES
32	a	102.08	0.65325	YES	YES

33	a	107.51	0.19671	YES	YES
34	a	115.62	1.12462	YES	YES
35	a	126.16	1.69324	YES	YES
36	a	128.14	1.19873	YES	YES
37	a	140.98	0.82648	YES	YES
38	a	147.40	0.68539	YES	YES
39	a	161.04	1.84470	YES	YES
40	a	169.17	0.60601	YES	YES
41	a	173.42	1.00393	YES	YES
42	a	177.17	3.51441	YES	YES
43	a	189.09	7.62515	YES	YES
44	a	192.14	3.80213	YES	YES
45	a	197.39	1.77220	YES	YES
46	a	201.23	2.69884	YES	YES
47	a	206.92	0.75101	YES	YES
48	a	209.87	2.91585	YES	YES
49	a	219.81	1.39674	YES	YES
50	a	224.55	1.00293	YES	YES

./10/a

BP86/SV(P) energy (au): -3330.9224459670

PBE0/def2-TZVPP energy (au): -3330.425245755
cosmo_dcm Total energy + OC corr. = -3330.4843308390
cosmo_acetone Total energy + OC corr. = -3330.4912535792

Zero point energy (au): 0.9148702
Entropy (kJ mol^-1): 1.44011
Chemical potential (kJ mol^-1): 2135.62

XYZ coordinates:

117

C	0.97620	-3.66926	-2.59055
C	0.18873	-3.04659	-3.62974
C	2.24299	-2.99776	-2.54144
C	0.97457	-2.00638	-4.21698
C	2.23363	-1.95894	-3.53083
H	0.69842	-4.56533	-2.02436
H	-0.81460	-3.35646	-3.94779
H	3.09302	-3.25912	-1.89751
H	0.67447	-1.35059	-5.04437
H	3.06241	-1.27681	-3.76253
Ru	0.57094	-1.49851	-1.98064
C	1.31710	-3.04466	0.69283
C	1.09375	-1.63226	0.07717
P	1.46220	0.71592	-1.77572
C	0.36361	2.04347	-1.08962
C	0.12528	3.23293	-1.74045
N	-0.17238	1.81894	0.16595
C	-0.68609	4.24868	-1.11635
C	-1.22164	4.00744	0.18582
C	-0.94408	2.73634	0.87728
O	-1.34985	2.47126	2.02233
P	-1.68681	-1.58330	-1.09191
C	-2.01237	-1.82806	0.74445
C	-2.63582	-2.98956	1.23648
N	-1.58241	-0.83123	1.53707
C	-2.75965	-3.11529	2.63465
C	-2.28281	-2.11257	3.47517
C	-1.71385	-0.94947	2.88013
N	-1.27525	0.14251	3.62118
C	-0.97073	0.14686	4.98865
O	-1.03564	-0.87201	5.67245
O	1.18171	-0.66125	0.80969
H	0.28624	-3.37731	0.96512
C	1.87878	1.37965	-3.46052
C	3.03320	0.95510	-0.82473
H	0.56498	3.42840	-2.72722
H	0.00917	0.90888	0.63458
C	-0.96109	5.49154	-1.74794

C	-2.00838	4.99195	0.82492
C	-2.73932	-0.11986	-1.53477
C	-2.62253	-3.01089	-1.84055
H	-3.02737	-3.76935	0.57139
H	1.67560	-3.75323	-0.07654
H	-3.23933	-4.00956	3.06561
H	-2.33818	-2.18562	4.56788
H	-1.15196	1.01165	3.05421
C	-0.54906	1.51711	5.57656
H	-0.33057	-0.38148	-2.68747
C	-4.01493	-5.23658	-2.90990
C	-2.83876	-5.43174	-2.16319
C	-2.14745	-4.32901	-1.63837
C	-3.81329	-2.82781	-2.57576
C	-4.49870	-3.93460	-3.11049
H	-4.55590	-6.10110	-3.32752
H	-2.45774	-6.45073	-1.98538
H	-1.23992	-4.50077	-1.03858
H	-4.22323	-1.81881	-2.73104
H	-5.42652	-3.77055	-3.68242
C	-4.42320	2.01653	-2.31689
C	-4.37929	1.60248	-0.97649
C	-3.54919	0.53673	-0.58445
C	-2.78646	0.30652	-2.88300
C	-3.62722	1.36093	-3.27273
H	-5.07795	2.84984	-2.61917
H	-4.99688	2.11125	-0.21891
H	-3.52608	0.23544	0.47192
H	-2.18502	-0.21018	-3.65028
H	-3.66197	1.67052	-4.33011
C	2.50224	2.32609	-6.05511
C	3.51147	2.19855	-5.08798
C	3.20396	1.73393	-3.79595
C	0.86857	1.50736	-4.44326
C	1.17747	1.98463	-5.72684
H	2.74474	2.69508	-7.06489
H	4.55142	2.46902	-5.33305
H	4.00658	1.65362	-3.04675
H	-0.17665	1.25471	-4.20111
H	0.37680	2.09176	-6.47701
C	5.49540	1.37700	0.48911
C	5.18185	0.10946	-0.03033
C	3.95558	-0.10076	-0.68042
C	3.35269	2.22710	-0.30114
C	4.57827	2.43271	0.35399
H	6.45378	1.53984	1.00833
H	5.88979	-0.72694	0.08414
H	3.70620	-1.10362	-1.05939
H	2.64563	3.06601	-0.40194
H	4.81356	3.42780	0.76528
C	-1.73153	2.51146	5.44509
C	0.69229	2.06216	4.82671
C	-0.20527	1.31135	7.06432
H	0.63561	0.59700	7.19146
H	-1.07157	0.90539	7.62737
H	0.08754	2.28297	7.51932
H	0.46995	2.30014	3.76470
H	1.53463	1.33618	4.85815

H	1.03571	3.00265	5.31244
H	-1.98472	2.71997	4.38399
H	-1.45856	3.47810	5.92456
H	-2.63911	2.12451	5.95928
C	-2.26874	6.20576	0.18458
H	-2.40099	4.77716	1.83071
H	-0.54816	5.68875	-2.75111
C	-1.74155	6.45376	-1.10522
H	-1.94608	7.41506	-1.60449
H	-2.88095	6.97374	0.68432
C	2.22138	-3.08010	1.90738
C	3.93820	-3.15326	4.15873
C	4.41363	-3.54794	2.89668
C	3.55961	-3.50998	1.78146
C	1.75599	-2.69001	3.18066
C	2.60583	-2.72634	4.29746
H	4.60372	-3.18809	5.03687
H	5.45286	-3.89761	2.78064
H	3.93860	-3.83866	0.79710
H	0.71102	-2.36493	3.30899
H	2.21575	-2.42678	5.28387

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	6.09	0.11953	YES	YES
8	a	13.54	0.32593	YES	YES
9	a	15.64	0.11624	YES	YES
10	a	17.57	0.00663	YES	YES
11	a	21.96	0.16495	YES	YES
12	a	23.03	0.06962	YES	YES
13	a	27.57	0.38390	YES	YES
14	a	35.18	0.83496	YES	YES
15	a	38.11	0.29383	YES	YES
16	a	39.70	0.74206	YES	YES
17	a	41.73	0.18168	YES	YES
18	a	45.64	0.26262	YES	YES
19	a	48.90	0.05556	YES	YES
20	a	53.48	0.22322	YES	YES
21	a	57.18	0.76139	YES	YES
22	a	59.37	0.86134	YES	YES
23	a	60.67	0.48680	YES	YES
24	a	65.60	0.30493	YES	YES
25	a	69.64	0.01038	YES	YES
26	a	72.37	0.68849	YES	YES
27	a	75.41	0.05791	YES	YES
28	a	78.43	1.22712	YES	YES
29	a	80.36	0.54227	YES	YES

30	a	87.72	0.29840	YES	YES
31	a	89.03	0.16639	YES	YES
32	a	100.11	1.33811	YES	YES
33	a	103.34	0.27259	YES	YES
34	a	108.09	0.58000	YES	YES
35	a	119.44	1.37909	YES	YES
36	a	126.01	2.60181	YES	YES
37	a	130.16	1.69540	YES	YES
38	a	139.35	1.35412	YES	YES
39	a	148.75	1.49503	YES	YES
40	a	156.73	1.05900	YES	YES
41	a	167.62	0.21060	YES	YES
42	a	173.05	2.87492	YES	YES
43	a	178.85	1.58540	YES	YES
44	a	181.19	3.30900	YES	YES
45	a	186.37	1.65097	YES	YES
46	a	192.05	0.35136	YES	YES
47	a	200.80	1.54203	YES	YES
48	a	206.00	0.27240	YES	YES
49	a	212.01	1.50292	YES	YES
50	a	215.85	1.41164	YES	YES

./10/b

BP86/SV(P) energy (au): -3330.9223790040

PBE0/def2-TZVPP energy (au): -3330.425281972
cosmo_dcm Total energy + OC corr. = -3330.4791859415 Total energy + OC corr. = -3330.4839068311
cosmo_acetone Total energy + OC corr. = -3330.4854714278 Total energy + OC corr. = -3330.4907601168

Zero point energy (au): 0.9148948
Entropy (kJ mol^-1): 1.44259
Chemical potential (kJ mol^-1): 2134.98

XYZ coordinates:

117

C	0.92896	-3.46987	-2.34805
C	0.10047	-2.84799	-3.35581
C	2.19019	-2.78628	-2.33747
C	0.85518	-1.79597	-3.96174
C	2.13638	-1.74067	-3.31839
H	0.67926	-4.37319	-1.78018
H	-0.90952	-3.16680	-3.64231
H	3.06464	-3.04370	-1.72528
H	0.52115	-1.13734	-4.77379
H	2.94976	-1.04840	-3.57292
Ru	0.52284	-1.30835	-1.70966
C	1.37618	-2.86420	0.92503
C	1.11302	-1.45027	0.32938
P	1.40306	0.91199	-1.51847
C	0.31516	2.22473	-0.78701
C	0.04340	3.41535	-1.42231
N	-0.18132	1.98539	0.48165
C	-0.76035	4.41720	-0.76733
C	-1.25599	4.16067	0.54737
C	-0.94290	2.88885	1.22144
O	-1.31160	2.61167	2.37605
P	-1.70345	-1.42307	-0.74285
C	-1.96062	-1.68931	1.10224
C	-2.53395	-2.87121	1.60644
N	-1.52746	-0.68789	1.88675
C	-2.61130	-3.00692	3.00699
C	-2.13566	-1.99581	3.83835
C	-1.60902	-0.81834	3.23280
N	-1.16710	0.27832	3.96469
C	-0.83786	0.28974	5.32626
O	-0.88080	-0.72712	6.01471
O	1.20956	-0.48439	1.06721
H	0.36015	-3.21056	1.23323
C	1.76088	1.59150	-3.21026
C	3.00105	1.15686	-0.61504
H	0.45138	3.62310	-2.42030

H	0.02624	1.07502	0.93876
C	-1.06776	5.66090	-1.38178
C	-2.03633	5.13082	1.21546
C	-2.78328	0.03536	-1.13168
C	-2.65217	-2.85159	-1.47224
H	-2.92567	-3.65726	0.94914
H	1.71474	-3.56263	0.13795
H	-3.05338	-3.91589	3.44733
H	-2.15566	-2.07475	4.93195
H	-1.07069	1.14979	3.39609
C	-0.41833	1.66570	5.90327
H	-0.41388	-0.19426	-2.37388
C	-4.06699	-5.07859	-2.50833
C	-2.85996	-5.27090	-1.81189
C	-2.15789	-4.16730	-1.30333
C	-3.87239	-2.67148	-2.15808
C	-4.56920	-3.77892	-2.67629
H	-4.61736	-5.94369	-2.91229
H	-2.46320	-6.28813	-1.66052
H	-1.22581	-4.33686	-0.74171
H	-4.29622	-1.66446	-2.28692
H	-5.52039	-3.61766	-3.20925
C	-4.51318	2.16280	-1.83308
C	-4.42729	1.72814	-0.50125
C	-3.57464	0.66642	-0.14922
C	-2.87367	0.48159	-2.47097
C	-3.73676	1.53171	-2.82077
H	-5.18565	2.99304	-2.10339
H	-5.02935	2.21758	0.28114
H	-3.51784	0.34931	0.90094
H	-2.28853	-0.01622	-3.26272
H	-3.80454	1.85705	-3.87174
C	2.29522	2.56293	-5.81526
C	3.33484	2.43797	-4.88065
C	3.07173	1.96050	-3.58373
C	0.71997	1.71597	-4.16060
C	0.98467	2.20591	-5.44915
H	2.50292	2.94159	-6.82925
H	4.36420	2.72023	-5.15541
H	3.89818	1.88212	-2.86043
H	-0.31468	1.45042	-3.88894
H	0.16062	2.30915	-6.17422
C	5.49636	1.58664	0.63154
C	5.17933	0.32238	0.10624
C	3.93667	0.10822	-0.51038
C	3.32415	2.42561	-0.08608
C	4.56646	2.63520	0.53530
H	6.46798	1.75212	1.12471
H	5.89816	-0.50844	0.18989
H	3.68479	-0.89186	-0.89473
H	2.60692	3.25921	-0.15644
H	4.80446	3.62741	0.95193
C	-1.61668	2.64442	5.80249
C	0.79651	2.22688	5.12267
C	-0.03459	1.46458	7.38183
H	0.82002	0.76318	7.48763
H	-0.88035	1.04516	7.96587
H	0.25493	2.44051	7.82967

H	0.54401	2.46311	4.06705
H	1.64885	1.51171	5.13171
H	1.14072	3.17127	5.60003
H	-1.90026	2.84839	4.74843
H	-1.34357	3.61517	6.27374
H	-2.50529	2.24604	6.34055
C	-2.32925	6.34555	0.59152
H	-2.39768	4.90369	2.23022
H	-0.68605	5.87067	-2.39478
C	-1.84111	6.60899	-0.71040
H	-2.07086	7.57131	-1.19670
H	-2.93664	7.10245	1.11356
C	2.32458	-2.89884	2.10550
C	4.12275	-2.97377	4.29238
C	4.55144	-3.36779	3.01346
C	3.65744	-3.32825	1.93003
C	1.90587	-2.51076	3.39555
C	2.79612	-2.54789	4.48047
H	4.82001	-3.00867	5.14550
H	5.58572	-3.71744	2.85940
H	4.00024	-3.65486	0.93184
H	0.86585	-2.18663	3.56215
H	2.44256	-2.24998	5.48095

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	6.92	0.03238	YES	YES
8	a	9.36	0.80330	YES	YES
9	a	15.52	0.08393	YES	YES
10	a	18.30	0.01097	YES	YES
11	a	20.36	0.23475	YES	YES
12	a	23.75	0.02002	YES	YES
13	a	27.38	0.39956	YES	YES
14	a	33.72	0.66256	YES	YES
15	a	37.28	0.34619	YES	YES
16	a	40.69	0.42490	YES	YES
17	a	42.51	0.25324	YES	YES
18	a	45.19	0.17235	YES	YES
19	a	49.50	0.08834	YES	YES
20	a	53.86	0.15811	YES	YES
21	a	57.76	0.34057	YES	YES
22	a	59.15	0.93065	YES	YES
23	a	59.96	0.88367	YES	YES
24	a	64.19	0.31934	YES	YES
25	a	70.16	0.11014	YES	YES
26	a	71.46	0.65513	YES	YES
27	a	75.83	0.11778	YES	YES

28	a	78.41	1.46017	YES	YES
29	a	80.36	0.11896	YES	YES
30	a	88.01	0.37892	YES	YES
31	a	88.56	0.25015	YES	YES
32	a	99.25	1.34056	YES	YES
33	a	104.25	0.23703	YES	YES
34	a	106.81	0.62263	YES	YES
35	a	119.39	1.42116	YES	YES
36	a	125.98	2.86991	YES	YES
37	a	129.42	1.70334	YES	YES
38	a	139.57	1.19189	YES	YES
39	a	148.10	1.35403	YES	YES
40	a	156.37	1.17028	YES	YES
41	a	166.42	0.16063	YES	YES
42	a	173.36	2.65347	YES	YES
43	a	176.70	1.45296	YES	YES
44	a	180.80	4.50386	YES	YES
45	a	184.76	0.26227	YES	YES
46	a	193.00	0.39077	YES	YES
47	a	199.72	1.80134	YES	YES
48	a	208.25	0.38400	YES	YES
49	a	215.13	1.07486	YES	YES
50	a	217.25	2.26643	YES	YES

./10/c

BP86/SV(P) energy (au): -3330.9239595320

Single point data not present for this isomer

Zero point energy (au): 0.9153940
Entropy (kJ mol^-1): 1.42592
Chemical potential (kJ mol^-1): 2140.69

XYZ coordinates:

117

C	0.51870	-4.04611	-1.80015
C	-0.49520	-3.65733	-2.75321
C	1.73691	-3.37741	-2.15207
C	0.10599	-2.75945	-3.69145
C	1.47585	-2.56728	-3.30758
H	0.40748	-4.80571	-1.01842
H	-1.52643	-4.03120	-2.78422
H	2.70501	-3.49020	-1.64479
H	-0.38607	-2.29144	-4.55391
H	2.20747	-1.94793	-3.84348
Ru	0.13553	-1.79618	-1.58429
C	1.56865	-2.67883	1.12044
C	1.14322	-1.46428	0.24978
P	0.87025	0.42381	-2.10612
C	-0.09160	1.84719	-1.40859
C	-0.61790	2.86151	-2.17579
N	-0.21249	1.88414	-0.03153
C	-1.29667	3.96576	-1.54244
C	-1.40466	3.99339	-0.11759
C	-0.82773	2.90424	0.69045
O	-0.86083	2.86743	1.93257
P	-1.81996	-1.71133	-0.14853
C	-1.63300	-1.63026	1.72111
C	-2.01311	-2.70175	2.54856
N	-1.09132	-0.49245	2.18905
C	-1.75046	-2.57658	3.92735
C	-1.15930	-1.42013	4.43009
C	-0.86895	-0.36190	3.51963
N	-0.35863	0.86916	3.91776
C	0.12279	1.20671	5.19232
O	0.15904	0.39619	6.11343
O	1.41326	-0.35316	0.68575
H	1.15782	-2.44880	2.13060
C	0.75003	0.70894	-3.93807
C	2.61981	0.89630	-1.72170
H	-0.50909	2.85160	-3.26834
H	0.19456	1.10689	0.52466
C	-1.85331	5.03894	-2.28922
C	-2.05320	5.07142	0.52553
C	-3.00618	-0.33826	-0.54108

C	-2.87261	-3.23476	-0.37322
H	-2.50459	-3.60005	2.15460
H	1.08983	-3.61324	0.77543
H	-2.01963	-3.39578	4.61453
H	-0.92415	-1.28731	5.49311
H	-0.38583	1.59481	3.16812
C	0.59889	2.67217	5.36423
H	-1.00505	-0.90065	-2.26316
C	-4.43202	-5.58875	-0.64339
C	-3.09112	-5.67350	-0.22739
C	-2.31953	-4.50835	-0.09848
C	-4.22495	-3.16076	-0.77172
C	-4.99393	-4.33100	-0.91069
H	-5.03809	-6.50292	-0.75040
H	-2.64268	-6.65401	0.00197
H	-1.27928	-4.59207	0.25152
H	-4.69585	-2.18657	-0.96901
H	-6.04764	-4.25035	-1.22383
C	-4.93160	1.62763	-1.20547
C	-4.51186	1.46671	0.12412
C	-3.56029	0.48675	0.46008
C	-3.43228	-0.16698	-1.87918
C	-4.39239	0.80268	-2.20828
H	-5.67987	2.39478	-1.46236
H	-4.92614	2.10941	0.91749
H	-3.24047	0.38501	1.50610
H	-3.03928	-0.82241	-2.67511
H	-4.72286	0.91227	-3.25416
C	0.55538	1.06478	-6.74065
C	1.80281	1.14777	-6.10261
C	1.90215	0.97703	-4.70959
C	-0.50234	0.62063	-4.59099
C	-0.59894	0.80596	-5.97920
H	0.47945	1.20415	-7.83126
H	2.71277	1.35444	-6.68910
H	2.88760	1.05951	-4.22594
H	-1.41850	0.42610	-4.01027
H	-1.58406	0.74780	-6.47056
C	5.30954	1.65567	-1.32495
C	4.96421	0.29557	-1.39667
C	3.62531	-0.08218	-1.58964
C	2.97130	2.26259	-1.64416
C	4.31029	2.63670	-1.44467
H	6.35930	1.95231	-1.16728
H	5.73734	-0.48155	-1.28729
H	3.36375	-1.15063	-1.61268
H	2.20003	3.04347	-1.74167
H	4.57154	3.70556	-1.38056
C	-0.62580	3.61540	5.23691
C	1.66282	3.02908	4.29702
C	1.21298	2.80806	6.77112
H	2.08785	2.13547	6.89873
H	0.47762	2.54645	7.56009
H	1.54866	3.85584	6.93353
H	1.24692	3.02101	3.26706
H	2.52662	2.32883	4.33883
H	2.05039	4.05451	4.48856
H	-1.07551	3.57838	4.22224

H	-0.30735	4.66446	5.42941
H	-1.40712	3.35724	5.98567
C	-2.59491	6.11512	-0.22855
H	-2.11369	5.06595	1.62476
H	-1.77136	5.02900	-3.38874
C	-2.49268	6.09623	-1.63991
H	-2.91795	6.92415	-2.23061
H	-3.09846	6.95653	0.27424
C	3.07565	-2.87441	1.22491
C	5.86760	-3.29668	1.48022
C	5.04314	-4.31865	0.98152
C	3.65877	-4.10680	0.85616
C	3.91453	-1.85530	1.72828
C	5.29710	-2.06659	1.85433
H	6.95199	-3.46229	1.58836
H	5.47575	-5.29246	0.69872
H	3.01788	-4.92839	0.49036
H	3.47413	-0.89063	2.02478
H	5.93454	-1.26356	2.25981

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.17	0.20789	YES	YES
8	a	14.56	0.03278	YES	YES
9	a	15.39	0.03789	YES	YES
10	a	17.39	0.01190	YES	YES
11	a	21.11	0.05998	YES	YES
12	a	24.99	0.21579	YES	YES
13	a	29.41	0.22981	YES	YES
14	a	37.10	0.12604	YES	YES
15	a	39.43	0.07989	YES	YES
16	a	40.43	0.20945	YES	YES
17	a	45.62	0.78784	YES	YES
18	a	51.44	0.13869	YES	YES
19	a	52.14	0.83035	YES	YES
20	a	55.81	0.33895	YES	YES
21	a	57.78	0.24892	YES	YES
22	a	59.66	0.73313	YES	YES
23	a	63.50	0.38680	YES	YES
24	a	67.50	0.42366	YES	YES
25	a	70.93	0.48498	YES	YES
26	a	75.80	0.20204	YES	YES
27	a	75.95	0.21356	YES	YES
28	a	77.52	0.71703	YES	YES
29	a	82.56	0.28963	YES	YES
30	a	86.12	0.80013	YES	YES
31	a	88.10	0.32450	YES	YES

32	a	98.41	2.05325	YES	YES
33	a	104.01	0.13821	YES	YES
34	a	107.33	0.42690	YES	YES
35	a	119.43	0.58375	YES	YES
36	a	126.69	2.06151	YES	YES
37	a	136.05	0.97337	YES	YES
38	a	142.19	3.21865	YES	YES
39	a	151.49	2.50438	YES	YES
40	a	166.33	0.16689	YES	YES
41	a	168.68	0.15539	YES	YES
42	a	173.62	2.83727	YES	YES
43	a	179.02	1.11681	YES	YES
44	a	184.92	2.05716	YES	YES
45	a	186.56	2.66898	YES	YES
46	a	192.10	4.51272	YES	YES
47	a	200.97	2.14912	YES	YES
48	a	208.65	0.40349	YES	YES
49	a	211.85	1.18061	YES	YES
50	a	215.29	0.81479	YES	YES

./4

BP86/SV(P) energy (au): -3254.5111535530

PBE0/def2-TZVPP energy (au): -3254.017892510
cosmo_dcm Total energy + OC corr. = -3254.0666210077
cosmo_acetone Total energy + OC corr. = -3254.0720655779

Zero point energy (au): 0.8906804
Entropy (kJ mol^-1): 1.40549
Chemical potential (kJ mol^-1): 2078.67

XYZ coordinates:

114

C	-1.60912	1.33179	3.62573
C	-1.70383	2.56517	2.89419
C	-2.70468	0.49373	3.24016
C	-2.87576	2.47647	2.05613
C	-3.50205	1.20810	2.26465
H	-0.83080	1.08436	4.35960
H	-1.05057	3.43766	3.00827
H	-2.93423	-0.49699	3.65451
H	-3.24489	3.27854	1.40273
H	-4.43544	0.85376	1.80912
Ru	-1.40734	0.85849	1.40910
C	1.73900	0.37250	2.02966
C	0.55383	0.51631	1.64724
C	-3.51401	-1.82602	0.48072
P	-1.75019	-1.36269	0.80084
C	-1.19687	-2.63933	2.04911
C	-0.82231	-2.05812	-0.65012
C	-1.31835	-2.77973	-1.70918
N	0.54472	-1.84706	-0.54755
C	-0.41415	-3.33030	-2.69055
C	0.99522	-3.11163	-2.55338
C	1.50879	-2.31166	-1.43150
O	2.71211	-2.03161	-1.24637
C	-2.28604	1.57982	-1.98342
P	-1.08888	1.92263	-0.60625
C	-1.10482	3.78919	-0.43748
C	0.55049	1.92242	-1.57112
C	0.72373	2.73365	-2.69362
N	1.63494	1.25079	-1.07664
C	2.00429	2.85834	-3.26880
C	3.09151	2.16368	-2.74297
C	2.89278	1.30282	-1.63557
N	3.85156	0.47483	-1.10126
C	5.25083	0.67891	-1.26488
C	6.15100	-0.53233	-0.95298
O	5.67223	1.74846	-1.67944
H	-2.39786	-2.96666	-1.79726
H	0.89765	-1.31416	0.27223

H	-0.13229	3.29172	-3.09932
H	2.14868	3.50383	-4.15022
H	4.09757	2.24776	-3.16910
H	3.50508	-0.46294	-0.78839
C	1.89671	-3.65830	-3.49582
C	-0.87427	-4.10349	-3.79118
H	1.51461	0.78817	-0.12406
C	-0.34676	-4.60228	3.89695
C	-0.95178	-4.98804	2.68663
C	-1.37096	-4.01498	1.76661
C	-0.57718	-2.26205	3.25708
C	-0.15765	-3.23995	4.17797
H	-0.01779	-5.36797	4.61838
H	-1.09679	-6.05600	2.45518
H	-1.83812	-4.33300	0.81985
H	-0.39867	-1.19695	3.46526
H	0.32449	-2.92971	5.11932
C	-6.26134	-2.35660	0.05387
C	-5.51963	-1.64715	-0.90691
C	-4.15989	-1.37032	-0.69138
C	-4.26739	-2.53377	1.44460
C	-5.63303	-2.79172	1.23203
H	-7.32990	-2.56756	-0.11514
H	-6.00322	-1.29752	-1.83359
H	-3.60161	-0.79260	-1.44391
H	-3.78931	-2.89623	2.36811
H	-6.20623	-3.34440	1.99430
C	-0.92257	6.59175	-0.10350
C	-1.83473	6.04687	-1.02087
C	-1.92168	4.65279	-1.19678
C	-0.18288	4.34524	0.47982
C	-0.08994	5.73635	0.64094
H	-0.85517	7.68374	0.02898
H	-2.48678	6.70928	-1.61366
H	-2.62945	4.25070	-1.93825
H	0.47267	3.68144	1.06907
H	0.63810	6.15588	1.35458
C	-4.23197	0.99354	-3.95729
C	-2.89963	0.58491	-4.13386
C	-1.93106	0.87904	-3.15720
C	-3.63928	1.94918	-1.79582
C	-4.59949	1.67443	-2.78248
H	-4.98547	0.77765	-4.73217
H	-2.60337	0.03746	-5.04340
H	-0.89207	0.55345	-3.32301
H	-3.95401	2.45341	-0.86816
H	-5.64434	1.98974	-2.62789
C	5.71252	-1.28701	0.32199
C	7.59649	-0.02068	-0.79373
C	6.05448	-1.47692	-2.18425
H	8.28298	-0.88206	-0.64434
H	7.69034	0.65330	0.08500
H	7.92726	0.54524	-1.68882
H	6.44904	-2.09210	0.53603
H	4.72263	-1.78030	0.21161
H	5.68003	-0.61570	1.20686
H	5.02224	-1.86860	-2.31206
H	6.73406	-2.34483	-2.03335

H	6.36702	-0.95761	-3.11692
C	1.41935	-4.41729	-4.56581
H	2.97392	-3.47571	-3.36042
C	0.02863	-4.63795	-4.71110
H	-1.95602	-4.28277	-3.90569
H	2.12332	-4.84730	-5.29627
H	-0.34386	-5.24002	-5.55606
C	3.03341	0.27443	2.64474
C	5.52852	0.12986	3.99624
C	5.15136	1.31061	3.33062
C	3.92101	1.38515	2.66226
C	3.43575	-0.91565	3.31089
C	4.66606	-0.98143	3.98010
H	6.49344	0.07622	4.52627
H	5.82056	2.18681	3.33867
H	3.62344	2.31802	2.15695
H	2.76118	-1.78674	3.30417
H	4.95589	-1.91135	4.49690

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	6.23	0.07278	YES	YES
8	a	10.48	0.00991	YES	YES
9	a	16.53	0.02959	YES	YES
10	a	24.65	0.04029	YES	YES
11	a	26.99	0.06555	YES	YES
12	a	29.62	0.10372	YES	YES
13	a	33.85	0.05009	YES	YES
14	a	37.81	0.33528	YES	YES
15	a	43.18	0.24778	YES	YES
16	a	45.75	0.08736	YES	YES
17	a	47.81	0.03239	YES	YES
18	a	49.36	0.57003	YES	YES
19	a	52.31	0.69580	YES	YES
20	a	52.98	0.06840	YES	YES
21	a	55.51	0.21143	YES	YES
22	a	58.23	0.00830	YES	YES
23	a	64.38	1.08236	YES	YES
24	a	66.37	0.25950	YES	YES
25	a	67.55	0.77980	YES	YES
26	a	71.46	0.83539	YES	YES
27	a	75.60	1.54705	YES	YES
28	a	80.47	0.41700	YES	YES
29	a	86.41	0.62395	YES	YES
30	a	87.33	0.24466	YES	YES
31	a	96.39	1.04757	YES	YES
32	a	99.99	0.71760	YES	YES

33	a	101.45	0.37975	YES	YES
34	a	111.80	1.02028	YES	YES
35	a	118.61	5.98835	YES	YES
36	a	127.66	0.86599	YES	YES
37	a	134.58	3.68436	YES	YES
38	a	137.05	2.99553	YES	YES
39	a	161.56	0.93342	YES	YES
40	a	168.64	1.45528	YES	YES
41	a	175.48	0.20186	YES	YES
42	a	177.84	4.85370	YES	YES
43	a	181.98	0.66967	YES	YES
44	a	192.71	0.83363	YES	YES
45	a	196.97	1.57873	YES	YES
46	a	205.79	0.92427	YES	YES
47	a	211.98	4.06190	YES	YES
48	a	213.35	1.28006	YES	YES
49	a	221.47	1.12818	YES	YES
50	a	227.12	0.68274	YES	YES

./5/a

BP86/SV(P) energy (au): -3254.5242183060

PBE0/def2-TZVPP energy (au): -3254.021085297
cosmo_dcm Total energy + OC corr. = -3254.0721951040
cosmo_acetone Total energy + OC corr. = -3254.0780131378

Zero point energy (au): 0.8907793
Entropy (kJ mol^-1): 1.40305
Chemical potential (kJ mol^-1): 2079.11

XYZ coordinates:

114

C	2.12817	-2.84996	-2.72663
C	2.84461	-3.21073	-1.53450
C	0.80081	-3.37149	-2.61239
C	1.95954	-3.98958	-0.70366
C	0.70508	-4.09898	-1.36391
H	2.53462	-2.27817	-3.57169
H	3.90108	-2.99960	-1.33139
H	0.01221	-3.30109	-3.37266
H	2.22540	-4.43548	0.26410
H	-0.16965	-4.65990	-1.01427
Ru	1.12278	-1.82021	-0.94386
C	2.84955	0.75609	-1.55912
C	-2.22824	-2.53725	-1.73924
P	-1.13363	-1.10706	-1.26333
C	-1.33614	0.04343	-2.70851
C	-2.18684	-0.27453	0.02792
C	-3.50734	-0.62033	0.21978
N	-1.66129	0.82842	0.67772
C	-4.34885	0.15353	1.09674
C	-3.80418	1.30798	1.73518
C	-2.40096	1.67970	1.50201
O	-1.86471	2.68769	1.99883
C	-0.03232	-1.64256	2.49731
P	1.38243	-1.30118	1.36033
C	2.75339	-2.32890	2.09275
C	1.94544	0.44323	1.77627
C	3.19269	0.65379	2.38526
N	1.13708	1.45561	1.39319
C	3.64075	1.98193	2.52785
C	2.83828	3.03612	2.10827
C	1.54695	2.73655	1.58915
N	0.62019	3.72728	1.28391
C	0.88002	5.09734	1.12691
C	-0.37203	5.99218	0.93319
O	2.01678	5.55691	1.15497
H	-3.94536	-1.46863	-0.32059
H	-0.62391	1.03385	0.69102
H	3.81232	-0.18071	2.73502

H	4.62548	2.18602	2.98010
H	3.14920	4.08511	2.18145
H	-0.36930	3.39814	1.34771
C	-4.60891	2.09997	2.58493
C	-5.71089	-0.17751	1.33046
C	4.90112	-3.82934	3.16967
C	3.64734	-3.83512	3.80051
C	2.58000	-3.08505	3.27186
C	4.02353	-2.32370	1.46872
C	5.08896	-3.06373	2.00411
H	5.73570	-4.41494	3.58802
H	3.49325	-4.42228	4.72044
H	1.60949	-3.09306	3.79015
H	4.18791	-1.71320	0.56674
H	6.07410	-3.04049	1.50991
C	-2.11972	-2.31356	4.27567
C	-1.68953	-3.24580	3.31477
C	-0.65710	-2.90856	2.42498
C	-0.46350	-0.71485	3.46852
C	-1.50869	-1.05086	4.34767
H	-2.93394	-2.57315	4.97164
H	-2.15859	-4.24200	3.26065
H	-0.31516	-3.64582	1.67899
H	0.00960	0.27582	3.54460
H	-1.84215	-0.31659	5.09827
C	-3.84778	-4.74933	-2.44069
C	-3.53705	-3.76958	-3.39677
C	-2.73669	-2.66520	-3.04969
C	-2.54412	-3.52961	-0.78192
C	-3.35332	-4.62302	-1.12957
H	-4.47971	-5.60981	-2.71404
H	-3.92485	-3.85560	-4.42487
H	-2.51513	-1.89973	-3.80910
H	-2.17343	-3.43451	0.25099
H	-3.60145	-5.38176	-0.36936
C	-1.73849	1.63053	-5.01210
C	-0.59754	0.81847	-4.90606
C	-0.39248	0.03569	-3.75779
C	-2.48161	0.86362	-2.82111
C	-2.67474	1.65662	-3.96413
H	-1.89498	2.25074	-5.90969
H	0.14967	0.80376	-5.71589
H	0.52088	-0.57262	-3.67048
H	-3.23417	0.88447	-2.01702
H	-3.56862	2.29780	-4.03465
C	-1.13605	6.05656	2.28243
C	-1.29764	5.43271	-0.17314
C	0.10978	7.40235	0.54108
H	-2.13600	6.14252	-0.35031
H	-1.74958	4.45691	0.10686
H	-0.74924	5.30789	-1.13317
H	0.78670	7.82522	1.31188
H	-0.76436	8.08047	0.42642
H	0.67018	7.38650	-0.41814
H	-2.00338	6.74801	2.18773
H	-0.48071	6.44492	3.09298
H	-1.52619	5.06181	2.58653
C	-5.94386	1.75335	2.80575

H	-4.15864	2.98578	3.05859
H	-6.14303	-1.06336	0.83651
C	-6.49383	0.61206	2.17395
H	-7.54968	0.34682	2.34727
H	-6.57254	2.37026	3.46791
C	2.71861	2.04278	-2.26816
C	2.56966	4.51642	-3.64799
C	3.81840	3.92425	-3.39235
C	3.89290	2.70189	-2.70922
C	1.46735	2.65786	-2.51595
C	1.39767	3.87789	-3.20371
H	2.51061	5.47846	-4.18235
H	4.74503	4.42056	-3.72433
H	4.87767	2.24489	-2.51366
H	0.54490	2.18220	-2.14938
H	0.41411	4.33975	-3.38857
C	1.97978	-0.22006	-1.29579
H	3.86527	0.53096	-1.16400

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	6.66	0.19021	YES	YES
8	a	14.86	0.09991	YES	YES
9	a	19.90	0.01182	YES	YES
10	a	20.99	0.06633	YES	YES
11	a	26.78	0.00828	YES	YES
12	a	28.21	0.15919	YES	YES
13	a	31.64	0.05636	YES	YES
14	a	34.00	0.49782	YES	YES
15	a	35.91	0.06688	YES	YES
16	a	41.47	0.82398	YES	YES
17	a	44.58	0.13603	YES	YES
18	a	48.26	0.00200	YES	YES
19	a	51.51	0.22008	YES	YES
20	a	52.76	0.11556	YES	YES
21	a	57.46	0.31709	YES	YES
22	a	57.85	0.46078	YES	YES
23	a	63.42	0.12958	YES	YES
24	a	66.86	0.58942	YES	YES
25	a	69.63	0.33684	YES	YES
26	a	76.25	0.18497	YES	YES
27	a	77.02	0.38628	YES	YES
28	a	78.15	0.45275	YES	YES
29	a	86.51	1.41022	YES	YES
30	a	90.76	0.37177	YES	YES
31	a	93.39	1.36930	YES	YES
32	a	95.53	0.03274	YES	YES

33	a	104.24	0.58463	YES	YES
34	a	107.53	1.12602	YES	YES
35	a	115.38	0.65491	YES	YES
36	a	125.29	1.63500	YES	YES
37	a	127.85	0.50389	YES	YES
38	a	135.72	1.90139	YES	YES
39	a	162.93	0.50496	YES	YES
40	a	166.12	1.11057	YES	YES
41	a	168.64	1.49090	YES	YES
42	a	183.06	0.88822	YES	YES
43	a	189.20	0.90102	YES	YES
44	a	197.19	0.84349	YES	YES
45	a	206.37	0.11562	YES	YES
46	a	211.07	1.21679	YES	YES
47	a	213.39	2.21905	YES	YES
48	a	217.09	2.80914	YES	YES
49	a	223.22	1.89346	YES	YES
50	a	228.36	1.49364	YES	YES

./5/b

BP86/SV(P) energy (au): -3254.5287065190

PBE0/def2-TZVPP energy (au): -3254.025901436
cosmo_dcm Total energy + OC corr. = -3254.0757090953
cosmo_acetone Total energy + OC corr. = -3254.0813325256

Zero point energy (au): 0.8902358
Entropy (kJ mol^-1): 1.41728
Chemical potential (kJ mol^-1): 2073.64

XYZ coordinates:

114

C	2.15607	-2.97843	-2.38153
C	2.76982	-3.21463	-1.10099
C	0.82752	-3.50526	-2.33251
C	1.82418	-3.93296	-0.28134
C	0.63361	-4.11501	-1.03096
H	2.62974	-2.48552	-3.24122
H	3.80239	-2.97494	-0.82258
H	0.10531	-3.52132	-3.15915
H	2.00854	-4.28092	0.74397
H	-0.26587	-4.64956	-0.70379
Ru	1.00873	-1.79056	-0.81206
C	2.23308	0.94559	-1.84976
C	-2.29608	-2.62416	-1.73571
P	-1.25819	-1.15821	-1.24935
C	-1.41726	-0.03676	-2.72459
C	-2.38398	-0.30652	-0.03045
C	-3.68880	-0.70381	0.16799
N	-1.92145	0.86172	0.54840
C	-4.57378	0.07985	0.99309
C	-4.09412	1.29958	1.55876
C	-2.71236	1.73278	1.30030
O	-2.24067	2.81076	1.71157
C	-0.15886	-1.22758	2.58339
P	1.24514	-0.98312	1.40923
C	2.65076	-1.85229	2.26349
C	1.70236	0.82375	1.58417
C	2.93546	1.22406	2.11939
N	0.80564	1.70190	1.08321
C	3.26561	2.59302	2.07016
C	2.36761	3.50315	1.52166
C	1.10851	3.02099	1.07212
N	0.09944	3.87995	0.63755
C	0.30244	5.12043	0.02876
C	-0.97620	5.96570	-0.19733
O	1.42326	5.50391	-0.29991
H	-4.08149	-1.60285	-0.32289
H	-0.89395	1.12900	0.54103
H	3.63203	0.50009	2.56071

H	4.23178	2.94203	2.46903
H	2.59536	4.57366	1.45035
H	-0.86318	3.55326	0.88882
C	-4.94316	2.09988	2.35577
C	-5.91825	-0.30636	1.24482
C	4.82732	-3.16554	3.50916
C	3.54702	-3.21952	4.08214
C	2.46417	-2.56327	3.46857
C	3.94514	-1.80248	1.69275
C	5.02492	-2.44839	2.31508
H	5.67426	-3.67702	3.99477
H	3.38397	-3.77064	5.02262
H	1.47140	-2.60599	3.94165
H	4.11795	-1.22976	0.76691
H	6.02958	-2.38850	1.86511
C	-2.20923	-1.75085	4.45205
C	-1.87917	-2.71456	3.48256
C	-0.86577	-2.44963	2.54699
C	-0.48891	-0.26781	3.56425
C	-1.51565	-0.52918	4.48820
H	-3.00973	-1.95340	5.18197
H	-2.41537	-3.67741	3.45492
H	-0.60323	-3.20747	1.78984
H	0.04950	0.69130	3.61041
H	-1.77090	0.23053	5.24452
C	-3.83986	-4.88426	-2.45682
C	-3.50235	-3.92157	-3.42102
C	-2.74007	-2.79345	-3.06462
C	-2.63886	-3.59981	-0.76987
C	-3.41065	-4.71681	-1.12740
H	-4.44190	-5.76350	-2.73776
H	-3.83981	-4.03959	-4.46364
H	-2.49784	-2.04177	-3.83151
H	-2.31991	-3.47473	0.27702
H	-3.68019	-5.46197	-0.36099
C	-1.72436	1.54768	-5.04671
C	-0.61913	0.69007	-4.91923
C	-0.46253	-0.09324	-3.76329
C	-2.53145	0.82129	-2.86432
C	-2.67742	1.61180	-4.01617
H	-1.84215	2.16851	-5.94982
H	0.13467	0.63334	-5.72151
H	0.41764	-0.74740	-3.66657
H	-3.29739	0.87579	-2.07490
H	-3.54726	2.28276	-4.10659
C	-1.99219	5.17917	-1.06253
C	-0.57245	7.26227	-0.92379
C	-1.60613	6.30348	1.17846
H	-1.47002	7.89798	-1.08928
H	-0.10857	7.04659	-1.90992
H	0.16539	7.84304	-0.33190
H	-1.95146	5.39362	1.71565
H	-2.48937	6.96477	1.03280
H	-0.88330	6.84427	1.82868
H	-2.87444	5.82274	-1.27652
H	-2.36561	4.26797	-0.54763
H	-1.54711	4.87812	-2.03670
C	-6.25858	1.69712	2.59737

H	-4.54117	3.03586	2.77293
H	-6.30160	-1.24246	0.80614
C	-6.74508	0.49135	2.03729
H	-7.78608	0.18204	2.22628
H	-6.92137	2.31944	3.22014
C	3.62767	1.42171	-1.73292
C	6.28629	2.38715	-1.52148
C	5.21670	3.28421	-1.68803
C	3.89984	2.81027	-1.79401
C	4.71517	0.52633	-1.57628
C	6.02930	1.00511	-1.46847
H	7.31983	2.76227	-1.44647
H	5.40629	4.36910	-1.73749
H	3.07061	3.52915	-1.90161
H	4.52424	-0.55988	-1.58050
H	6.86403	0.29268	-1.35985
C	1.69619	-0.18292	-1.39103
H	1.50886	1.62335	-2.35022

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	5.90	0.06353	YES	YES
8	a	11.33	0.30193	YES	YES
9	a	13.78	0.57558	YES	YES
10	a	19.37	0.02919	YES	YES
11	a	20.56	0.05267	YES	YES
12	a	24.36	0.01907	YES	YES
13	a	27.83	0.07910	YES	YES
14	a	30.73	0.15983	YES	YES
15	a	35.77	0.05028	YES	YES
16	a	42.93	0.07916	YES	YES
17	a	44.13	0.20305	YES	YES
18	a	47.46	0.54543	YES	YES
19	a	48.88	1.18878	YES	YES
20	a	50.35	0.13820	YES	YES
21	a	52.96	0.14927	YES	YES
22	a	58.91	0.11684	YES	YES
23	a	62.87	0.58831	YES	YES
24	a	65.01	0.39929	YES	YES
25	a	67.50	0.25586	YES	YES
26	a	69.87	0.64518	YES	YES
27	a	75.72	0.32887	YES	YES
28	a	84.24	0.38760	YES	YES
29	a	86.79	2.11661	YES	YES
30	a	88.38	0.44813	YES	YES
31	a	93.56	0.00766	YES	YES
32	a	96.92	0.95435	YES	YES

33	a	101.26	0.48227	YES	YES
34	a	107.94	0.33874	YES	YES
35	a	114.07	0.84823	YES	YES
36	a	124.59	1.33965	YES	YES
37	a	128.08	0.91455	YES	YES
38	a	141.01	2.96084	YES	YES
39	a	163.00	1.66753	YES	YES
40	a	167.68	0.16944	YES	YES
41	a	171.14	1.64963	YES	YES
42	a	182.71	2.46247	YES	YES
43	a	193.46	0.80878	YES	YES
44	a	198.54	0.56582	YES	YES
45	a	204.13	0.23580	YES	YES
46	a	209.39	0.63670	YES	YES
47	a	210.32	2.05084	YES	YES
48	a	219.49	2.18767	YES	YES
49	a	220.56	2.56807	YES	YES
50	a	226.43	1.09338	YES	YES

./6/a

BP86/SV(P) energy (au): -3330.8880173630

PBE0/def2-TZVPP energy (au): -3330.406499831
cosmo_dcm Total energy + OC corr. = -3330.4567296649
cosmo_acetone Total energy + OC corr. = -3330.4624220161

Zero point energy (au): 0.9147901
Entropy (kJ mol^-1): 1.42346
Chemical potential (kJ mol^-1): 2141.79

XYZ coordinates:

117

C	-1.60188	3.72923	1.67518
C	-1.31886	4.12714	0.31863
C	-2.75889	2.89329	1.65258
C	-2.34724	3.57451	-0.52947
C	-3.22957	2.81834	0.28037
H	-1.02427	4.01604	2.56415
H	-0.52560	4.80941	-0.00899
H	-3.25631	2.45159	2.52579
H	-2.42319	3.72912	-1.61394
H	-4.12895	2.28971	-0.05547
Ru	-1.06699	1.87056	0.47842
C	1.74379	1.91351	1.94102
C	0.58427	1.81619	1.29509
P	-1.94542	-0.26365	1.21857
C	-1.61645	-1.88499	0.35234
C	-2.56414	-2.64931	-0.29190
N	-0.30765	-2.32055	0.40711
C	-2.18525	-3.89233	-0.91650
C	-0.81801	-4.30832	-0.88001
C	0.17765	-3.47837	-0.18605
O	1.39019	-3.76854	-0.09727
P	0.00798	1.23432	-1.54854
C	1.78555	0.58375	-1.68578
C	2.61935	1.12184	-2.68222
N	2.18598	-0.43842	-0.89663
C	3.91402	0.59095	-2.83441
C	4.33001	-0.47387	-2.04046
C	3.41046	-0.99418	-1.09359
N	3.68823	-2.12430	-0.31732
C	4.97200	-2.59807	0.00380
O	5.98525	-1.99324	-0.32723
H	1.95735	0.98996	2.52500
C	-3.80698	-0.25431	1.29009
C	-1.47450	-0.69976	2.95772
H	-3.61588	-2.34040	-0.32136
H	0.40474	-1.81240	1.00694
C	-3.13215	-4.72573	-1.57253
C	-0.42520	-5.52119	-1.49085

C	-0.93412	0.05107	-2.61722
C	0.14374	2.76207	-2.60962
H	2.28170	1.93492	-3.33719
H	4.59139	1.00579	-3.59891
H	5.32760	-0.91998	-2.12917
H	2.84952	-2.70475	-0.08143
C	5.01400	-3.92749	0.79994
O	1.69183	-1.06956	1.79540
H	2.35369	-1.76619	2.00730
H	1.93808	-0.72434	0.87568
C	-6.63774	-0.20270	1.37946
C	-5.96872	-0.15654	0.14324
C	-4.56524	-0.17180	0.09800
C	-4.48704	-0.29938	2.52632
C	-5.89317	-0.26840	2.56727
H	-7.73908	-0.18566	1.41482
H	-6.54461	-0.10552	-0.79543
H	-4.05551	-0.12393	-0.87735
H	-3.92328	-0.36268	3.46986
H	-6.40699	-0.30279	3.54192
C	-0.89790	-1.36640	5.63969
C	-0.66631	-0.06255	5.17159
C	-0.94896	0.26929	3.83509
C	-1.70968	-2.01025	3.43481
C	-1.41821	-2.33962	4.76772
H	-0.66980	-1.62759	6.68595
H	-0.25307	0.70371	5.84748
H	-0.73940	1.28545	3.46749
H	-2.12816	-2.78009	2.76621
H	-1.60031	-3.36562	5.12678
C	0.43125	5.13072	-4.13360
C	1.07716	5.00787	-2.88928
C	0.93111	3.83617	-2.13054
C	-0.48289	2.88420	-3.86753
C	-0.34480	4.06675	-4.61943
H	0.54288	6.05225	-4.72755
H	1.70606	5.82887	-2.50790
H	1.46070	3.74760	-1.16730
H	-1.07448	2.05259	-4.27931
H	-0.84207	4.14597	-5.59991
C	-2.44605	-1.64824	-4.29782
C	-3.05012	-0.52488	-3.70490
C	-2.30297	0.31001	-2.85884
C	-0.33505	-1.07554	-3.21899
C	-1.09217	-1.92301	-4.04741
H	-3.03251	-2.30915	-4.95628
H	-4.11078	-0.29776	-3.90305
H	-2.78368	1.18714	-2.39475
H	0.72793	-1.30126	-3.04730
H	-0.61289	-2.80349	-4.50457
C	4.09396	-3.85844	2.04425
C	6.46959	-4.16711	1.24455
C	4.55228	-5.07556	-0.13582
H	4.22939	-4.77364	2.66163
H	3.01700	-3.82202	1.76671
H	4.34969	-2.98713	2.69015
H	5.19693	-5.13352	-1.04021
H	3.49565	-4.94919	-0.45439

H	4.63190	-6.04741	0.40066
H	6.54239	-5.13351	1.78947
H	6.82771	-3.35790	1.91665
H	7.15503	-4.19993	0.37275
H	0.63486	-5.81413	-1.44104
C	-1.37263	-6.32252	-2.13142
C	-2.73001	-5.92125	-2.16905
H	-4.19025	-4.41732	-1.60146
H	-3.47507	-6.55999	-2.67122
H	-1.06669	-7.26984	-2.60396
C	2.77438	2.96780	1.93207
C	4.82062	4.93840	1.95666
C	5.08005	3.64045	2.43003
C	4.07001	2.66724	2.42097
C	2.52363	4.28479	1.47099
C	3.53548	5.25572	1.48107
H	5.61316	5.70390	1.96911
H	6.08057	3.38226	2.81418
H	4.28355	1.65168	2.79361
H	1.51119	4.55455	1.13005
H	3.31618	6.27652	1.12618

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	13.54	0.05183	YES	YES
8	a	17.85	0.12967	YES	YES
9	a	19.14	0.02844	YES	YES
10	a	21.79	0.04588	YES	YES
11	a	27.51	0.08133	YES	YES
12	a	30.02	0.17297	YES	YES
13	a	38.23	0.01893	YES	YES
14	a	40.96	0.48673	YES	YES
15	a	43.74	0.32206	YES	YES
16	a	44.58	0.04586	YES	YES
17	a	48.00	0.92220	YES	YES
18	a	50.89	0.01895	YES	YES
19	a	54.36	0.58549	YES	YES
20	a	56.84	0.24063	YES	YES
21	a	58.19	0.04223	YES	YES
22	a	61.31	0.04587	YES	YES
23	a	63.38	0.37304	YES	YES
24	a	69.54	1.10292	YES	YES
25	a	73.22	0.33192	YES	YES
26	a	73.93	1.03710	YES	YES
27	a	76.04	0.03648	YES	YES
28	a	82.06	0.59540	YES	YES
29	a	83.04	1.27107	YES	YES

30	a	89.35	0.62440	YES	YES
31	a	93.19	0.93366	YES	YES
32	a	96.24	0.55837	YES	YES
33	a	101.45	0.38727	YES	YES
34	a	104.61	1.09061	YES	YES
35	a	110.58	0.69701	YES	YES
36	a	123.17	0.28040	YES	YES
37	a	129.83	3.26193	YES	YES
38	a	136.75	2.45050	YES	YES
39	a	149.49	0.43080	YES	YES
40	a	158.43	1.66098	YES	YES
41	a	164.22	2.66774	YES	YES
42	a	171.67	1.82364	YES	YES
43	a	180.31	1.09965	YES	YES
44	a	189.29	1.38109	YES	YES
45	a	190.77	1.28633	YES	YES
46	a	193.67	1.39865	YES	YES
47	a	201.35	1.12455	YES	YES
48	a	209.57	3.92256	YES	YES
49	a	213.36	1.86683	YES	YES
50	a	215.78	2.79148	YES	YES

./6/6a_open

BP86/SV(P) energy (au): -3330.8745927940

PBE0/def2-TZVPP energy (au): -3330.391003605
cosmo_dcm Total energy + OC corr. = -3330.4467126723
cosmo_acetone Total energy + OC corr. = -3330.4531615968

Zero point energy (au): 0.9143085
Entropy (kJ mol^-1): 1.45065
Chemical potential (kJ mol^-1): 2133.53

XYZ coordinates:

117

C	3.37200	-1.25092	-1.50515
C	2.61116	-2.12082	-2.37095
C	3.11659	0.09478	-1.91847
C	1.88574	-1.32768	-3.30128
C	2.16624	0.05930	-2.99755
H	4.06541	-1.56869	-0.71762
H	2.62822	-3.21826	-2.32462
H	3.56539	0.99748	-1.48284
H	1.25898	-1.68526	-4.12645
H	1.79866	0.92821	-3.55735
Ru	1.14133	-0.74363	-1.13884
C	1.78929	1.04879	1.38136
C	1.34872	0.31554	0.35723
C	-2.56402	0.18568	-0.98566
P	-0.88259	0.36460	-1.77410
C	-1.43888	0.04752	-3.52602
C	-0.58295	2.19855	-1.66067
C	-0.11383	2.96814	-2.70499
N	-0.76945	2.76053	-0.41390
C	0.14596	4.37576	-2.50493
C	-0.08578	4.95332	-1.21856
C	-0.56627	4.12037	-0.09099
O	-0.79127	4.52780	1.04682
C	-0.69532	-3.86483	-0.52264
P	0.50004	-2.63433	0.19195
C	2.02449	-3.66765	0.49787
C	-0.04098	-2.45303	1.99402
C	0.11413	-3.58556	2.81437
N	-0.48060	-1.27160	2.46654
C	-0.19493	-3.46273	4.18152
C	-0.61327	-2.23780	4.69471
C	-0.74861	-1.14116	3.79990
N	-1.15357	0.12199	4.21538
C	-1.43139	0.55691	5.52472
C	-1.91569	2.02594	5.62146
O	-1.31450	-0.17624	6.49924
H	1.62006	0.58273	2.37413
H	0.04312	2.53361	-3.70250

H	-1.07212	2.16528	0.39875
H	0.48745	-4.53619	2.40769
H	-0.08770	-4.33130	4.85174
H	-0.83506	-2.07962	5.75791
H	-1.28564	0.80498	3.44213
C	0.14563	6.32857	-1.00432
C	0.61137	5.21600	-3.55289
C	-5.18151	-0.17015	0.02373
C	-4.26088	-1.23099	0.05688
C	-2.95898	-1.05205	-0.44349
C	-3.50079	1.24354	-1.03881
C	-4.79702	1.06613	-0.52727
H	-6.20046	-0.30581	0.42122
H	-4.55520	-2.20793	0.47397
H	-2.25077	-1.89340	-0.41749
H	-3.22162	2.21941	-1.46583
H	-5.51327	1.90306	-0.56373
C	-2.52249	-0.63426	-6.05265
C	-2.60279	0.68610	-5.58004
C	-2.07937	1.02578	-4.32100
C	-1.39212	-1.28256	-3.99617
C	-1.92788	-1.62176	-5.24956
H	-2.93805	-0.89693	-7.03905
H	-3.08742	1.46452	-6.19162
H	-2.18516	2.05970	-3.96085
H	-0.95687	-2.06850	-3.35988
H	-1.88769	-2.66728	-5.59658
C	-2.42226	-5.77270	-1.70448
C	-2.60943	-5.37958	-0.36937
C	-1.75053	-4.43675	0.22248
C	-0.52399	-4.25725	-1.87042
C	-1.37290	-5.21202	-2.45304
H	-3.09437	-6.51562	-2.16343
H	-3.43007	-5.81367	0.22490
H	-1.91329	-4.14850	1.27235
H	0.29026	-3.82023	-2.47079
H	-1.21489	-5.51730	-3.50031
C	4.36970	-5.13589	1.07439
C	3.34378	-5.71462	0.31151
C	2.17138	-4.98833	0.02684
C	3.06188	-3.08976	1.26670
C	4.22335	-3.82145	1.55575
H	5.28293	-5.70982	1.30048
H	3.44588	-6.74664	-0.06207
H	1.36883	-5.46904	-0.55405
H	2.96030	-2.05964	1.64879
H	5.01983	-3.36287	2.16435
H	-1.13771	0.17245	1.64298
O	-1.60559	1.07704	1.64580
H	-2.55121	0.88925	1.44709
C	-3.31715	2.12668	4.96416
C	-0.92815	2.98584	4.91060
C	-2.01686	2.39247	7.11477
H	-1.23566	4.03715	5.10258
H	-0.90691	2.86464	3.80518
H	0.10635	2.86463	5.30133
H	-2.39570	3.43224	7.22042
H	-1.02654	2.32936	7.61393

H	-2.70436	1.70853	7.65434
H	-3.28753	1.89409	3.87727
H	-3.70515	3.16413	5.06905
H	-4.04303	1.43987	5.45298
C	0.60443	7.13702	-2.04834
H	-0.04569	6.73311	0.00199
C	0.83767	6.57511	-3.32543
H	0.78990	4.78406	-4.55198
H	1.19746	7.21464	-4.14822
H	0.78292	8.21144	-1.87947
C	2.51394	2.33370	1.38002
C	4.00788	4.74504	1.45905
C	3.43187	4.30551	0.25340
C	2.68917	3.11748	0.21207
C	3.08703	2.79513	2.59058
C	3.82809	3.98513	2.62753
H	4.58848	5.68122	1.48840
H	3.55082	4.90252	-0.66536
H	2.21720	2.80338	-0.73287
H	2.95389	2.20501	3.51288
H	4.26576	4.32416	3.58085

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	8.42	0.06224	YES	YES
8	a	15.42	0.00665	YES	YES
9	a	18.83	0.00921	YES	YES
10	a	20.57	0.02250	YES	YES
11	a	24.59	0.01769	YES	YES
12	a	28.31	0.05227	YES	YES
13	a	32.45	0.39552	YES	YES
14	a	35.33	0.03190	YES	YES
15	a	37.01	0.48349	YES	YES
16	a	40.32	0.19910	YES	YES
17	a	44.07	0.72087	YES	YES
18	a	45.70	0.25345	YES	YES
19	a	49.62	0.12999	YES	YES
20	a	51.08	0.22343	YES	YES
21	a	52.93	0.19499	YES	YES
22	a	53.61	0.00406	YES	YES
23	a	58.74	0.20290	YES	YES
24	a	62.80	0.11569	YES	YES
25	a	63.51	0.55196	YES	YES
26	a	70.06	0.59646	YES	YES
27	a	71.73	0.15252	YES	YES
28	a	74.08	0.92347	YES	YES
29	a	80.21	1.25332	YES	YES

30	a	83.47	0.06450	YES	YES
31	a	87.75	0.22712	YES	YES
32	a	90.90	0.28331	YES	YES
33	a	95.53	1.44695	YES	YES
34	a	109.29	0.24472	YES	YES
35	a	113.89	0.63182	YES	YES
36	a	120.25	0.79352	YES	YES
37	a	127.40	1.04452	YES	YES
38	a	134.34	0.86700	YES	YES
39	a	141.55	1.72284	YES	YES
40	a	154.66	4.91913	YES	YES
41	a	159.09	1.82706	YES	YES
42	a	175.76	0.18435	YES	YES
43	a	178.03	3.62673	YES	YES
44	a	185.57	0.23281	YES	YES
45	a	188.16	2.06339	YES	YES
46	a	193.51	3.20440	YES	YES
47	a	198.09	3.16834	YES	YES
48	a	206.47	0.38052	YES	YES
49	a	207.57	0.49546	YES	YES
50	a	210.89	1.85522	YES	YES

./6/b

BP86/SV(P) energy (au): -3330.8856981390

PBE0/def2-TZVPP energy (au): -3330.403068237
cosmo_dcm Total energy + OC corr. = -3330.4538683581
cosmo_acetone Total energy + OC corr. = -3330.4596378132

Zero point energy (au): 0.9142040
Entropy (kJ mol^-1): 1.43356
Chemical potential (kJ mol^-1): 2138.12

XYZ coordinates:

117

C	-2.34779	3.19668	2.00281
C	-2.40164	3.71565	0.66423
C	-3.20902	2.05432	2.06307
C	-3.33564	2.91123	-0.08449
C	-3.84316	1.89565	0.77083
H	-1.74823	3.60682	2.82623
H	-1.88285	4.60999	0.29914
H	-3.41998	1.45116	2.95591
H	-3.61758	3.07736	-1.13263
H	-4.60387	1.14804	0.51838
Ru	-1.50994	1.61314	0.58592
C	1.28374	2.99272	1.04528
C	0.21489	2.19657	0.92898
P	-1.52076	-0.66321	1.42581
C	-0.85905	-2.14845	0.50341
C	-1.61989	-3.21453	0.07485
N	0.50066	-2.14389	0.27910
C	-0.98901	-4.31385	-0.61411
C	0.41619	-4.26834	-0.87739
C	1.20600	-3.11507	-0.41793
O	2.43269	-2.97958	-0.60662
P	-0.80275	1.22340	-1.65686
C	1.01673	1.19112	-2.17892
C	1.41601	1.89506	-3.32787
N	1.87835	0.42761	-1.47353
C	2.76519	1.81131	-3.72513
C	3.65786	1.01301	-3.01521
C	3.16268	0.29231	-1.89601
N	3.94224	-0.60607	-1.16627
C	5.34711	-0.60518	-1.10365
O	6.01722	0.25285	-1.66711
H	1.27657	3.79245	0.27075
C	-3.25865	-1.22616	1.80344
C	-0.68899	-0.85644	3.07277
H	-2.69910	-3.25524	0.26673
H	1.10929	-1.38859	0.71552
C	-1.72382	-5.45125	-1.04738
C	1.04905	-5.33201	-1.55971

C	-1.49599	-0.26793	-2.50310
C	-1.39456	2.64077	-2.71778
H	0.70716	2.49674	-3.91092
H	3.11067	2.36443	-4.61415
H	4.71422	0.92023	-3.29324
H	3.41044	-1.39793	-0.73851
C	5.97930	-1.75628	-0.28227
O	1.92099	-0.09988	1.22326
H	2.84465	-0.09779	1.55661
H	1.93851	0.25805	0.27403
C	-5.91428	-2.05505	2.33686
C	-5.50158	-1.81141	1.01467
C	-4.18797	-1.39149	0.75033
C	-3.68036	-1.47687	3.12733
C	-5.00174	-1.88302	3.38915
H	-6.94690	-2.37932	2.54466
H	-6.20939	-1.94897	0.18054
H	-3.87860	-1.20312	-0.29010
H	-2.97861	-1.35994	3.96729
H	-5.31364	-2.07186	4.42928
C	0.38625	-1.18259	5.66408
C	0.03129	0.09653	5.20346
C	-0.49580	0.25966	3.91067
C	-0.33554	-2.14128	3.54326
C	0.20568	-2.29930	4.82950
H	0.80611	-1.30958	6.67537
H	0.17406	0.97776	5.85008
H	-0.74498	1.26642	3.54150
H	-0.48830	-3.02929	2.90875
H	0.48463	-3.30558	5.18213
C	-2.17368	4.87582	-4.27436
C	-1.35599	5.05330	-3.14306
C	-0.97399	3.94642	-2.37052
C	-2.19583	2.46989	-3.86608
C	-2.58795	3.58385	-4.63304
H	-2.47882	5.74494	-4.87943
H	-1.01013	6.06168	-2.86265
H	-0.31947	4.09826	-1.49709
H	-2.51177	1.46438	-4.18236
H	-3.21647	3.43186	-5.52577
C	-2.65183	-2.47620	-3.83583
C	-3.47498	-1.51491	-3.22206
C	-2.90074	-0.42518	-2.54842
C	-0.67731	-1.23557	-3.12182
C	-1.25612	-2.33619	-3.77820
H	-3.10056	-3.33471	-4.36115
H	-4.57208	-1.61334	-3.26993
H	-3.55408	0.32616	-2.07392
H	0.41829	-1.13909	-3.09678
H	-0.60477	-3.08756	-4.25274
C	5.30890	-1.88470	1.10755
C	7.47876	-1.44666	-0.10859
C	5.80305	-3.07590	-1.08004
H	5.84317	-2.65448	1.70718
H	4.24817	-2.20972	1.03727
H	5.36527	-0.92689	1.67291
H	6.27034	-2.99664	-2.08617
H	4.73246	-3.34682	-1.19990

H	6.30696	-3.90709	-0.53768
H	7.97050	-2.27381	0.44848
H	7.63535	-0.50238	0.45592
H	7.98261	-1.33374	-1.09055
H	2.13275	-5.26575	-1.74286
C	0.30599	-6.43847	-1.97683
C	-1.08455	-6.49563	-1.71641
H	-2.80675	-5.50028	-0.84544
H	-1.66608	-7.37377	-2.04221
H	0.80049	-7.27022	-2.50422
C	2.44747	3.03228	1.94698
C	4.73964	3.20256	3.61787
C	4.62853	4.02525	2.48404
C	3.49592	3.94260	1.66033
C	2.56844	2.21366	3.09904
C	3.70246	2.29990	3.91956
H	5.62763	3.26760	4.26730
H	5.43136	4.73875	2.23621
H	3.42075	4.59230	0.77201
H	1.76601	1.50390	3.34613
H	3.77536	1.65670	4.81240

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.36	0.03239	YES	YES
8	a	17.06	0.15966	YES	YES
9	a	21.17	0.12823	YES	YES
10	a	23.74	0.04089	YES	YES
11	a	27.10	0.11957	YES	YES
12	a	29.00	0.03885	YES	YES
13	a	31.01	0.06600	YES	YES
14	a	37.50	0.82369	YES	YES
15	a	41.35	0.05633	YES	YES
16	a	44.46	0.02892	YES	YES
17	a	48.61	0.03162	YES	YES
18	a	51.82	0.75615	YES	YES
19	a	52.63	0.55800	YES	YES
20	a	55.59	0.24761	YES	YES
21	a	56.07	0.14574	YES	YES
22	a	60.33	0.03815	YES	YES
23	a	64.04	0.55267	YES	YES
24	a	68.28	0.19767	YES	YES
25	a	71.15	0.42237	YES	YES
26	a	71.95	0.88997	YES	YES
27	a	76.85	0.71856	YES	YES
28	a	80.50	2.25691	YES	YES
29	a	85.76	1.48856	YES	YES

30	a	89.71	0.92167	YES	YES
31	a	90.08	0.04906	YES	YES
32	a	93.78	0.15261	YES	YES
33	a	100.46	0.69831	YES	YES
34	a	102.97	2.06585	YES	YES
35	a	107.05	0.61045	YES	YES
36	a	123.52	0.83604	YES	YES
37	a	129.56	3.47104	YES	YES
38	a	129.79	3.41571	YES	YES
39	a	133.46	0.14145	YES	YES
40	a	153.62	0.07577	YES	YES
41	a	163.65	4.30332	YES	YES
42	a	170.90	0.93141	YES	YES
43	a	177.08	4.72495	YES	YES
44	a	179.88	0.90893	YES	YES
45	a	189.10	2.21520	YES	YES
46	a	192.79	0.83194	YES	YES
47	a	203.17	0.67160	YES	YES
48	a	208.60	1.60260	YES	YES
49	a	210.09	4.83898	YES	YES
50	a	215.23	1.96575	YES	YES

./6/6b_open

BP86/SV(P) energy (au): -3330.8798263200

PBE0/def2-TZVPP energy (au): -3330.395188262
cosmo_dcm Total energy + OC corr. = -3330.4479970218
cosmo_acetone Total energy + OC corr. = -3330.4540645630

Zero point energy (au): 0.9147197
Entropy (kJ mol^-1): 1.45510
Chemical potential (kJ mol^-1): 2132.85

XYZ coordinates:

117

C	3.52204	-0.82903	0.76912
C	3.14329	-1.00567	2.14497
C	3.04995	-1.96687	0.03142
C	2.46332	-2.26343	2.27480
C	2.38844	-2.83874	0.96202
H	4.08601	0.01778	0.35575
H	3.39178	-0.32375	2.96711
H	3.18240	-2.14708	-1.04315
H	2.15040	-2.72745	3.21805
H	1.94088	-3.80891	0.70775
Ru	1.24749	-0.81870	0.85795
C	1.61244	1.11914	-1.62277
C	1.28581	0.39115	-0.55682
C	-2.42642	-1.63170	-0.19841
P	-0.64187	-2.13232	0.03954
C	-0.96053	-3.79757	0.81046
C	-0.10635	-2.54530	-1.69079
C	0.41332	-3.75928	-2.07987
N	-0.07863	-1.46785	-2.55688
C	0.99648	-3.90357	-3.39513
C	1.09037	-2.75833	-4.24773
C	0.57437	-1.44896	-3.79794
O	0.68914	-0.38316	-4.41628
C	-1.19826	0.25346	3.37845
P	0.21356	0.77580	2.29073
C	1.43635	1.39991	3.56036
C	-0.38818	2.42218	1.59025
C	-0.29121	3.57126	2.39504
N	-0.89692	2.45653	0.34124
C	-0.73979	4.79588	1.86313
C	-1.23378	4.85311	0.56309
C	-1.29229	3.64763	-0.18909
N	-1.74453	3.60006	-1.50224
C	-2.19375	4.66171	-2.30500
C	-2.60030	4.24566	-3.74202
O	-2.26370	5.81467	-1.89635
H	1.30582	0.67187	-2.60076
H	0.40279	-4.62062	-1.39636

H	-0.54378	-0.56202	-2.27968
H	0.11744	3.52064	3.41377
H	-0.68801	5.71424	2.47083
H	-1.57079	5.78486	0.09171
H	-1.71036	2.65377	-1.92896
C	1.68751	-2.86584	-5.52241
C	1.51002	-5.14222	-3.86481
C	-5.19151	-1.07650	-0.44788
C	-4.53768	-0.88206	0.77965
C	-3.16561	-1.15933	0.90550
C	-3.09302	-1.84171	-1.42942
C	-4.46480	-1.55864	-1.55066
H	-6.26708	-0.85800	-0.54629
H	-5.09699	-0.51368	1.65447
H	-2.67553	-1.01566	1.87836
H	-2.54700	-2.21835	-2.30838
H	-4.96794	-1.72369	-2.51760
C	-1.58650	-6.29308	1.98984
C	-2.09461	-5.96319	0.72048
C	-1.79492	-4.72263	0.13752
C	-0.46851	-4.13317	2.08694
C	-0.77756	-5.37289	2.67439
H	-1.82841	-7.26652	2.44681
H	-2.73869	-6.67536	0.17923
H	-2.21828	-4.47641	-0.84918
H	0.15812	-3.41339	2.63184
H	-0.38336	-5.61859	3.67403
C	-3.25282	-0.60072	5.12470
C	-3.34195	0.64668	4.48373
C	-2.31979	1.07697	3.61873
C	-1.11778	-0.99970	4.02570
C	-2.13437	-1.42269	4.89709
H	-4.05460	-0.93332	5.80379
H	-4.21312	1.29843	4.66024
H	-2.40494	2.05893	3.12926
H	-0.24566	-1.64835	3.84694
H	-2.05587	-2.40132	5.39778
C	3.33757	2.40043	5.40759
C	2.19096	1.73280	5.86382
C	1.24135	1.23929	4.94792
C	2.59963	2.06841	3.10989
C	3.53773	2.56954	4.02442
H	4.07536	2.79146	6.12678
H	2.02169	1.59735	6.94465
H	0.34145	0.73582	5.33205
H	2.78018	2.19862	2.03041
H	4.43295	3.09465	3.65347
H	-1.17475	1.19591	-0.83349
O	-1.51376	0.79294	-1.71431
H	-2.40881	0.43162	-1.51982
C	-3.80820	3.27648	-3.66950
C	-1.40945	3.55869	-4.45835
C	-3.00616	5.51928	-4.50778
H	-1.68570	3.34995	-5.51561
H	-1.12364	2.58713	-3.99961
H	-0.51247	4.21559	-4.46679
H	-3.32033	5.25355	-5.54078
H	-2.16142	6.23741	-4.57308

H	-3.84702	6.04262	-4.00642
H	-3.55347	2.32055	-3.16053
H	-4.14491	3.02084	-4.69865
H	-4.66810	3.73937	-3.13663
C	2.17980	-4.09619	-5.96620
H	1.74495	-1.96050	-6.14678
C	2.08971	-5.23521	-5.13209
H	1.44575	-6.03297	-3.21777
H	2.48034	-6.20392	-5.48432
H	2.63876	-4.18064	-6.96449
C	2.32466	2.40636	-1.75084
C	3.74621	4.83470	-2.11516
C	3.22147	4.50225	-0.85350
C	2.51627	3.30334	-0.67221
C	2.84071	2.76205	-3.02259
C	3.54761	3.96069	-3.19848
H	4.29844	5.77801	-2.25570
H	3.35297	5.19141	-0.00267
H	2.07570	3.07258	0.31029
H	2.68219	2.08128	-3.87526
H	3.94475	4.21685	-4.19449

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	4.77	0.04860	YES	YES
8	a	12.78	0.03593	YES	YES
9	a	16.34	0.01704	YES	YES
10	a	19.71	0.04766	YES	YES
11	a	21.51	0.08069	YES	YES
12	a	25.16	0.04976	YES	YES
13	a	30.82	0.03384	YES	YES
14	a	34.41	0.09514	YES	YES
15	a	37.47	0.05083	YES	YES
16	a	40.62	0.37992	YES	YES
17	a	43.54	0.31156	YES	YES
18	a	49.06	0.30883	YES	YES
19	a	50.42	0.40862	YES	YES
20	a	50.67	0.43904	YES	YES
21	a	53.63	0.99778	YES	YES
22	a	54.68	1.09135	YES	YES
23	a	58.98	0.19497	YES	YES
24	a	61.44	1.25692	YES	YES
25	a	68.11	0.07503	YES	YES
26	a	72.15	0.09521	YES	YES
27	a	75.02	1.25943	YES	YES
28	a	78.10	1.32632	YES	YES
29	a	79.64	0.26135	YES	YES

30	a	83.14	0.52406	YES	YES
31	a	90.59	0.46899	YES	YES
32	a	90.94	0.92228	YES	YES
33	a	99.83	2.81117	YES	YES
34	a	110.22	0.92207	YES	YES
35	a	112.96	1.43989	YES	YES
36	a	119.66	0.23362	YES	YES
37	a	129.71	0.09180	YES	YES
38	a	138.71	2.30159	YES	YES
39	a	150.29	1.75616	YES	YES
40	a	158.69	3.03033	YES	YES
41	a	162.35	2.80502	YES	YES
42	a	170.28	0.47733	YES	YES
43	a	180.57	3.34266	YES	YES
44	a	186.52	4.36984	YES	YES
45	a	188.03	0.59139	YES	YES
46	a	199.03	4.13868	YES	YES
47	a	200.97	3.52751	YES	YES
48	a	203.30	3.66160	YES	YES
49	a	210.19	1.93609	YES	YES
50	a	210.59	3.15102	YES	YES

./7/a

BP86/SV(P) energy (au): -3330.8963288340

PBE0/def2-TZVPP energy (au): -3330.412125205
cosmo_dcm Total energy + OC corr. = -3330.4612262075
cosmo_acetone Total energy + OC corr. = -3330.4667080755

Zero point energy (au): 0.9179134
Entropy (kJ mol^-1): 1.39961
Chemical potential (kJ mol^-1): 2154.11

XYZ coordinates:

117

C	-1.17683	0.40138	3.88067
C	0.19484	0.01678	4.06118
C	-1.20573	1.74702	3.39569
C	1.01235	1.15453	3.70448
C	0.16266	2.22150	3.29917
H	-2.04914	-0.22832	4.09545
H	0.54385	-0.92622	4.49351
H	-2.10562	2.34769	3.20871
H	2.10747	1.19589	3.77356
H	0.47336	3.23290	3.01141
Ru	-0.15301	0.46079	1.85726
C	-1.99180	-2.16610	1.75029
C	-1.26844	-1.16122	1.16637
P	-1.08874	1.88454	0.21056
C	-0.49813	1.89406	-1.56685
C	-0.03140	2.94574	-2.31894
N	-0.60624	0.64688	-2.15461
C	0.33140	2.73138	-3.70007
C	0.21284	1.42358	-4.27626
C	-0.27976	0.31263	-3.45440
O	-0.41453	-0.87189	-3.84764
P	1.81868	-0.27650	0.87584
C	2.00133	-1.86475	-0.17500
C	3.13197	-2.68481	-0.15653
N	0.97577	-2.21716	-1.00622
C	3.16225	-3.84437	-0.96168
C	2.10587	-4.16139	-1.81544
C	0.99465	-3.28740	-1.86599
N	-0.07937	-3.38297	-2.72271
C	-0.49023	-4.58488	-3.35970
O	0.03938	-5.65075	-3.08483
H	-2.64628	-2.75710	1.06584
C	-1.00940	3.70006	0.61832
C	-2.91768	1.66419	-0.11432
H	0.04599	3.95290	-1.88750
H	-1.02067	-0.10242	-1.56456
C	0.80038	3.79021	-4.52518
C	0.55938	1.20448	-5.63002

C	2.73971	0.90056	-0.23843
C	3.13323	-0.75027	2.12349
H	3.98408	-2.42825	0.48642
H	4.04794	-4.50015	-0.93443
H	2.11342	-5.04862	-2.45882
H	-0.44852	-2.45684	-3.06714
C	-1.61789	-4.42503	-4.40027
O	-1.43127	-1.19860	-0.28557
H	-2.14425	-1.84939	-0.51721
H	0.04302	-1.72685	-0.86826
C	-0.83523	6.43993	1.32012
C	0.32163	5.72745	0.95635
C	0.23756	4.36675	0.61911
C	-2.16551	4.42409	0.98211
C	-2.07524	5.78261	1.33666
H	-0.76805	7.50600	1.59153
H	1.30027	6.23544	0.93874
H	1.15329	3.81755	0.34932
H	-3.15030	3.93151	0.98788
H	-2.98856	6.32964	1.62225
C	-5.70616	1.42639	-0.52687
C	-4.90707	2.09469	-1.47167
C	-3.52330	2.21662	-1.26643
C	-3.72547	0.99045	0.82508
C	-5.11252	0.87680	0.62128
H	-6.79293	1.33464	-0.68729
H	-5.36430	2.52916	-2.37585
H	-2.91295	2.75494	-2.00996
H	-3.26138	0.53503	1.71305
H	-5.73179	0.35040	1.36615
C	5.02969	-1.60276	4.04764
C	3.76531	-2.21627	3.98133
C	2.82482	-1.78945	3.03132
C	4.41092	-0.15482	2.18290
C	5.34816	-0.57493	3.14640
H	5.76707	-1.93131	4.79791
H	3.50949	-3.03331	4.67563
H	1.83840	-2.27821	2.98440
H	4.69330	0.63654	1.47239
H	6.33948	-0.09420	3.18235
C	4.15015	2.80027	-1.79547
C	3.80801	3.09290	-0.46311
C	3.09399	2.15802	0.30357
C	3.09198	0.61532	-1.57425
C	3.78322	1.56387	-2.34946
H	4.70418	3.53623	-2.40039
H	4.09786	4.05882	-0.01716
H	2.81989	2.40205	1.34318
H	2.83579	-0.35299	-2.03120
H	4.04135	1.32642	-3.39409
C	-1.00669	-3.74883	-5.65858
C	-2.77595	-3.55890	-3.84574
C	-2.13730	-5.83135	-4.75721
H	-2.92220	-5.75211	-5.54041
H	-2.57762	-6.33867	-3.87193
H	-1.32093	-6.47799	-5.13992
H	-0.63593	-2.72456	-5.43861
H	-1.78781	-3.66645	-6.44661

H	-0.17104	-4.35527	-6.07165
H	-3.17878	-3.97768	-2.89653
H	-3.60902	-3.54312	-4.58245
H	-2.47388	-2.50167	-3.68034
H	0.89267	4.80170	-4.09664
C	1.13524	3.55827	-5.85931
C	1.01633	2.26222	-6.41732
H	0.45377	0.18892	-6.04216
H	1.49338	4.39169	-6.48574
H	1.28116	2.09206	-7.47339
C	-2.11578	-2.61497	3.15666
C	-2.44113	-3.59589	5.80975
C	-3.55758	-3.16406	5.07213
C	-3.39653	-2.68678	3.76169
C	-1.01059	-3.08306	3.90498
C	-1.16738	-3.56146	5.21639
H	-2.56576	-3.97493	6.83716
H	-4.56424	-3.20334	5.52048
H	-4.28040	-2.35848	3.18821
H	-0.01942	-3.10375	3.42415
H	-0.29058	-3.92942	5.77527

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	10.95	0.03002	YES	YES
8	a	19.48	0.05727	YES	YES
9	a	19.98	0.02127	YES	YES
10	a	27.23	0.04007	YES	YES
11	a	29.80	0.01956	YES	YES
12	a	34.35	0.60274	YES	YES
13	a	37.04	0.07575	YES	YES
14	a	39.28	0.40231	YES	YES
15	a	40.90	0.32387	YES	YES
16	a	46.12	0.31122	YES	YES
17	a	48.44	0.74966	YES	YES
18	a	51.02	0.49858	YES	YES
19	a	54.28	0.19772	YES	YES
20	a	55.13	0.15542	YES	YES
21	a	58.44	0.06138	YES	YES
22	a	60.58	0.44228	YES	YES
23	a	62.37	0.53042	YES	YES
24	a	69.39	0.55472	YES	YES
25	a	71.73	1.79921	YES	YES
26	a	74.20	1.40689	YES	YES
27	a	80.06	1.75773	YES	YES
28	a	84.12	0.19727	YES	YES
29	a	87.13	0.46260	YES	YES

30	a	92.26	0.57774	YES	YES
31	a	94.54	0.19219	YES	YES
32	a	98.52	0.41904	YES	YES
33	a	109.42	0.25525	YES	YES
34	a	113.03	3.25776	YES	YES
35	a	121.58	0.11907	YES	YES
36	a	131.33	1.58220	YES	YES
37	a	134.12	1.28477	YES	YES
38	a	147.02	1.58982	YES	YES
39	a	165.69	0.86937	YES	YES
40	a	172.78	0.90297	YES	YES
41	a	174.31	2.11972	YES	YES
42	a	180.67	0.71289	YES	YES
43	a	185.09	1.35206	YES	YES
44	a	189.35	2.88831	YES	YES
45	a	196.12	1.35805	YES	YES
46	a	203.52	2.70145	YES	YES
47	a	205.54	2.39198	YES	YES
48	a	208.73	3.81912	YES	YES
49	a	214.79	0.14911	YES	YES
50	a	219.90	1.21421	YES	YES

./7/b

BP86/SV(P) energy (au): -3330.9088577380

PBE0/def2-TZVPP energy (au): -3330.423916758
cosmo_dcm Total energy + OC corr. = -3330.4718202481
cosmo_acetone Total energy + OC corr. = -3330.4771596120

Zero point energy (au): 0.9186625
Entropy (kJ mol^-1): 1.41046
Chemical potential (kJ mol^-1): 2152.70

XYZ coordinates:

117

C	-2.62201	1.77968	2.85699
C	-1.41489	1.79389	3.63626
C	-2.55022	2.84044	1.89905
C	-0.60859	2.89209	3.15535
C	-1.29926	3.54480	2.09357
H	-3.46097	1.08221	2.98046
H	-1.18590	1.15656	4.49831
H	-3.33769	3.11800	1.18611
H	0.36119	3.19338	3.57385
H	-0.97147	4.43715	1.54665
Ru	-0.88583	1.35118	1.46755
C	-2.01157	-1.39262	2.36712
C	-1.43556	-0.64056	1.37052
P	-1.29533	1.72979	-0.80840
C	-0.16158	1.11460	-2.16042
C	0.49286	1.84183	-3.12605
N	-0.02933	-0.26301	-2.14926
C	1.29691	1.16208	-4.11364
C	1.42007	-0.26567	-4.07111
C	0.73201	-1.02206	-3.01859
O	0.79639	-2.26606	-2.86969
P	1.36325	0.81302	1.54044
C	2.11822	-0.92960	1.28469
C	3.31225	-1.31894	1.89418
N	1.47486	-1.84267	0.49778
C	3.79238	-2.63265	1.70839
C	3.11157	-3.54078	0.89899
C	1.93197	-3.11446	0.24349
N	1.19911	-3.85419	-0.65658
C	1.21857	-5.27478	-0.72359
O	1.81867	-5.93234	0.11335
H	-2.08982	-0.92943	3.36373
C	-1.44559	3.52917	-1.25604
C	-2.89348	1.02271	-1.47283
H	0.39154	2.93501	-3.16673
H	-0.57230	-0.78271	-1.43134
C	1.97254	1.86657	-5.14790
C	2.19831	-0.94530	-5.03734

C	2.54767	1.79263	0.49127
C	2.05060	1.00300	3.27243
H	3.85979	-0.60695	2.52710
H	4.72899	-2.94442	2.19925
H	3.46215	-4.56680	0.73998
H	0.78195	-3.30486	-1.45287
C	0.45762	-5.88959	-1.91591
O	-1.19579	-1.35148	0.14229
H	-1.61210	-2.25872	0.20556
H	0.48630	-1.61113	0.18970
C	-1.62807	6.29647	-1.82971
C	-0.39746	5.73302	-1.44611
C	-0.30880	4.36312	-1.14948
C	-2.67657	4.10220	-1.64260
C	-2.76549	5.47875	-1.92080
H	-1.69916	7.37313	-2.05445
H	0.50139	6.36706	-1.37102
H	0.65592	3.93840	-0.82908
H	-3.57781	3.47604	-1.73105
H	-3.73576	5.90992	-2.21705
C	-5.34516	0.01684	-2.46106
C	-4.37285	0.50659	-3.35161
C	-3.15573	1.00762	-2.86248
C	-3.87030	0.52194	-0.58864
C	-5.09168	0.02621	-1.07940
H	-6.30125	-0.37361	-2.84671
H	-4.56344	0.50092	-4.43748
H	-2.40672	1.39510	-3.57282
H	-3.66280	0.50346	0.49253
H	-5.84731	-0.35820	-0.37471
C	2.97570	1.14228	5.94204
C	1.92321	0.27136	5.60370
C	1.46043	0.20530	4.28059
C	3.11773	1.85891	3.61381
C	3.56973	1.93260	4.94579
H	3.33401	1.20031	6.98261
H	1.45896	-0.36124	6.37802
H	0.63687	-0.48182	4.02168
H	3.61475	2.46923	2.84397
H	4.40055	2.61140	5.19931
C	4.27401	3.41303	-1.06439
C	3.43979	3.99739	-0.09428
C	2.57142	3.19685	0.66508
C	3.38681	1.21718	-0.48671
C	4.23646	2.02402	-1.26448
H	4.95255	4.04147	-1.66376
H	3.46259	5.08711	0.07167
H	1.90639	3.67043	1.40589
H	3.39051	0.12902	-0.65577
H	4.87913	1.55648	-2.02801
C	1.32484	-5.66346	-3.18576
C	-0.93276	-5.23547	-2.10462
C	0.29573	-7.39876	-1.64873
H	-0.20549	-7.87943	-2.51652
H	-0.32058	-7.58444	-0.74281
H	1.27818	-7.89019	-1.49274
H	1.44748	-4.58250	-3.41358
H	0.82834	-6.14172	-4.05904

H	2.32967	-6.12608	-3.07130
H	-1.54197	-5.29593	-1.17580
H	-1.48398	-5.77583	-2.90520
H	-0.86234	-4.17316	-2.42501
H	1.88452	2.96443	-5.19438
C	2.73200	1.18038	-6.09590
C	2.84800	-0.22994	-6.04435
H	2.27167	-2.04204	-4.97622
H	3.24495	1.74088	-6.89482
H	3.44855	-0.76041	-6.80060
C	-2.47242	-2.79626	2.27237
C	-3.31734	-5.51974	2.14005
C	-2.61727	-5.04309	3.26472
C	-2.20264	-3.70564	3.32892
C	-3.21423	-3.28825	1.16118
C	-3.61948	-4.63447	1.09304
H	-3.64235	-6.57163	2.09141
H	-2.39286	-5.72477	4.10182
H	-1.65090	-3.34716	4.21438
H	-3.55243	-2.58972	0.37427
H	-4.20474	-4.98214	0.22549

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	6.49	0.03438	YES	YES
8	a	16.87	0.02911	YES	YES
9	a	18.66	0.03334	YES	YES
10	a	21.07	0.02336	YES	YES
11	a	27.44	0.05032	YES	YES
12	a	30.91	0.53892	YES	YES
13	a	32.96	0.17450	YES	YES
14	a	36.33	0.10351	YES	YES
15	a	41.28	0.22852	YES	YES
16	a	44.71	0.80201	YES	YES
17	a	47.88	0.18998	YES	YES
18	a	49.94	0.20374	YES	YES
19	a	52.98	0.41400	YES	YES
20	a	54.49	0.17199	YES	YES
21	a	55.84	0.27418	YES	YES
22	a	59.51	0.02526	YES	YES
23	a	64.18	0.45928	YES	YES
24	a	69.12	0.93523	YES	YES
25	a	70.95	0.23054	YES	YES
26	a	75.31	2.45116	YES	YES
27	a	78.40	0.71411	YES	YES
28	a	84.86	0.20503	YES	YES
29	a	86.55	0.09371	YES	YES

30	a	91.78	0.83483	YES	YES
31	a	96.28	0.64026	YES	YES
32	a	101.22	0.32506	YES	YES
33	a	115.21	2.69067	YES	YES
34	a	116.47	0.22411	YES	YES
35	a	126.56	0.45142	YES	YES
36	a	133.19	1.00817	YES	YES
37	a	135.96	1.81419	YES	YES
38	a	144.81	1.61249	YES	YES
39	a	157.67	0.25109	YES	YES
40	a	165.46	0.87528	YES	YES
41	a	176.36	0.55670	YES	YES
42	a	179.57	2.85272	YES	YES
43	a	185.57	1.16046	YES	YES
44	a	187.12	1.84880	YES	YES
45	a	196.33	0.94355	YES	YES
46	a	202.05	3.20965	YES	YES
47	a	205.08	0.80877	YES	YES
48	a	209.03	0.38145	YES	YES
49	a	211.18	1.50370	YES	YES
50	a	220.31	4.11069	YES	YES

./8/a

BP86/SV(P) energy (au): -3330.9110922350

PBE0/def2-TZVPP energy (au): -3330.426936755
cosmo_dcm Total energy + OC corr. = -3330.4798285825
cosmo_acetone Total energy + OC corr. = -3330.4858594977

Zero point energy (au): 0.9180849
Entropy (kJ mol^-1): 1.43730
Chemical potential (kJ mol^-1): 2144.80

XYZ coordinates:

117

C	1.27738	1.83864	3.45630
C	2.10732	2.44984	2.45333
C	-0.03794	2.39442	3.32565
C	1.32437	3.39682	1.71745
C	-0.01130	3.34351	2.24624
H	1.60088	1.14931	4.24538
H	3.18116	2.26555	2.31306
H	-0.89576	2.16377	3.97081
H	1.68398	4.06721	0.92905
H	-0.85123	3.97131	1.91964
Ru	0.42630	1.26589	1.37422
C	-0.20369	-1.22373	3.09611
C	-0.42859	-0.41487	1.81667
P	-1.15158	1.74929	-0.31445
C	-1.18012	0.82758	-1.93290
C	-1.09452	1.40593	-3.17892
N	-1.39939	-0.53042	-1.82120
C	-1.24177	0.58555	-4.36171
C	-1.49486	-0.81622	-4.22198
C	-1.59346	-1.43200	-2.88105
O	-1.81864	-2.62156	-2.64597
P	2.10461	0.16486	0.08258
C	1.70683	-1.25460	-1.07697
C	2.18140	-1.34491	-2.39567
N	1.04799	-2.25434	-0.46497
C	1.95867	-2.55370	-3.08732
C	1.29310	-3.60837	-2.46610
C	0.83966	-3.40520	-1.13704
N	0.14160	-4.37179	-0.41350
C	-0.38317	-5.59307	-0.85159
O	-0.12884	-6.06168	-1.95233
O	-1.38072	-0.98207	1.04344
H	-0.36739	-2.30733	2.85934
C	-1.12478	3.52312	-0.88354
C	-2.93811	1.54452	0.18780
H	-0.95792	2.49150	-3.28220
H	-1.43325	-0.94706	-0.87897
C	-1.16716	1.13183	-5.67147

C	-1.66434	-1.62765	-5.36479
C	3.11012	1.34759	-0.93836
C	3.43788	-0.71736	1.05490
H	2.73284	-0.52330	-2.87206
H	0.85845	-1.15136	3.39402
H	2.32012	-2.66875	-4.12235
H	1.09463	-4.56704	-2.96123
H	-0.09475	-4.06419	0.53327
C	-1.31469	-6.28776	0.17852
H	-1.68293	-1.86062	1.39252
C	5.49549	-2.08552	2.44128
C	4.50228	-1.39584	3.15293
C	3.48157	-0.71774	2.46145
C	4.44188	-1.42007	0.34698
C	5.46158	-2.09454	1.03504
H	6.29601	-2.61823	2.97991
H	4.51814	-1.38346	4.25509
H	2.70781	-0.17983	3.02412
H	4.43161	-1.44433	-0.75454
H	6.23525	-2.63510	0.46566
C	4.60293	3.20342	-2.47348
C	5.11021	2.72410	-1.25432
C	4.37448	1.79782	-0.49488
C	2.59928	1.85071	-2.15778
C	3.34708	2.76094	-2.92432
H	5.18828	3.91764	-3.07519
H	6.09516	3.06210	-0.89306
H	4.80356	1.41143	0.44275
H	1.61274	1.52184	-2.52416
H	2.94261	3.12553	-3.88277
C	-1.03153	6.21532	-1.76062
C	-2.23910	5.65965	-1.30816
C	-2.29049	4.32184	-0.87697
C	0.08802	4.09465	-1.32963
C	0.13223	5.42653	-1.77345
H	-0.99566	7.26311	-2.10055
H	-3.15744	6.26895	-1.29108
H	-3.24960	3.90569	-0.53465
H	1.01071	3.49428	-1.33524
H	1.08672	5.85109	-2.12567
C	-5.66089	1.41873	0.95043
C	-4.66899	1.67714	1.91150
C	-3.31663	1.73161	1.53319
C	-3.94210	1.28944	-0.77363
C	-5.29266	1.22095	-0.39138
H	-6.72167	1.37171	1.24608
H	-4.94639	1.83570	2.96645
H	-2.54598	1.91272	2.29757
H	-3.67685	1.15156	-1.83370
H	-6.06279	1.01584	-1.15301
C	-1.84954	-7.58274	-0.46253
C	-2.50088	-5.34938	0.51680
C	-0.51758	-6.63155	1.46145
H	-2.17754	-4.44189	1.07997
H	-3.23704	-5.88190	1.15900
H	-3.02281	-5.00719	-0.40312
H	-1.17122	-7.17441	2.17973
H	-0.13267	-5.72726	1.98693

H	0.35182	-7.28558	1.23241
H	-1.01895	-8.26296	-0.74411
H	-2.42612	-7.36472	-1.38578
H	-2.51415	-8.11405	0.25320
H	-1.86299	-2.70045	-5.21374
C	-1.58357	-1.06830	-6.64283
C	-1.33443	0.31597	-6.79258
H	-0.98111	2.21201	-5.79419
H	-1.27646	0.75596	-7.80184
H	-1.71813	-1.70222	-7.53410
C	-1.08819	-0.83061	4.27989
C	-2.68916	-0.19299	6.53190
C	-1.30029	-0.34774	6.67333
C	-0.50893	-0.66329	5.55571
C	-2.48578	-0.67671	4.15058
C	-3.27846	-0.36038	5.26682
H	-3.31276	0.05148	7.40694
H	-0.82663	-0.22731	7.66138
H	0.57897	-0.79960	5.68351
H	-2.97418	-0.79670	3.16934
H	-4.36880	-0.25104	5.14585

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	7.49	0.05583	YES	YES
8	a	12.28	0.06207	YES	YES
9	a	14.58	0.08895	YES	YES
10	a	19.06	0.12361	YES	YES
11	a	21.81	0.13211	YES	YES
12	a	26.20	0.07710	YES	YES
13	a	28.51	0.04700	YES	YES
14	a	32.21	0.24912	YES	YES
15	a	34.67	0.08694	YES	YES
16	a	42.00	0.27702	YES	YES
17	a	45.34	0.15280	YES	YES
18	a	48.97	0.39651	YES	YES
19	a	50.66	0.10350	YES	YES
20	a	53.28	0.88658	YES	YES
21	a	59.51	0.07238	YES	YES
22	a	59.95	0.17547	YES	YES
23	a	62.30	0.20787	YES	YES
24	a	65.12	0.02471	YES	YES
25	a	66.72	0.21487	YES	YES
26	a	70.51	0.11348	YES	YES
27	a	77.43	0.73865	YES	YES
28	a	79.39	0.36509	YES	YES
29	a	80.34	0.53469	YES	YES

30	a	88.62	1.04113	YES	YES
31	a	89.52	1.61448	YES	YES
32	a	91.66	0.94412	YES	YES
33	a	107.01	0.18406	YES	YES
34	a	110.78	0.42562	YES	YES
35	a	114.77	0.53458	YES	YES
36	a	116.62	3.50347	YES	YES
37	a	130.46	0.95670	YES	YES
38	a	140.18	0.68409	YES	YES
39	a	154.96	0.13837	YES	YES
40	a	160.38	2.00782	YES	YES
41	a	163.30	0.28735	YES	YES
42	a	166.33	0.24533	YES	YES
43	a	173.66	0.87378	YES	YES
44	a	186.74	1.08771	YES	YES
45	a	195.46	0.46115	YES	YES
46	a	199.88	2.85061	YES	YES
47	a	204.27	3.45211	YES	YES
48	a	205.74	0.70581	YES	YES
49	a	211.93	2.05040	YES	YES
50	a	218.46	0.40302	YES	YES

./8/b

BP86/SV(P) energy (au): -3330.9201243620

PBE0/def2-TZVPP energy (au): -3330.436054314
cosmo_dcm Total energy + OC corr. = -3330.4881931505
cosmo_acetone Total energy + OC corr. = -3330.4941502791

Zero point energy (au): 0.9178797
Entropy (kJ mol^-1): 1.44191
Chemical potential (kJ mol^-1): 2143.16

XYZ coordinates:

117

C	-1.17488	1.83734	3.81884
C	-0.00185	2.57665	3.44424
C	-2.26005	2.31237	3.01026
C	-0.35704	3.52963	2.42997
C	-1.75117	3.34692	2.15104
H	-1.24702	1.10659	4.63470
H	0.98775	2.47509	3.90925
H	-3.31008	1.99842	3.08442
H	0.30516	4.28144	1.98635
H	-2.34380	3.93393	1.43666
Ru	-0.69686	1.36994	1.60312
C	-2.05536	-1.15091	2.73747
C	-1.41737	-0.43296	1.52522
P	-1.28626	1.73425	-0.64735
C	-0.30701	1.02081	-2.06189
C	0.25588	1.76026	-3.07779
N	-0.25438	-0.35878	-2.10539
C	0.89635	1.08779	-4.18639
C	0.90928	-0.34216	-4.22937
C	0.28834	-1.13248	-3.14494
O	0.22682	-2.36365	-3.09866
P	1.56934	0.67882	1.33439
C	2.20632	-0.54331	0.05780
C	3.33398	-0.29463	-0.74373
N	1.58572	-1.73478	0.10332
C	3.83823	-1.36618	-1.50896
C	3.22344	-2.61510	-1.46008
C	2.06844	-2.74952	-0.64428
N	1.33544	-3.93215	-0.55593
C	1.44973	-5.08107	-1.34789
O	2.40152	-5.27344	-2.09292
O	-1.49419	-1.17136	0.41478
H	-1.28214	-1.21159	3.53112
C	-1.39286	3.53058	-1.12843
C	-2.99016	1.11774	-1.10129
H	0.18648	2.85692	-3.07384
H	-0.63780	-0.89456	-1.31148
C	1.49787	1.80278	-5.25691

C	1.51008	-1.01771	-5.31359
C	2.67400	2.15836	1.12309
C	2.30742	-0.16652	2.82738
H	3.83459	0.68261	-0.75795
H	-2.84853	-0.48185	3.13670
H	4.72882	-1.21837	-2.14153
H	3.57831	-3.48043	-2.03308
H	0.49508	-3.83385	0.02130
C	0.28781	-6.09584	-1.18019
H	-1.95694	-2.04569	0.59704
C	3.46667	-1.50005	5.03997
C	2.11122	-1.13695	5.06638
C	1.53843	-0.47518	3.96493
C	3.67106	-0.54331	2.80768
C	4.24471	-1.20002	3.90699
H	3.91892	-2.01926	5.90065
H	1.49269	-1.36875	5.94901
H	0.47658	-0.19253	3.98458
H	4.29496	-0.32695	1.92537
H	5.30910	-1.48467	3.87547
C	4.27434	4.47219	0.77636
C	4.19947	3.84509	2.03080
C	3.41128	2.69301	2.20321
C	2.74490	2.80561	-0.13302
C	3.54794	3.94559	-0.30648
H	4.90309	5.36702	0.64017
H	4.76840	4.24620	2.88547
H	3.39010	2.19994	3.18761
H	2.18190	2.40674	-0.99352
H	3.60692	4.42384	-1.29800
C	-1.50284	6.26960	-1.84125
C	-2.59451	5.42571	-2.10240
C	-2.54199	4.06424	-1.75355
C	-0.30307	4.38956	-0.86115
C	-0.35448	5.74585	-1.22198
H	-1.54738	7.33569	-2.11736
H	-3.50083	5.82574	-2.58566
H	-3.40753	3.42128	-1.97175
H	0.59828	3.99633	-0.36723
H	0.50843	6.39856	-1.01091
C	-5.62412	0.33127	-1.77812
C	-5.31571	0.70485	-0.45862
C	-4.00620	1.08812	-0.12330
C	-3.31142	0.75040	-2.42686
C	-4.61836	0.35356	-2.75889
H	-6.64949	0.02554	-2.04294
H	-6.10087	0.70047	0.31558
H	-3.76739	1.36847	0.91429
H	-2.54297	0.77867	-3.21547
H	-4.85026	0.06357	-3.79677
C	0.41743	-7.15055	-2.29615
C	-1.08176	-5.38160	-1.29762
C	0.42567	-6.78049	0.20351
H	-1.31446	-4.74878	-0.40934
H	-1.89557	-6.13736	-1.36520
H	-1.12526	-4.73591	-2.20094
H	-0.38324	-7.53323	0.33771
H	0.35053	-6.05130	1.04168

H	1.40068	-7.30704	0.29449
H	1.41151	-7.64199	-2.26928
H	0.30219	-6.68838	-3.29980
H	-0.36842	-7.92808	-2.17452
H	1.49706	-2.11889	-5.30948
C	2.09942	-0.29337	-6.35318
C	2.09052	1.12087	-6.32174
H	1.48852	2.90537	-5.24009
H	2.55220	1.68964	-7.14565
H	2.56847	-0.82135	-7.19922
C	-2.62267	-2.53634	2.47515
C	-3.69286	-5.12045	2.01875
C	-4.40689	-3.98119	1.61097
C	-3.87745	-2.69924	1.83935
C	-1.90908	-3.69321	2.86527
C	-2.44259	-4.97370	2.64543
H	-4.11239	-6.12540	1.85044
H	-5.38898	-4.08822	1.12257
H	-4.45313	-1.80960	1.52943
H	-0.93174	-3.58580	3.36633
H	-1.88111	-5.86378	2.97271

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	9.01	0.06436	YES	YES
8	a	11.23	0.18703	YES	YES
9	a	14.65	0.06951	YES	YES
10	a	19.73	0.12170	YES	YES
11	a	24.11	0.10081	YES	YES
12	a	26.50	0.07299	YES	YES
13	a	27.88	0.27197	YES	YES
14	a	33.30	0.02793	YES	YES
15	a	36.66	0.07942	YES	YES
16	a	40.28	0.12475	YES	YES
17	a	41.89	0.89378	YES	YES
18	a	43.29	0.24088	YES	YES
19	a	49.64	0.30682	YES	YES
20	a	52.07	0.04828	YES	YES
21	a	53.95	0.23932	YES	YES
22	a	58.06	0.27475	YES	YES
23	a	60.19	0.24970	YES	YES
24	a	62.91	0.70474	YES	YES
25	a	64.56	0.15490	YES	YES
26	a	69.76	0.94843	YES	YES
27	a	70.92	0.36583	YES	YES
28	a	78.41	0.17421	YES	YES
29	a	81.95	0.14091	YES	YES

30	a	87.46	0.23478	YES	YES
31	a	90.51	0.37900	YES	YES
32	a	93.71	2.47119	YES	YES
33	a	106.68	0.31002	YES	YES
34	a	110.68	0.28942	YES	YES
35	a	115.19	0.38094	YES	YES
36	a	117.38	3.98657	YES	YES
37	a	125.22	0.06096	YES	YES
38	a	132.51	0.43985	YES	YES
39	a	133.96	0.43174	YES	YES
40	a	151.30	0.19872	YES	YES
41	a	161.10	0.07781	YES	YES
42	a	162.96	0.64119	YES	YES
43	a	171.37	0.97119	YES	YES
44	a	181.66	0.08462	YES	YES
45	a	189.02	1.61497	YES	YES
46	a	197.48	0.39148	YES	YES
47	a	207.73	5.46737	YES	YES
48	a	209.74	1.09351	YES	YES
49	a	214.30	0.93927	YES	YES
50	a	219.50	1.78345	YES	YES

./8/c

BP86/SV(P) energy (au): -3330.9083426580

PBE0/def2-TZVPP energy (au): -3330.425014254
cosmo_dcm Total energy + OC corr. = -3330.4797155973
cosmo_acetone Total energy + OC corr. = -3330.4859735306

Zero point energy (au): 0.9178665
Entropy (kJ mol^-1): 1.43663
Chemical potential (kJ mol^-1): 2144.36

XYZ coordinates:

117

C	0.25285	0.98265	-3.74201
C	1.33310	0.04849	-3.56093
C	-0.95555	0.22185	-3.84770
C	0.81031	-1.27956	-3.56477
C	-0.61922	-1.17021	-3.72360
H	0.33802	2.06919	-3.85908
H	2.39299	0.32246	-3.47470
H	-1.95463	0.63005	-4.04910
H	1.38403	-2.21093	-3.49611
H	-1.31357	-2.01575	-3.82002
Ru	-0.12391	-0.15515	-1.75012
C	-2.19294	2.16276	-1.31661
C	-1.34920	0.99568	-0.78485
P	-1.06471	-2.03291	-0.66022
C	-0.69546	-2.49813	1.10696
C	-0.45977	-3.78644	1.53113
N	-0.72595	-1.46939	2.02911
C	-0.25374	-4.05663	2.93629
C	-0.30606	-2.97997	3.87728
C	-0.57365	-1.59673	3.42431
O	-0.66069	-0.60539	4.14861
P	1.72115	0.23636	-0.28454
C	1.47531	1.01684	1.41189
C	2.18503	0.62327	2.55905
N	0.67194	2.09447	1.38873
C	2.00345	1.37911	3.73212
C	1.16078	2.49022	3.73191
C	0.51575	2.82131	2.51487
N	-0.33137	3.92872	2.37023
C	-0.71964	4.87274	3.32917
O	-0.34412	4.81664	4.49285
O	-1.73535	0.69003	0.47368
H	-3.02839	1.68768	-1.88214
C	-0.71971	-3.63835	-1.52749
C	-2.93294	-1.98311	-0.60426
H	-0.43399	-4.61567	0.81124
H	-0.93751	-0.51586	1.69694
C	-0.00579	-5.36958	3.42247

C	-0.11616	-3.22675	5.25429
C	2.75887	-1.29031	-0.06087
C	3.01368	1.46223	-0.86036
H	2.87286	-0.23260	2.55073
H	-2.69284	2.65766	-0.44350
H	2.52933	1.09291	4.65712
H	0.98393	3.10426	4.62350
H	-0.66525	4.05871	1.41043
C	-1.66074	5.98738	2.79464
H	-2.37252	1.34891	0.85484
C	4.95444	3.40018	-1.56096
C	3.66965	3.45025	-2.12416
C	2.70501	2.48892	-1.77208
C	4.30408	1.43112	-0.28048
C	5.26636	2.38992	-0.63352
H	5.71314	4.14968	-1.83929
H	3.41048	4.24179	-2.84619
H	1.69548	2.54972	-2.20226
H	4.56791	0.65290	0.45290
H	6.26902	2.34614	-0.17766
C	4.29209	-3.67515	0.08584
C	4.46709	-2.78619	-0.99052
C	3.70999	-1.60633	-1.06245
C	2.57597	-2.20334	1.00213
C	3.34454	-3.37946	1.07861
H	4.89660	-4.59444	0.15035
H	5.20904	-3.00465	-1.77601
H	3.88167	-0.91380	-1.90153
H	1.83394	-2.00454	1.78728
H	3.19303	-4.06721	1.92593
C	-0.12262	-6.06708	-2.84551
C	-1.45390	-5.63700	-2.72810
C	-1.75499	-4.43159	-2.06780
C	0.61996	-4.07466	-1.65291
C	0.91275	-5.28490	-2.30177
H	0.11028	-7.01406	-3.35918
H	-2.27204	-6.24531	-3.14702
H	-2.80563	-4.11612	-1.97270
H	1.44030	-3.47286	-1.22989
H	1.96012	-5.61847	-2.38307
C	-5.76606	-1.96665	-0.60413
C	-5.05631	-1.34760	-1.64731
C	-3.65107	-1.35023	-1.64246
C	-3.65555	-2.60925	0.43495
C	-5.06124	-2.59455	0.43604
H	-6.86820	-1.96032	-0.60292
H	-5.59997	-0.85762	-2.47188
H	-3.10453	-0.85260	-2.45778
H	-3.12300	-3.11785	1.25391
H	-5.60777	-3.08264	1.25954
C	-2.02685	6.90515	3.97697
C	-2.95033	5.35737	2.21122
C	-0.92761	6.80863	1.70455
H	-2.75321	4.73568	1.30705
H	-3.65592	6.15939	1.90128
H	-3.46773	4.72380	2.96495
H	-1.57115	7.65327	1.37194
H	-0.68708	6.20559	0.80011

H	0.02089	7.23778	2.09476
H	-1.12004	7.36024	4.42656
H	-2.54504	6.34090	4.78037
H	-2.69737	7.72075	3.62865
H	-0.17083	-2.37159	5.94617
C	0.12757	-4.52545	5.70899
C	0.18208	-5.59752	4.78736
H	0.03138	-6.20929	2.70852
H	0.37081	-6.62150	5.14938
H	0.27426	-4.71702	6.78433
C	-1.57153	3.25670	-2.16308
C	-0.53983	5.43617	-3.65003
C	0.05697	5.06301	-2.43206
C	-0.45464	3.98137	-1.69530
C	-2.16602	3.64418	-3.38186
C	-1.65316	4.72239	-4.12400
H	-0.14144	6.28792	-4.22511
H	0.92690	5.62153	-2.04848
H	0.02992	3.67626	-0.75130
H	-3.05475	3.10515	-3.75403
H	-2.13250	5.01086	-5.07376

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	6.39	0.02559	YES	YES
8	a	10.50	0.07475	YES	YES
9	a	15.13	0.18955	YES	YES
10	a	19.81	0.18142	YES	YES
11	a	24.49	0.01392	YES	YES
12	a	25.37	0.02314	YES	YES
13	a	27.04	0.30365	YES	YES
14	a	37.26	0.24767	YES	YES
15	a	38.82	0.27492	YES	YES
16	a	42.36	0.77536	YES	YES
17	a	45.58	0.13778	YES	YES
18	a	46.82	0.11297	YES	YES
19	a	49.59	0.26788	YES	YES
20	a	53.74	0.20829	YES	YES
21	a	55.03	0.12430	YES	YES
22	a	59.35	0.12147	YES	YES
23	a	64.10	0.17307	YES	YES
24	a	67.36	0.03409	YES	YES
25	a	68.89	2.64741	YES	YES
26	a	71.05	0.51098	YES	YES
27	a	75.72	0.61455	YES	YES
28	a	77.28	0.44675	YES	YES
29	a	80.43	1.37324	YES	YES

30	a	88.68	2.21803	YES	YES
31	a	94.00	0.07037	YES	YES
32	a	99.32	0.09183	YES	YES
33	a	106.24	0.24744	YES	YES
34	a	113.49	0.07768	YES	YES
35	a	114.19	2.50603	YES	YES
36	a	121.50	0.39645	YES	YES
37	a	125.99	0.26399	YES	YES
38	a	139.82	0.02842	YES	YES
39	a	140.26	0.68698	YES	YES
40	a	161.79	0.38974	YES	YES
41	a	166.71	0.21150	YES	YES
42	a	169.55	3.06578	YES	YES
43	a	176.27	1.22799	YES	YES
44	a	187.00	1.72574	YES	YES
45	a	194.92	0.04475	YES	YES
46	a	199.70	2.35879	YES	YES
47	a	200.96	4.95274	YES	YES
48	a	207.02	0.97641	YES	YES
49	a	208.26	1.05304	YES	YES
50	a	214.67	0.09807	YES	YES

./9/a

BP86/SV(P) energy (au): -3330.9413971650

PBE0/def2-TZVPP energy (au): -3330.448735942
cosmo_dcm Total energy + OC corr. = -3330.4979444538
cosmo_acetone Total energy + OC corr. = -3330.5034658659

Zero point energy (au): 0.9183405
Entropy (kJ mol^-1): 1.42735
Chemical potential (kJ mol^-1): 2147.20

XYZ coordinates:

117

C	1.83720	-3.45040	-1.67725
C	0.48006	-2.47682	-3.28694
C	0.51474	-3.91065	-1.43884
C	-0.34100	-3.27205	-2.41600
C	1.83043	-2.56307	-2.81880
H	2.73460	-3.74516	-1.11649
H	0.12561	-1.92644	-4.16810
H	0.19235	-4.61797	-0.66467
H	-1.41731	-3.45258	-2.53873
Ru	0.52353	-1.56158	-1.20038
C	0.95713	0.76205	-3.22055
C	0.35355	0.33084	-1.85312
P	-1.54987	-1.47054	-0.10608
C	-1.81090	-0.41058	1.40411
C	-2.31648	-0.78740	2.62524
N	-1.49894	0.91660	1.17007
C	-2.53335	0.21012	3.64572
C	-2.21373	1.58087	3.37558
C	-1.65496	1.95700	2.06906
O	-1.31631	3.11979	1.74914
P	2.03162	-0.89625	0.45808
C	2.51012	0.90181	0.90950
C	3.74331	1.19823	1.49290
N	1.66828	1.94430	0.62867
C	4.09170	2.54349	1.74044
C	3.21717	3.58321	1.43321
C	1.94916	3.26596	0.88766
N	0.94969	4.16224	0.60467
C	1.14983	5.55105	0.38028
O	2.27634	6.02309	0.34540
O	-0.15616	1.31149	-1.22229
H	1.61401	1.62995	-2.97271
C	-2.17687	-3.12399	0.46350
C	-2.97755	-0.82839	-1.12238
H	-2.57938	-1.83598	2.82255
H	-1.11850	1.15787	0.21940
C	-3.07032	-0.11967	4.92023
C	-2.43161	2.57142	4.36125

C	1.79677	-1.57023	2.17549
C	3.78329	-1.39858	0.02020
H	4.44253	0.38691	1.73719
H	0.82142	1.73782	0.02221
H	5.06914	2.77651	2.19360
H	3.46670	4.63602	1.60755
H	-0.02646	3.79183	0.73452
C	-0.13897	6.37974	0.20777
H	1.60641	-0.02836	-3.63976
C	6.42878	-2.01428	-0.77791
C	5.92292	-2.50613	0.43552
C	4.61047	-2.19403	0.84015
C	4.30310	-0.90282	-1.19825
C	5.61646	-1.20274	-1.59098
H	7.45761	-2.25737	-1.08906
H	6.55424	-3.13508	1.08443
H	4.24638	-2.57089	1.80807
H	3.67469	-0.26732	-1.84384
H	6.00836	-0.80101	-2.53970
C	1.40611	-2.71332	4.73626
C	1.67390	-3.53721	3.62844
C	1.84898	-2.97306	2.35441
C	1.51780	-0.75304	3.29190
C	1.31597	-1.32321	4.56133
H	1.26401	-3.15691	5.73516
H	1.74270	-4.63033	3.75480
H	2.02841	-3.63470	1.49121
H	1.45507	0.34120	3.18593
H	1.09348	-0.66956	5.42019
C	-5.17388	0.06161	-2.66241
C	-3.93452	-0.17911	-3.27582
C	-2.84174	-0.61971	-2.50823
C	-4.22786	-0.57498	-0.51011
C	-5.31736	-0.13436	-1.27668
H	-6.03053	0.40978	-3.26248
H	-3.80482	-0.01339	-4.35715
H	-1.86795	-0.78499	-2.99406
H	-4.35601	-0.72543	0.57464
H	-6.28576	0.05901	-0.78662
C	-3.02190	-5.69328	1.29986
C	-1.92030	-5.07449	1.91853
C	-1.49359	-3.80456	1.49716
C	-3.28213	-3.75103	-0.15187
C	-3.69585	-5.03073	0.26151
H	-3.35212	-6.69291	1.62621
H	-1.38473	-5.58722	2.73451
H	-0.61743	-3.34095	1.97664
H	-3.83147	-3.24147	-0.95817
H	-4.55801	-5.50774	-0.23249
H	2.71833	-2.12700	-3.29236
C	-1.12804	5.69455	-0.76659
C	0.25879	7.76664	-0.33443
C	-0.79159	6.52524	1.61053
H	-1.99866	6.36590	-0.93240
H	-1.52829	4.73741	-0.36820
H	-0.65856	5.50143	-1.75660
H	0.98146	8.27207	0.33884
H	-0.64629	8.40545	-0.42520

H	0.73255	7.68975	-1.33686
H	-1.09854	5.54113	2.02599
H	-1.70154	7.15999	1.52778
H	-0.09691	7.01924	2.32492
H	-2.17948	3.61597	4.12103
C	-2.96125	2.22121	5.60425
C	-3.28050	0.86993	5.88094
H	-3.32489	-1.16993	5.13867
H	-3.70191	0.59775	6.86263
H	-3.13465	2.99463	6.36974
C	-0.05129	1.20192	-4.27643
C	-1.86411	2.03228	-6.29639
C	-1.86606	2.65860	-5.03664
C	-0.96896	2.24933	-4.03684
C	-0.05800	0.58249	-5.54572
C	-0.95506	0.99158	-6.54853
H	-2.56307	2.36126	-7.08274
H	-2.57108	3.48131	-4.83166
H	-0.97602	2.74013	-3.05131
H	0.67112	-0.21631	-5.76796
H	-0.93412	0.49958	-7.53500

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	4.44	0.06076	YES	YES
8	a	11.07	0.09623	YES	YES
9	a	16.61	0.05582	YES	YES
10	a	18.20	0.05471	YES	YES
11	a	23.38	0.19972	YES	YES
12	a	27.02	0.03959	YES	YES
13	a	33.03	0.19124	YES	YES
14	a	37.42	0.26952	YES	YES
15	a	39.22	0.51300	YES	YES
16	a	41.85	0.76579	YES	YES
17	a	47.23	0.15661	YES	YES
18	a	49.90	0.58778	YES	YES
19	a	52.88	0.60030	YES	YES
20	a	56.70	0.10568	YES	YES
21	a	58.50	0.07196	YES	YES
22	a	60.58	0.26644	YES	YES
23	a	60.83	0.12473	YES	YES
24	a	65.97	0.26468	YES	YES
25	a	70.75	0.26643	YES	YES
26	a	72.77	0.20318	YES	YES
27	a	75.11	3.66884	YES	YES
28	a	77.52	0.73163	YES	YES
29	a	85.49	0.01959	YES	YES

30	a	88.03	0.50095	YES	YES
31	a	89.52	0.59368	YES	YES
32	a	96.64	1.21931	YES	YES
33	a	108.22	0.27955	YES	YES
34	a	109.66	3.88624	YES	YES
35	a	119.76	0.82830	YES	YES
36	a	133.64	3.03052	YES	YES
37	a	135.98	2.89338	YES	YES
38	a	143.59	2.01153	YES	YES
39	a	164.11	1.09506	YES	YES
40	a	166.93	1.50431	YES	YES
41	a	173.70	1.41402	YES	YES
42	a	178.30	3.45767	YES	YES
43	a	183.98	1.44489	YES	YES
44	a	184.53	3.39654	YES	YES
45	a	194.00	1.20586	YES	YES
46	a	198.60	3.76945	YES	YES
47	a	205.36	0.90829	YES	YES
48	a	206.39	1.29699	YES	YES
49	a	216.52	2.35298	YES	YES
50	a	217.58	4.11632	YES	YES

./9/b

BP86/SV(P) energy (au): -3330.9380912130

PBE0/def2-TZVPP energy (au): -3330.445835776
cosmo_dcm Total energy + OC corr. = -3330.4952250943
cosmo_acetone Total energy + OC corr. = -3330.5007563315

Zero point energy (au): 0.9181898
Entropy (kJ mol^-1): 1.42005
Chemical potential (kJ mol^-1): 2149.14

XYZ coordinates:

117

C	3.52905	-2.44263	-0.85435
C	2.36311	-2.19510	-2.83882
C	2.55226	-3.49233	-0.90260
C	1.81909	-3.31944	-2.11893
C	3.43385	-1.65676	-2.04736
H	4.27499	-2.30568	-0.06394
H	2.06022	-1.86926	-3.84113
H	2.44493	-4.30831	-0.17759
H	1.01983	-3.98201	-2.47747
Ru	1.44050	-1.38927	-0.91720
C	1.55194	0.87779	-3.03328
C	1.06656	0.47241	-1.61200
P	-0.87091	-1.79023	-1.14944
C	-2.08979	-0.97944	0.00542
C	-3.12418	-1.60548	0.65930
N	-1.89935	0.38120	0.18136
C	-4.01412	-0.83703	1.49589
C	-3.80617	0.57223	1.64726
C	-2.67817	1.22177	0.96515
O	-2.39438	2.43656	1.04854
P	1.57148	-0.78985	1.35607
C	1.61300	0.99090	2.05059
C	2.33474	1.34996	3.19143
N	0.87659	1.95477	1.42536
C	2.31300	2.69316	3.62721
C	1.55016	3.65543	2.96929
C	0.77227	3.25384	1.85510
N	-0.11965	4.04170	1.17151
C	-0.14555	5.45937	1.19315
O	0.73161	6.09499	1.75900
O	0.37824	1.38348	-1.05494
H	2.54728	0.43620	-3.23000
C	-1.50706	-3.54050	-1.14085
C	-1.49389	-1.21225	-2.81436
H	-3.28475	-2.68585	0.54463
H	-1.10054	0.83358	-0.31691
C	-5.11103	-1.43493	2.17454
C	-4.67836	1.33953	2.45364

C	0.31493	-1.50358	2.53392
C	3.20514	-1.28261	2.12564
H	2.91884	0.59727	3.73700
H	0.51594	1.70883	0.43639
H	2.89514	2.98354	4.51734
H	1.51163	4.70297	3.29001
H	-0.92795	3.52264	0.75885
C	-1.36051	6.10252	0.49401
H	0.84548	0.37091	-3.73225
C	5.75155	-1.89864	3.20152
C	4.60738	-2.56785	3.66101
C	3.33800	-2.25749	3.13345
C	4.36518	-0.61099	1.66870
C	5.62576	-0.91180	2.20501
H	6.74199	-2.13996	3.62032
H	4.69361	-3.33593	4.44694
H	2.45263	-2.77558	3.53165
H	4.28187	0.15906	0.88237
H	6.51676	-0.37360	1.84221
C	-1.56360	-2.73151	4.26149
C	-0.75412	-3.51967	3.42486
C	0.16675	-2.90876	2.55924
C	-0.50182	-0.72190	3.37896
C	-1.43918	-1.33353	4.23011
H	-2.29241	-3.20812	4.93687
H	-0.84348	-4.61820	3.44102
H	0.79041	-3.53252	1.89966
H	-0.42039	0.37567	3.38713
H	-2.07402	-0.70641	4.87665
C	-2.31570	-0.40084	-5.40456
C	-1.47010	-1.51358	-5.24697
C	-1.06079	-1.91258	-3.96523
C	-2.34922	-0.10297	-2.98280
C	-2.75298	0.29961	-4.26979
H	-2.63772	-0.08669	-6.41060
H	-1.13035	-2.08111	-6.12882
H	-0.41501	-2.79931	-3.86512
H	-2.71966	0.46006	-2.11398
H	-3.42619	1.16569	-4.37853
C	-2.52768	-6.17889	-1.08284
C	-1.33239	-5.86970	-0.41260
C	-0.82791	-4.55834	-0.44211
C	-2.71017	-3.86046	-1.81290
C	-3.21491	-5.17079	-1.78128
H	-2.92268	-7.20785	-1.06527
H	-0.78480	-6.65554	0.13305
H	0.11194	-4.31813	0.07476
H	-3.25953	-3.08374	-2.36794
H	-4.15214	-5.40509	-2.31225
H	4.10311	-0.83022	-2.31975
C	-1.67123	5.42498	-0.86196
C	-1.04916	7.59678	0.28022
C	-2.57376	5.94393	1.45336
H	-2.48016	5.99159	-1.37346
H	-2.03504	4.38068	-0.74502
H	-0.78436	5.41592	-1.53279
H	-0.80690	8.09973	1.23913
H	-1.92998	8.10145	-0.17263

H	-0.18115	7.73516	-0.40000
H	-2.82441	4.87405	1.62284
H	-3.46403	6.43773	1.00459
H	-2.37475	6.42748	2.43516
H	-4.49244	2.42072	2.54667
C	-5.75035	0.72894	3.10698
C	-5.96397	-0.66355	2.96457
H	-5.28237	-2.51838	2.06463
H	-6.81309	-1.14173	3.47997
H	-6.43243	1.32871	3.73084
C	1.58445	2.36640	-3.31373
C	1.68034	5.14910	-3.84697
C	2.79680	4.49649	-3.29621
C	2.74680	3.11700	-3.03563
C	0.47013	3.03426	-3.86194
C	0.51666	4.41244	-4.13054
H	1.72133	6.22887	-4.06574
H	3.71743	5.06372	-3.08022
H	3.63507	2.61091	-2.61754
H	-0.44399	2.46067	-4.09154
H	-0.35917	4.91408	-4.57492

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	11.29	0.05461	YES	YES
8	a	13.20	0.02899	YES	YES
9	a	15.74	0.08547	YES	YES
10	a	20.70	0.20278	YES	YES
11	a	23.22	0.05014	YES	YES
12	a	29.50	0.11029	YES	YES
13	a	33.34	0.07589	YES	YES
14	a	36.06	0.13654	YES	YES
15	a	39.10	0.73092	YES	YES
16	a	41.29	0.07105	YES	YES
17	a	42.77	0.61030	YES	YES
18	a	47.92	0.68265	YES	YES
19	a	49.18	0.43417	YES	YES
20	a	50.50	0.07899	YES	YES
21	a	55.33	0.79955	YES	YES
22	a	57.61	0.49835	YES	YES
23	a	59.07	0.84559	YES	YES
24	a	62.31	0.52990	YES	YES
25	a	66.76	1.57992	YES	YES
26	a	71.32	0.42639	YES	YES
27	a	80.84	0.61613	YES	YES
28	a	83.80	1.19991	YES	YES
29	a	86.09	0.32816	YES	YES

30	a	89.31	0.99376	YES	YES
31	a	98.25	0.30617	YES	YES
32	a	101.57	0.31627	YES	YES
33	a	108.31	0.75704	YES	YES
34	a	112.81	4.02096	YES	YES
35	a	128.15	2.45985	YES	YES
36	a	133.98	2.51638	YES	YES
37	a	138.46	1.27445	YES	YES
38	a	143.86	1.21182	YES	YES
39	a	159.65	0.52159	YES	YES
40	a	166.76	1.43362	YES	YES
41	a	171.85	5.49140	YES	YES
42	a	176.13	3.56614	YES	YES
43	a	186.99	6.13380	YES	YES
44	a	192.44	2.12355	YES	YES
45	a	194.71	0.48235	YES	YES
46	a	201.56	4.23903	YES	YES
47	a	206.95	1.10729	YES	YES
48	a	207.75	0.74133	YES	YES
49	a	215.83	2.06777	YES	YES
50	a	217.94	0.55646	YES	YES

./9/c

BP86/SV(P) energy (au): -3330.9388412130

PBE0/def2-TZVPP energy (au): -3330.445161212
cosmo_dcm Total energy + OC corr. = -3330.4936513521
cosmo_acetone Total energy + OC corr. = -3330.4990589193

Zero point energy (au): 0.9187742
Entropy (kJ mol^-1): 1.42482
Chemical potential (kJ mol^-1): 2148.63

XYZ coordinates:

117

C	0.53746	-1.26473	-3.88238
C	-1.62062	-1.88891	-3.33142
C	0.60750	-2.58036	-3.28856
C	-0.72094	-2.95014	-2.93995
C	-0.83227	-0.85767	-3.93996
H	1.38354	-0.71453	-4.30850
H	-2.71457	-1.92102	-3.25679
H	1.51237	-3.19186	-3.18086
H	-1.02689	-3.90405	-2.49013
Ru	-0.25158	-1.01208	-1.72958
C	-2.61731	0.99876	-2.02732
C	-1.32532	0.62311	-1.25929
P	-1.15740	-2.00505	0.21595
C	-0.66633	-1.37125	1.90019
C	-0.30060	-2.14164	2.97870
N	-0.68743	0.00831	2.03167
C	0.02419	-1.51202	4.23582
C	-0.02049	-0.08448	4.34839
C	-0.37602	0.72794	3.17795
O	-0.41150	1.97758	3.15562
P	1.83336	-0.27563	-0.91391
C	2.25073	1.50077	-0.34482
C	3.51718	2.07725	-0.47772
N	1.26608	2.23103	0.24795
C	3.71672	3.40303	-0.03685
C	2.68919	4.12782	0.56667
C	1.43519	3.49631	0.74736
N	0.35160	4.02602	1.41002
C	0.14364	5.40467	1.66385
O	0.90221	6.24877	1.20974
O	-1.11850	1.44995	-0.30609
H	-3.04207	0.13762	-2.57310
C	-1.00688	-3.84308	0.47695
C	-3.01515	-1.81055	0.25813
H	-0.25818	-3.23555	2.89416
H	-0.94039	0.58892	1.20349
C	0.38167	-2.26919	5.38477
C	0.28510	0.54502	5.57735

C	2.60298	-1.18262	0.52377
C	3.17176	-0.32069	-2.22560
H	4.34083	1.50793	-0.92878
H	0.24944	1.84086	0.13782
H	4.70880	3.87008	-0.15225
H	2.82029	5.15737	0.91951
H	-0.24769	3.31813	1.89398
C	-1.07468	5.72947	2.55352
H	-3.35324	1.28123	-1.23987
C	5.12639	-0.23304	-4.27467
C	5.23413	-1.16498	-3.23195
C	4.26803	-1.20538	-2.20720
C	3.07543	0.62158	-3.27833
C	4.04527	0.66790	-4.29063
H	5.88656	-0.20054	-5.07198
H	6.08384	-1.86668	-3.20226
H	4.39685	-1.92342	-1.38336
H	2.23486	1.33700	-3.30536
H	3.95601	1.41352	-5.09770
C	3.73862	-2.68132	2.64400
C	3.38874	-3.31546	1.43967
C	2.81458	-2.57362	0.39536
C	2.95518	-0.55702	1.73953
C	3.51187	-1.30390	2.79231
H	4.18544	-3.26172	3.46741
H	3.55961	-4.39678	1.31156
H	2.53837	-3.08299	-0.54094
H	2.80119	0.52278	1.88538
H	3.77357	-0.79813	3.73586
C	-5.83346	-1.53897	0.15061
C	-5.18078	-2.46827	-0.67944
C	-3.78461	-2.60103	-0.62751
C	-3.67994	-0.89074	1.09655
C	-5.07946	-0.75580	1.03841
H	-6.92983	-1.43390	0.11080
H	-5.76371	-3.10171	-1.36804
H	-3.29420	-3.35240	-1.26780
H	-3.11831	-0.27238	1.81217
H	-5.58156	-0.03431	1.70344
C	-0.78132	-6.62820	0.92469
C	0.13699	-5.97134	0.08923
C	0.02395	-4.58737	-0.13021
C	-1.93044	-4.51397	1.31373
C	-1.81385	-5.89566	1.53659
H	-0.69756	-7.71407	1.09442
H	0.94484	-6.53937	-0.40045
H	0.73775	-4.07619	-0.79181
H	-2.75072	-3.95694	1.79336
H	-2.54256	-6.40465	2.18846
H	-1.20023	0.07673	-4.38325
C	-2.33292	4.94993	2.09834
C	-1.33579	7.24573	2.46725
C	-0.70562	5.33651	4.01072
H	-3.20374	5.27349	2.70949
H	-2.23190	3.85126	2.23626
H	-2.57532	5.15165	1.03169
H	-0.44114	7.82707	2.77216
H	-2.18025	7.51874	3.13658

H	-1.59837	7.55399	1.43232
H	-0.51569	4.24569	4.10896
H	-1.54880	5.59985	4.68718
H	0.19375	5.89101	4.35819
H	0.23906	1.64372	5.63090
C	0.63007	-0.22185	6.69158
C	0.67750	-1.63348	6.59097
H	0.41720	-3.36857	5.31188
H	0.94718	-2.23530	7.47435
H	0.86221	0.26853	7.65068
C	-2.44383	2.17459	-2.98765
C	-2.20236	4.35380	-4.79402
C	-2.81240	3.15795	-5.20661
C	-2.92928	2.08039	-4.31111
C	-1.84309	3.38763	-2.58330
C	-1.72102	4.46407	-3.47769
H	-2.10909	5.20059	-5.49343
H	-3.20734	3.06160	-6.23151
H	-3.43025	1.15444	-4.64431
H	-1.48009	3.48598	-1.54848
H	-1.25269	5.40325	-3.13886

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	3.55	0.02117	YES	YES
8	a	13.09	0.12334	YES	YES
9	a	16.64	0.14056	YES	YES
10	a	20.43	0.07118	YES	YES
11	a	23.10	0.27633	YES	YES
12	a	28.01	0.05571	YES	YES
13	a	28.73	0.13198	YES	YES
14	a	32.68	0.19793	YES	YES
15	a	34.66	0.17041	YES	YES
16	a	42.02	0.47559	YES	YES
17	a	43.98	0.41987	YES	YES
18	a	47.40	0.29889	YES	YES
19	a	51.29	0.61386	YES	YES
20	a	53.73	0.69227	YES	YES
21	a	55.50	0.26116	YES	YES
22	a	56.91	0.22921	YES	YES
23	a	61.40	1.08626	YES	YES
24	a	64.82	0.45215	YES	YES
25	a	70.95	0.44858	YES	YES
26	a	73.84	1.56440	YES	YES
27	a	82.51	0.87948	YES	YES
28	a	85.56	0.60310	YES	YES
29	a	88.24	0.78440	YES	YES

30	a	91.48	0.26173	YES	YES
31	a	95.82	0.80798	YES	YES
32	a	104.78	0.33310	YES	YES
33	a	113.51	3.82904	YES	YES
34	a	114.34	0.21531	YES	YES
35	a	129.58	2.27138	YES	YES
36	a	138.02	1.20787	YES	YES
37	a	141.39	2.97437	YES	YES
38	a	160.40	2.69472	YES	YES
39	a	167.76	1.69997	YES	YES
40	a	169.48	3.07561	YES	YES
41	a	173.77	3.13351	YES	YES
42	a	179.83	0.89290	YES	YES
43	a	190.45	2.86284	YES	YES
44	a	194.75	2.86852	YES	YES
45	a	197.96	0.31091	YES	YES
46	a	201.61	7.02435	YES	YES
47	a	204.26	1.83734	YES	YES
48	a	206.71	2.54178	YES	YES
49	a	213.85	1.31304	YES	YES
50	a	216.75	2.71154	YES	YES

./11/a

BP86/SV(P) energy (au): -3330.9151544660

PBE0/def2-TZVPP energy (au): -3330.422874990
cosmo_dcm Total energy + OC corr. = -3330.4749015972
cosmo_acetone Total energy + OC corr. = -3330.4809184675

Zero point energy (au): 0.9154268
Entropy (kJ mol^-1): 1.41338
Chemical potential (kJ mol^-1): 2144.92

XYZ coordinates:

117

C	-0.40255	3.72188	1.87633
C	-1.28165	3.81054	0.75160
C	-1.06304	2.92140	2.87853
C	-2.47046	3.04425	1.02802
C	-2.32960	2.50877	2.36213
H	0.57148	4.21802	1.97076
H	-1.08072	4.38259	-0.16339
H	-0.68662	2.70244	3.88658
H	-3.36188	2.95593	0.39524
H	-3.08657	1.92062	2.89766
Ru	-0.74286	1.62319	1.00746
C	1.87925	1.23569	2.99996
C	0.95196	0.44030	2.07269
P	-2.02461	-0.38177	1.09380
C	-1.68496	-1.79517	-0.05925
C	-2.59834	-2.38563	-0.90149
N	-0.41153	-2.31674	0.05764
C	-2.22101	-3.55720	-1.65591
C	-0.90494	-4.09855	-1.50195
C	0.06005	-3.45117	-0.59525
O	1.22283	-3.84662	-0.39874
P	-0.08330	1.60242	-1.29967
C	1.38466	0.55912	-1.85841
C	2.00928	0.92068	-3.06777
N	1.85013	-0.39935	-1.04532
C	3.20406	0.26417	-3.40815
C	3.72193	-0.71171	-2.55566
C	2.99250	-1.04168	-1.38556
N	3.40577	-2.07338	-0.53270
C	4.73591	-2.42533	-0.29468
O	5.66739	-1.74647	-0.72595
O	0.96579	-0.78236	2.08746
H	1.34572	2.09317	3.45205
C	-3.84315	-0.08636	0.85480
C	-1.99131	-1.29953	2.71793
H	-3.62015	-1.99165	-0.98406
H	0.26180	-1.84112	0.69284
C	-3.12327	-4.20819	-2.54050

C	-0.52235	-5.25514	-2.21763
C	-1.37782	1.26898	-2.57559
C	0.61971	3.26850	-1.76443
H	1.59997	1.71106	-3.71422
H	3.73171	0.52125	-4.34135
H	4.66346	-1.23030	-2.77638
H	2.63610	-2.66908	-0.16232
C	4.94992	-3.71988	0.52869
H	2.15880	0.53082	3.81415
H	0.85210	0.97686	0.89586
C	-2.08706	-2.68401	5.18349
C	-1.66263	-1.34564	5.14126
C	-1.61113	-0.66116	3.91547
C	-2.41935	-2.64570	2.76997
C	-2.46340	-3.33176	3.99441
H	-2.11926	-3.22490	6.14326
H	-1.35898	-0.83170	6.06785
H	-1.25228	0.37836	3.89134
H	-2.72650	-3.16724	1.84917
H	-2.79333	-4.38312	4.01610
C	-6.59977	0.42143	0.45812
C	-5.67965	0.66242	-0.57749
C	-4.31051	0.42069	-0.37890
C	-4.77353	-0.32842	1.89007
C	-6.14159	-0.06930	1.69125
H	-7.67356	0.61598	0.30315
H	-6.02805	1.04427	-1.55114
H	-3.60314	0.62530	-1.19654
H	-4.43721	-0.72770	2.85897
H	-6.85373	-0.26199	2.51015
C	1.88698	5.71808	-2.39492
C	0.82911	5.24532	-3.18635
C	0.20051	4.02346	-2.87982
C	1.69294	3.74666	-0.97675
C	2.32172	4.95983	-1.29276
H	2.37995	6.67258	-2.64121
H	0.48904	5.82415	-4.06082
H	-0.60754	3.66144	-3.53363
H	2.05842	3.16331	-0.11387
H	3.16400	5.30897	-0.67364
C	-3.37286	0.77525	-4.51980
C	-3.42767	1.94107	-3.73411
C	-2.44576	2.18028	-2.75895
C	-1.33680	0.09684	-3.36175
C	-2.33309	-0.14867	-4.32356
H	-4.14260	0.58819	-5.28610
H	-4.24016	2.67133	-3.88134
H	-2.51352	3.09095	-2.14245
H	-0.51955	-0.62938	-3.23267
H	-2.28590	-1.06782	-4.92948
C	4.08455	-3.71964	1.81299
C	6.44155	-3.80768	0.90401
C	4.55870	-4.92416	-0.36900
H	4.32386	-4.62086	2.41951
H	2.99569	-3.75449	1.59392
H	4.29166	-2.82602	2.44251
H	7.08531	-3.78686	0.00063
H	6.63567	-4.75264	1.45707

H	6.74766	-2.95676	1.55001
H	3.48276	-4.89937	-0.64458
H	4.75037	-5.87403	0.17848
H	5.16640	-4.94084	-1.30037
C	-2.72947	-5.34885	-3.24197
H	-4.14208	-3.80429	-2.66190
H	0.49619	-5.64727	-2.07228
C	-1.42619	-5.87658	-3.08224
H	-3.44056	-5.84490	-3.92295
H	-1.12713	-6.77954	-3.63872
C	3.12467	1.74760	2.28497
C	5.48325	2.68204	1.02905
C	4.69885	3.55848	1.79928
C	3.52331	3.09562	2.41638
C	3.92472	0.87627	1.51514
C	5.09360	1.33844	0.88700
H	6.40502	3.04469	0.54546
H	5.00819	4.60844	1.93241
H	2.92641	3.78586	3.03791
H	3.63435	-0.18107	1.40611
H	5.69493	0.63445	0.28830

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	13.59	0.01991	YES	YES
8	a	19.33	0.08514	YES	YES
9	a	24.49	0.03855	YES	YES
10	a	26.61	0.18899	YES	YES
11	a	29.41	0.04365	YES	YES
12	a	33.59	0.23570	YES	YES
13	a	38.56	0.08255	YES	YES
14	a	41.50	0.37736	YES	YES
15	a	43.19	0.15668	YES	YES
16	a	46.37	0.29669	YES	YES
17	a	48.41	0.93438	YES	YES
18	a	49.57	0.14092	YES	YES
19	a	52.34	0.73211	YES	YES
20	a	56.57	0.21303	YES	YES
21	a	58.63	2.60451	YES	YES
22	a	60.97	0.02425	YES	YES
23	a	62.27	0.05487	YES	YES
24	a	64.38	0.46525	YES	YES
25	a	67.91	1.05128	YES	YES
26	a	70.52	0.68681	YES	YES
27	a	72.95	1.69161	YES	YES
28	a	75.64	1.65434	YES	YES
29	a	79.98	0.54938	YES	YES

30	a	83.33	0.16178	YES	YES
31	a	88.31	0.27539	YES	YES
32	a	100.03	1.36347	YES	YES
33	a	103.78	0.15282	YES	YES
34	a	110.68	2.59442	YES	YES
35	a	119.21	4.00057	YES	YES
36	a	123.82	3.07394	YES	YES
37	a	131.35	0.97266	YES	YES
38	a	134.34	1.22515	YES	YES
39	a	140.25	0.73280	YES	YES
40	a	145.84	2.24235	YES	YES
41	a	163.33	1.18743	YES	YES
42	a	168.62	3.69051	YES	YES
43	a	171.79	0.36194	YES	YES
44	a	176.62	0.13764	YES	YES
45	a	186.92	4.92392	YES	YES
46	a	189.86	4.72386	YES	YES
47	a	194.80	0.42715	YES	YES
48	a	204.08	0.28185	YES	YES
49	a	210.02	0.50413	YES	YES
50	a	212.26	2.63927	YES	YES

./11/b

BP86/SV(P) energy (au): -3330.9105244960

PBE0/def2-TZVPP energy (au): -3330.418579635
cosmo_dcm Total energy + OC corr. = -3330.4713425346
cosmo_acetone Total energy + OC corr. = -3330.4774034574

Zero point energy (au): 0.9155376
Entropy (kJ mol^-1): 1.44881
Chemical potential (kJ mol^-1): 2135.42

XYZ coordinates:

117

C	3.26573	0.80237	2.55406
C	3.52556	1.82818	1.60296
C	2.14241	1.20852	3.36816
C	2.55693	2.88050	1.79688
C	1.72577	2.50203	2.90751
H	3.85608	-0.11383	2.67497
H	4.34339	1.84238	0.87339
H	1.72373	0.66153	4.22281
H	2.54676	3.84301	1.27123
H	0.92864	3.12142	3.33899
Ru	1.41241	1.03534	1.22110
C	1.88429	-2.08457	2.22137
C	0.77670	-1.24256	1.57821
P	-0.92423	1.53719	1.36963
C	-2.02962	1.07251	-0.04838
C	-2.90277	1.92428	-0.68243
N	-1.92959	-0.24268	-0.46553
C	-3.72587	1.43548	-1.76194
C	-3.61317	0.06922	-2.17208
C	-2.66337	-0.82799	-1.49336
O	-2.49941	-2.02996	-1.76942
P	1.69690	1.09702	-1.17279
C	1.82304	-0.61306	-1.95455
C	2.77423	-0.90883	-2.94572
N	0.92874	-1.51137	-1.50535
C	2.82386	-2.23519	-3.42228
C	1.92198	-3.18552	-2.94816
C	0.93053	-2.76574	-2.01707
N	-0.11817	-3.58973	-1.61523
C	-0.11229	-4.99030	-1.62809
O	0.90824	-5.62608	-1.88157
O	-0.38734	-1.59400	1.54106
H	2.79637	-1.97890	1.59775
C	-1.41871	3.30788	1.66706
C	-1.77986	0.72180	2.81787
H	-2.98456	2.97409	-0.37176
H	-1.29791	-0.88246	0.05243
C	-4.66265	2.26883	-2.43145

C	-4.41683	-0.42939	-3.22168
C	0.48659	1.95404	-2.28424
C	3.32561	1.85027	-1.68611
H	3.46058	-0.14622	-3.33652
H	3.57185	-2.51945	-4.18089
H	1.93875	-4.22913	-3.28567
H	-0.99798	-3.08010	-1.38628
C	-1.47411	-5.66578	-1.33165
H	2.11203	-1.60472	3.20049
H	1.15438	-0.55407	0.57491
C	-3.06448	-0.39907	5.08046
C	-1.98741	0.48893	5.24734
C	-1.35038	1.04261	4.12558
C	-2.86979	-0.16003	2.66143
C	-3.50372	-0.71705	3.78598
H	-3.56464	-0.83578	5.96008
H	-1.64371	0.76069	6.25886
H	-0.52801	1.75646	4.28566
H	-3.23725	-0.42678	1.66018
H	-4.35075	-1.40710	3.64145
C	-2.23550	5.98357	2.11071
C	-0.97475	5.71391	1.55370
C	-0.57296	4.38503	1.33328
C	-2.68489	3.59025	2.23286
C	-3.08833	4.91806	2.44778
H	-2.55173	7.02423	2.28894
H	-0.29517	6.54153	1.29237
H	0.41896	4.18130	0.90509
H	-3.36248	2.76875	2.51330
H	-4.07756	5.11932	2.89033
C	5.84849	2.91236	-2.42457
C	4.66922	3.60593	-2.73536
C	3.41497	3.07735	-2.37535
C	4.52252	1.15671	-1.37916
C	5.77072	1.68025	-1.74934
H	6.82864	3.32395	-2.71492
H	4.71670	4.56557	-3.27544
H	2.50362	3.62666	-2.65671
H	4.48047	0.18356	-0.86175
H	6.68960	1.11875	-1.51348
C	-1.21443	3.37900	-4.03641
C	-0.71354	4.00167	-2.88032
C	0.12120	3.28882	-2.00534
C	-0.02673	1.33325	-3.44396
C	-0.87612	2.04354	-4.30949
H	-1.87315	3.93431	-4.72355
H	-0.97807	5.04719	-2.65231
H	0.49960	3.78311	-1.09869
H	0.23596	0.29195	-3.68358
H	-1.27281	1.54515	-5.20863
C	-2.10692	-5.10629	-0.03386
C	-1.23566	-7.18059	-1.18298
C	-2.41356	-5.39938	-2.53849
H	-3.03145	-5.67931	0.20156
H	-2.40160	-4.03951	-0.13335
H	-1.41451	-5.20424	0.83088
H	-0.75352	-7.60445	-2.08790
H	-2.20618	-7.69903	-1.02186

H	-0.57504	-7.40212	-0.31746
H	-2.62824	-4.31680	-2.66346
H	-3.38234	-5.92288	-2.37652
H	-1.97213	-5.78903	-3.48240
C	-5.45174	1.76145	-3.46466
H	-4.76295	3.32204	-2.12093
H	-4.30624	-1.48637	-3.50913
C	-5.32989	0.40924	-3.86468
H	-6.17858	2.41777	-3.97107
H	-5.96027	0.01872	-4.67992
C	1.52964	-3.54200	2.43583
C	0.90228	-6.26685	2.84428
C	1.59121	-5.86841	1.68573
C	1.90368	-4.51357	1.48474
C	0.83211	-3.95086	3.59171
C	0.52263	-5.30481	3.79716
H	0.66271	-7.33052	3.00727
H	1.88851	-6.61004	0.92744
H	2.44830	-4.21587	0.57315
H	0.53188	-3.20174	4.34407
H	-0.01009	-5.61282	4.71177

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	4.11	0.16418	YES	YES
8	a	8.61	0.17647	YES	YES
9	a	17.31	0.12021	YES	YES
10	a	20.72	0.07730	YES	YES
11	a	24.03	0.07780	YES	YES
12	a	24.99	0.10916	YES	YES
13	a	32.22	0.42986	YES	YES
14	a	37.74	0.69035	YES	YES
15	a	38.89	0.53725	YES	YES
16	a	42.57	0.75689	YES	YES
17	a	45.61	1.80344	YES	YES
18	a	48.23	0.16474	YES	YES
19	a	53.38	0.64551	YES	YES
20	a	53.96	0.20004	YES	YES
21	a	54.40	0.82627	YES	YES
22	a	56.86	0.72950	YES	YES
23	a	60.19	2.01980	YES	YES
24	a	62.75	1.45046	YES	YES
25	a	65.29	0.62849	YES	YES
26	a	68.65	1.86255	YES	YES
27	a	72.03	2.62006	YES	YES
28	a	79.97	0.06606	YES	YES
29	a	81.70	0.40711	YES	YES

30	a	84.18	2.24014	YES	YES
31	a	88.64	1.02438	YES	YES
32	a	94.01	2.33291	YES	YES
33	a	101.06	0.15659	YES	YES
34	a	106.08	0.51483	YES	YES
35	a	110.43	2.10915	YES	YES
36	a	122.16	1.55720	YES	YES
37	a	131.04	3.02115	YES	YES
38	a	133.07	0.96150	YES	YES
39	a	142.92	0.23437	YES	YES
40	a	147.61	1.51360	YES	YES
41	a	161.76	0.77300	YES	YES
42	a	168.96	0.14351	YES	YES
43	a	173.91	4.98500	YES	YES
44	a	176.50	3.50240	YES	YES
45	a	188.52	2.50911	YES	YES
46	a	192.80	1.06083	YES	YES
47	a	196.54	1.22443	YES	YES
48	a	198.38	0.29208	YES	YES
49	a	206.10	6.45214	YES	YES
50	a	212.17	1.44977	YES	YES

./11/c

BP86/SV(P) energy (au): -3330.9130024270

PBE0/def2-TZVPP energy (au): -3330.418484408
cosmo_dcm Total energy + OC corr. = -3330.4697551036
cosmo_acetone Total energy + OC corr. = -3330.4755971502

Zero point energy (au): 0.9160139
Entropy (kJ mol^-1): 1.42062
Chemical potential (kJ mol^-1): 2143.85

XYZ coordinates:

117

C	3.85368	-0.38296	0.25738
C	3.78890	0.15759	-1.06352
C	3.61497	0.66127	1.20537
C	3.52954	1.57476	-0.93504
C	3.44408	1.88960	0.45900
H	4.04289	-1.43497	0.51435
H	3.99555	-0.38026	-1.99475
H	3.62356	0.55269	2.29701
H	3.46005	2.28861	-1.76683
H	3.32766	2.89183	0.88951
Ru	1.73647	0.52888	-0.07742
C	1.73233	-2.73388	-0.03020
C	1.12068	-1.51546	0.66793
P	0.35861	1.66759	1.50030
C	-1.46429	1.31969	1.40043
C	-2.46019	2.26384	1.31575
N	-1.79354	-0.02405	1.33502
C	-3.83664	1.84750	1.18669
C	-4.14829	0.45383	1.08807
C	-3.06854	-0.54516	1.12924
O	-3.22205	-1.77402	1.00888
P	0.39887	0.79703	-2.06194
C	-0.35202	-0.83723	-2.62331
C	-0.46030	-1.16493	-3.98530
N	-0.81312	-1.62845	-1.64146
C	-1.04655	-2.40490	-4.30766
C	-1.51211	-3.24720	-3.29843
C	-1.40358	-2.80852	-1.94945
N	-1.89490	-3.54045	-0.86797
C	-2.19069	-4.91658	-0.86870
O	-1.97726	-5.61819	-1.85139
O	0.53519	-1.62754	1.74081
H	0.84402	-3.37224	-0.25876
C	0.42668	3.52473	1.55930
C	0.76891	1.28938	3.28072
H	-2.22023	3.33500	1.33464
H	-1.04570	-0.73152	1.46589
C	-4.90518	2.78412	1.15008

C	-5.49000	0.03016	0.95201
C	-1.09280	1.90547	-2.13703
C	1.40376	1.28382	-3.55281
H	-0.10759	-0.48515	-4.77316
H	-1.14414	-2.71051	-5.36252
H	-1.95402	-4.22792	-3.51101
H	-2.13900	-2.97001	-0.03215
C	-2.81081	-5.47245	0.43698
H	2.16286	-2.43767	-1.00680
H	0.53580	-0.72501	-0.18539
C	1.49634	0.78033	5.96927
C	2.26036	1.66452	5.18730
C	1.89826	1.91971	3.85523
C	0.00300	0.41184	4.07609
C	0.36643	0.16208	5.41120
H	1.77703	0.58254	7.01645
H	3.13874	2.17072	5.62007
H	2.49008	2.64367	3.27164
H	-0.89265	-0.07989	3.67162
H	-0.24857	-0.52147	6.01887
C	0.55837	6.34668	1.74144
C	1.16341	5.68063	0.66338
C	1.09400	4.27890	0.57345
C	-0.16601	4.20454	2.65081
C	-0.10680	5.60469	2.73375
H	0.61400	7.44494	1.81550
H	1.69769	6.25357	-0.11216
H	1.57584	3.76186	-0.27058
H	-0.66863	3.63665	3.44965
H	-0.57461	6.11841	3.58945
C	3.02571	1.92777	-5.78678
C	2.08288	2.84947	-5.30647
C	1.27162	2.52995	-4.20193
C	2.34743	0.35554	-4.05486
C	3.14802	0.67317	-5.16273
H	3.65601	2.17818	-6.65540
H	1.96235	3.82703	-5.80124
H	0.51864	3.25899	-3.86770
H	2.43377	-0.64307	-3.59746
H	3.86705	-0.06894	-5.54668
C	-3.33436	3.62797	-2.33908
C	-2.06872	4.15007	-2.02357
C	-0.96118	3.29417	-1.91244
C	-2.37277	1.38961	-2.44302
C	-3.48235	2.24625	-2.53944
H	-4.20551	4.29720	-2.42628
H	-1.93763	5.23203	-1.85846
H	0.01551	3.72529	-1.65492
H	-2.51788	0.31312	-2.61383
H	-4.47183	1.82360	-2.77696
C	-2.02813	-5.00051	1.68615
C	-2.78142	-7.01139	0.35645
C	-4.28064	-4.97861	0.51270
H	-2.45125	-5.48947	2.59154
H	-2.10153	-3.90349	1.84662
H	-0.95370	-5.28354	1.62376
H	-3.32222	-7.37924	-0.53973
H	-3.26037	-7.44306	1.26239

H	-1.73989	-7.39507	0.29651
H	-4.33966	-3.87244	0.59671
H	-4.77222	-5.41670	1.40998
H	-4.85645	-5.30403	-0.38187
C	-6.22560	2.35009	1.02361
H	-4.67893	3.86032	1.22810
H	-5.69390	-1.04930	0.87934
C	-6.52277	0.96973	0.92274
H	-7.04436	3.08813	1.00506
H	-7.56917	0.63860	0.82542
C	2.73205	-3.55777	0.77371
C	4.60077	-5.17060	2.16648
C	3.44578	-4.70019	2.81434
C	2.51552	-3.90392	2.12551
C	3.89409	-4.03989	0.13036
C	4.82080	-4.84084	0.81896
H	5.32560	-5.79879	2.70940
H	3.26043	-4.96042	3.86952
H	1.61179	-3.54399	2.64015
H	4.07292	-3.79656	-0.93175
H	5.71785	-5.21118	0.29604

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	8.06	0.04733	YES	YES
8	a	16.13	0.07032	YES	YES
9	a	20.01	0.00995	YES	YES
10	a	20.83	0.20220	YES	YES
11	a	26.29	0.07282	YES	YES
12	a	30.55	0.03824	YES	YES
13	a	34.20	0.09198	YES	YES
14	a	36.60	0.16856	YES	YES
15	a	39.72	1.36522	YES	YES
16	a	43.52	0.80007	YES	YES
17	a	48.27	0.02594	YES	YES
18	a	50.19	0.23008	YES	YES
19	a	51.82	0.00024	YES	YES
20	a	53.50	0.43210	YES	YES
21	a	55.01	0.04470	YES	YES
22	a	58.85	0.25923	YES	YES
23	a	61.60	0.19611	YES	YES
24	a	65.53	0.46920	YES	YES
25	a	67.74	0.82136	YES	YES
26	a	72.82	0.54958	YES	YES
27	a	79.95	0.88232	YES	YES
28	a	82.46	0.42257	YES	YES
29	a	86.09	0.35258	YES	YES

30	a	90.39	0.50892	YES	YES
31	a	94.88	0.81046	YES	YES
32	a	102.12	1.46275	YES	YES
33	a	104.75	0.11386	YES	YES
34	a	115.16	3.32236	YES	YES
35	a	117.64	0.99168	YES	YES
36	a	129.78	2.12847	YES	YES
37	a	132.94	0.43219	YES	YES
38	a	141.95	3.41646	YES	YES
39	a	151.32	0.57007	YES	YES
40	a	155.14	6.60928	YES	YES
41	a	168.37	0.73485	YES	YES
42	a	171.86	1.13238	YES	YES
43	a	180.87	1.54040	YES	YES
44	a	189.39	4.52405	YES	YES
45	a	191.03	1.27675	YES	YES
46	a	197.28	1.09907	YES	YES
47	a	202.60	1.74542	YES	YES
48	a	204.54	1.18421	YES	YES
49	a	207.95	3.15504	YES	YES
50	a	212.11	4.58666	YES	YES

./12/a

BP86/SV(P) energy (au): -3330.9414831690

PBE0/def2-TZVPP energy (au): -3330.450719552
cosmo_dcm Total energy + OC corr. = -3330.4985195989
cosmo_acetone Total energy + OC corr. = -3330.5038802345

Zero point energy (au): 0.9180830
Entropy (kJ mol^-1): 1.43187
Chemical potential (kJ mol^-1): 2146.19

XYZ coordinates:

117

C	-0.83379	4.43099	0.76077
C	-1.80153	4.01723	-0.21913
C	-1.27916	3.92962	2.03838
C	-2.82797	3.25563	0.43895
C	-2.50263	3.22303	1.85321
H	0.04569	5.05984	0.58242
H	-1.77620	4.26622	-1.28831
H	-0.74948	4.05760	2.99275
H	-3.75543	2.89330	-0.01731
H	-3.10558	2.75421	2.64091
Ru	-0.89773	2.17748	0.64530
C	2.87423	1.19465	2.91909
C	1.75833	0.99482	1.92868
P	-1.80012	0.06247	1.23912
C	-1.98878	-1.43731	0.12818
C	-3.15410	-2.17149	0.06757
N	-0.88043	-1.86166	-0.58525
C	-3.23700	-3.35601	-0.74856
C	-2.08501	-3.77816	-1.47781
C	-0.83283	-3.01891	-1.36302
O	0.23884	-3.36565	-1.90160
P	0.08256	1.67331	-1.44120
C	1.72969	0.76880	-1.42571
C	2.93631	1.39771	-1.76913
N	1.67682	-0.52622	-1.03613
C	4.12444	0.64389	-1.69720
C	4.07881	-0.69439	-1.31793
C	2.81398	-1.26612	-1.01781
N	2.65079	-2.62219	-0.73671
C	3.63074	-3.46851	-0.21071
O	4.71284	-3.04096	0.18683
O	0.93908	1.89487	1.67650
H	2.71636	2.16040	3.44293
C	-3.55912	0.21099	1.84905
C	-0.93734	-0.69501	2.70876
H	-4.02959	-1.87758	0.65872
H	0.01599	-1.29968	-0.62162
C	-4.42755	-4.12633	-0.84909

C	-2.13582	-4.93656	-2.28659
C	-0.89569	0.71381	-2.68298
C	0.51143	3.22715	-2.37748
H	2.96183	2.44050	-2.10960
H	5.08844	1.10839	-1.95960
H	4.98055	-1.31455	-1.26023
H	1.73273	-3.00596	-1.07172
C	3.25703	-4.97193	-0.16060
H	2.79009	0.37137	3.66714
H	1.68576	0.01016	1.40775
C	0.27555	-1.75869	5.03703
C	0.01554	-0.37970	4.94482
C	-0.57509	0.14946	3.78482
C	-0.67527	-2.07871	2.81310
C	-0.06680	-2.60309	3.96733
H	0.74304	-2.17516	5.94417
H	0.27327	0.29027	5.78147
H	-0.77023	1.23257	3.71725
H	-0.95292	-2.76220	1.99640
H	0.13023	-3.68559	4.03250
C	-6.24326	0.51076	2.70980
C	-5.91112	0.69027	1.35476
C	-4.58119	0.54524	0.92903
C	-3.90604	0.01279	3.20227
C	-5.23861	0.16898	3.62825
H	-7.28617	0.62989	3.04524
H	-6.69476	0.94197	0.62117
H	-4.34165	0.65992	-0.14017
H	-3.13907	-0.27201	3.93826
H	-5.48903	0.01105	4.68995
C	1.16802	5.62487	-3.73355
C	0.35391	4.66276	-4.35118
C	0.03058	3.46779	-3.68217
C	1.32229	4.20833	-1.75840
C	1.65627	5.39199	-2.43500
H	1.42252	6.55826	-4.26157
H	-0.03381	4.83654	-5.36837
H	-0.60179	2.72205	-4.18808
H	1.70683	4.03914	-0.73894
H	2.29906	6.14063	-1.94334
C	-2.44868	-0.60916	-4.63388
C	-3.07690	0.13876	-3.62325
C	-2.30363	0.79173	-2.64914
C	-0.26994	-0.03299	-3.70582
C	-1.04594	-0.69451	-4.67177
H	-3.05421	-1.12980	-5.39322
H	-4.17636	0.20908	-3.59024
H	-2.79042	1.37025	-1.84705
H	0.82778	-0.10588	-3.75373
H	-0.54789	-1.28331	-5.45903
C	1.97363	-5.17468	0.68274
C	4.42750	-5.73465	0.48876
C	3.02677	-5.48810	-1.60416
H	1.75295	-6.26150	0.77208
H	1.08650	-4.69627	0.21499
H	2.09870	-4.76847	1.71133
H	5.36620	-5.59984	-0.08808
H	4.19308	-6.82093	0.52964

H	4.62079	-5.37777	1.52287
H	2.15727	-4.99637	-2.09048
H	2.82666	-6.58247	-1.58004
H	3.92664	-5.32424	-2.23708
C	-4.46452	-5.26670	-1.65209
H	-5.32134	-3.81155	-0.28560
H	-1.22826	-5.23533	-2.83341
C	-3.31797	-5.67406	-2.37660
H	-5.39361	-5.85575	-1.72270
H	-3.36024	-6.57635	-3.00784
C	4.25089	1.14342	2.25953
C	6.81223	1.07719	1.06675
C	6.13694	2.30161	1.22101
C	4.86122	2.33364	1.80805
C	4.93119	-0.07980	2.09117
C	6.20378	-0.11392	1.49718
H	7.81765	1.05391	0.61514
H	6.61202	3.24127	0.89379
H	4.34370	3.29924	1.94052
H	4.47273	-1.02325	2.43135
H	6.71371	-1.08231	1.37405

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	5.86	0.05254	YES	YES
8	a	17.09	0.22632	YES	YES
9	a	18.85	0.17774	YES	YES
10	a	20.36	0.09171	YES	YES
11	a	26.76	0.05412	YES	YES
12	a	31.13	0.61132	YES	YES
13	a	34.07	0.24048	YES	YES
14	a	35.42	0.14338	YES	YES
15	a	36.19	0.34693	YES	YES
16	a	38.98	0.11118	YES	YES
17	a	41.67	0.05094	YES	YES
18	a	44.05	0.25977	YES	YES
19	a	46.12	0.19138	YES	YES
20	a	52.59	0.10941	YES	YES
21	a	55.36	0.34602	YES	YES
22	a	56.11	0.98581	YES	YES
23	a	61.01	0.15589	YES	YES
24	a	61.73	0.27947	YES	YES
25	a	66.63	0.42745	YES	YES
26	a	71.04	0.25759	YES	YES
27	a	76.45	0.09945	YES	YES
28	a	80.07	0.74485	YES	YES
29	a	84.90	1.05315	YES	YES

30	a	89.14	1.82574	YES	YES
31	a	91.65	0.23775	YES	YES
32	a	94.41	0.63012	YES	YES
33	a	97.42	0.10598	YES	YES
34	a	103.75	0.37949	YES	YES
35	a	117.89	0.45730	YES	YES
36	a	123.24	2.93483	YES	YES
37	a	128.86	1.30231	YES	YES
38	a	142.21	2.03294	YES	YES
39	a	157.34	0.68705	YES	YES
40	a	166.06	2.23452	YES	YES
41	a	169.17	0.91477	YES	YES
42	a	177.61	1.46951	YES	YES
43	a	182.02	0.22189	YES	YES
44	a	190.49	0.78494	YES	YES
45	a	191.76	0.32341	YES	YES
46	a	202.28	1.08878	YES	YES
47	a	203.57	1.01896	YES	YES
48	a	212.74	2.03495	YES	YES
49	a	213.37	0.98895	YES	YES
50	a	216.40	0.96807	YES	YES

./12/b

BP86/SV(P) energy (au): -3330.9379504140

PBE0/def2-TZVPP energy (au): -3330.448040386
cosmo_dcm Total energy + OC corr. = -3330.4969874543
cosmo_acetone Total energy + OC corr. = -3330.5024883455

Zero point energy (au): 0.9172105
Entropy (kJ mol^-1): 1.43963
Chemical potential (kJ mol^-1): 2142.23

XYZ coordinates:

117

C	3.94929	-1.01292	1.00196
C	4.11850	0.30999	0.45020
C	3.36588	-0.84805	2.31027
C	3.65682	1.27604	1.40831
C	3.20139	0.54632	2.57785
H	4.29268	-1.95382	0.55724
H	4.56865	0.54235	-0.52384
H	3.09386	-1.66453	2.99534
H	3.72332	2.36725	1.31778
H	2.83290	0.99215	3.51061
Ru	1.95841	0.02933	0.77652
C	1.00965	-3.63169	0.41586
C	0.10969	-2.57054	0.98365
P	0.30996	1.60041	1.48570
C	-1.02060	2.29013	0.37828
C	-1.40936	3.61030	0.37703
N	-1.75700	1.35539	-0.33248
C	-2.57562	4.02604	-0.36270
C	-3.35346	3.04051	-1.04525
C	-2.94508	1.62828	-1.00833
O	-3.59169	0.70469	-1.54254
P	1.58072	0.01421	-1.56769
C	0.34158	-1.25330	-2.19036
C	0.68733	-2.23498	-3.13713
N	-0.87460	-1.21353	-1.60111
C	-0.25598	-3.24053	-3.42753
C	-1.49700	-3.23288	-2.79308
C	-1.79051	-2.16454	-1.90400
N	-3.04604	-2.01261	-1.31655
C	-3.88084	-3.06787	-0.94667
O	-3.50061	-4.23739	-1.00041
O	0.36557	-1.36550	1.10383
H	0.76806	-3.68130	-0.67655
C	1.03362	3.14535	2.22108
C	-0.75138	0.94893	2.87830
H	-0.85773	4.35244	0.96983
H	-1.39695	0.38161	-0.48886
C	-3.00091	5.38115	-0.41123

C	-4.51703	3.41481	-1.75508
C	1.05229	1.58470	-2.39369
C	3.09518	-0.45207	-2.55509
H	1.66425	-2.22704	-3.63787
H	-0.01689	-4.02680	-4.16243
H	-2.25222	-4.00483	-2.98681
H	-3.34632	-1.01139	-1.22330
C	-5.29220	-2.65982	-0.46053
H	2.06521	-3.29129	0.48922
H	-0.90161	-2.90251	1.32990
C	-2.27565	0.03738	5.08315
C	-0.99290	-0.48526	4.84724
C	-0.23924	-0.03641	3.75019
C	-2.04142	1.46943	3.12484
C	-2.79684	1.01422	4.21848
H	-2.86955	-0.31766	5.94126
H	-0.57570	-1.25311	5.51942
H	0.76015	-0.45978	3.56773
H	-2.46422	2.24467	2.46650
H	-3.80161	1.43154	4.39579
C	2.22855	5.46684	3.31550
C	2.27250	5.23601	1.92864
C	1.68684	4.08115	1.38569
C	0.98531	3.38937	3.61037
C	1.58556	4.54089	4.15211
H	2.69292	6.37092	3.74177
H	2.76750	5.96206	1.26279
H	1.72136	3.91480	0.29755
H	0.47050	2.68357	4.28074
H	1.54037	4.71516	5.23958
C	5.39157	-1.24762	-4.01460
C	4.75253	-0.03295	-4.30592
C	3.60868	0.36167	-3.58724
C	3.74496	-1.67737	-2.27368
C	4.87829	-2.07471	-2.99903
H	6.28572	-1.55520	-4.58089
H	5.13934	0.61791	-5.10712
H	3.11595	1.31113	-3.84592
H	3.34371	-2.34203	-1.49195
H	5.36416	-3.03769	-2.77073
C	0.41792	4.01756	-3.68361
C	1.48778	3.96229	-2.77252
C	1.79462	2.75592	-2.12304
C	-0.01161	1.64459	-3.31742
C	-0.33039	2.85937	-3.95045
H	0.16894	4.96525	-4.18798
H	2.08561	4.86529	-2.56553
H	2.63819	2.71416	-1.41333
H	-0.60377	0.74596	-3.54849
H	-1.17019	2.89540	-4.66324
C	-5.17252	-1.73664	0.77804
C	-6.06192	-3.93909	-0.08317
C	-6.02872	-1.91478	-1.60318
H	-6.18811	-1.49856	1.16516
H	-4.67722	-0.77128	0.53625
H	-4.60514	-2.22971	1.59841
H	-6.15305	-4.62699	-0.95009
H	-7.08492	-3.67507	0.26405

H	-5.54827	-4.49626	0.72865
H	-5.52510	-0.96255	-1.87696
H	-7.06406	-1.66750	-1.27907
H	-6.10249	-2.54907	-2.51394
C	-4.15046	5.73686	-1.11826
H	-2.41311	6.14881	0.11868
H	-5.09343	2.62924	-2.26749
C	-4.91174	4.75365	-1.79501
H	-4.46974	6.79164	-1.14798
H	-5.81805	5.04657	-2.34928
C	0.78515	-4.99122	1.05866
C	0.34482	-7.49235	2.29558
C	-0.61673	-6.95802	1.42004
C	-0.40011	-5.71502	0.80265
C	1.74079	-5.53011	1.94410
C	1.52503	-6.77637	2.55642
H	0.17444	-8.47049	2.77434
H	-1.54394	-7.51546	1.20884
H	-1.16531	-5.31226	0.11481
H	2.67237	-4.97450	2.14995
H	2.28497	-7.18991	3.23954

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.05	0.42828	YES	YES
8	a	16.18	0.09806	YES	YES
9	a	18.09	0.11341	YES	YES
10	a	19.52	0.10461	YES	YES
11	a	22.23	0.10227	YES	YES
12	a	27.37	0.06600	YES	YES
13	a	31.19	0.09366	YES	YES
14	a	32.86	1.09739	YES	YES
15	a	37.03	0.45180	YES	YES
16	a	37.64	0.19852	YES	YES
17	a	42.12	0.01913	YES	YES
18	a	45.21	0.06769	YES	YES
19	a	47.87	0.08511	YES	YES
20	a	50.37	0.29210	YES	YES
21	a	55.07	0.40170	YES	YES
22	a	57.60	0.28707	YES	YES
23	a	57.98	1.14654	YES	YES
24	a	62.50	0.77932	YES	YES
25	a	64.31	0.37575	YES	YES
26	a	68.25	0.02297	YES	YES
27	a	73.12	0.00631	YES	YES
28	a	75.20	0.59006	YES	YES
29	a	77.88	1.28955	YES	YES

30	a	81.81	0.19640	YES	YES
31	a	87.21	0.24614	YES	YES
32	a	92.81	1.08776	YES	YES
33	a	96.42	0.39931	YES	YES
34	a	101.84	0.57872	YES	YES
35	a	105.33	0.14118	YES	YES
36	a	112.20	0.50532	YES	YES
37	a	123.48	1.84260	YES	YES
38	a	128.98	1.00292	YES	YES
39	a	139.55	0.87812	YES	YES
40	a	149.51	0.85041	YES	YES
41	a	164.36	1.31183	YES	YES
42	a	168.83	0.73819	YES	YES
43	a	173.79	0.14464	YES	YES
44	a	183.44	2.08734	YES	YES
45	a	192.39	2.74231	YES	YES
46	a	197.04	0.26014	YES	YES
47	a	203.92	1.00201	YES	YES
48	a	206.90	0.47182	YES	YES
49	a	208.85	3.39465	YES	YES
50	a	218.77	1.82289	YES	YES

./12/c

BP86/SV(P) energy (au): -3330.9436118700

PBE0/def2-TZVPP energy (au): -3330.453178176
cosmo_dcm Total energy + OC corr. = -3330.5016337591
cosmo_acetone Total energy + OC corr. = -3330.5070348195

Zero point energy (au): 0.9173692
Entropy (kJ mol^-1): 1.45677
Chemical potential (kJ mol^-1): 2137.27

XYZ coordinates:

117

C	3.21842	2.70275	0.64180
C	2.22304	3.53517	0.01763
C	2.78628	2.46553	1.99594
C	1.18320	3.80611	0.97139
C	1.55128	3.14872	2.21273
H	4.15888	2.35677	0.19829
H	2.26592	3.92479	-1.00803
H	3.31864	1.84366	2.72966
H	0.33188	4.48209	0.83057
H	0.99146	3.20046	3.15538
Ru	1.23579	1.62730	0.57809
C	2.43893	-2.63997	1.53848
C	1.57658	-1.46528	1.17022
P	-0.92257	1.16899	1.41989
C	-2.38219	0.53809	0.43519
C	-3.66182	1.02436	0.58647
N	-2.16127	-0.57016	-0.36742
C	-4.76691	0.40266	-0.09970
C	-4.52587	-0.76094	-0.89270
C	-3.16336	-1.29923	-1.00683
O	-2.88135	-2.34525	-1.62756
P	0.98338	1.06346	-1.71121
C	1.25428	-0.74647	-2.10564
C	2.33149	-1.21766	-2.87260
N	0.36301	-1.58211	-1.52215
C	2.49568	-2.61125	-3.00374
C	1.59070	-3.47995	-2.39687
C	0.49971	-2.91970	-1.68191
N	-0.51419	-3.70658	-1.13373
C	-0.31802	-4.98785	-0.61466
O	0.81403	-5.44007	-0.44528
O	2.01841	-0.32205	0.98121
H	2.00875	-3.03879	2.48997
C	-1.69667	2.64497	2.25605
C	-0.89262	-0.08836	2.80495
H	-3.85920	1.87485	1.25152
H	-1.18610	-0.88651	-0.61643
C	-6.09730	0.89210	0.00416

C	-5.59321	-1.40486	-1.55952
C	-0.59721	1.45034	-2.59001
C	2.24912	1.89540	-2.79537
H	3.02353	-0.52544	-3.36986
H	3.32873	-3.01391	-3.60344
H	1.68851	-4.56951	-2.48008
H	-1.47060	-3.27543	-1.21114
C	-1.60311	-5.77369	-0.26184
H	2.21925	-3.44577	0.79304
H	0.48291	-1.66630	1.07582
C	-0.79680	-1.89071	4.98891
C	0.27020	-1.00502	4.75793
C	0.22617	-0.11678	3.66985
C	-1.96177	-0.97831	3.04931
C	-1.90954	-1.87522	4.13083
H	-0.76129	-2.59150	5.83888
H	1.14415	-1.00295	5.43006
H	1.07101	0.56676	3.48764
H	-2.85245	-0.97109	2.40173
H	-2.75251	-2.56324	4.30675
C	-2.82484	4.93835	3.47870
C	-2.67410	4.88391	2.08127
C	-2.11000	3.74979	1.47565
C	-1.86584	2.70266	3.65597
C	-2.42071	3.84552	4.26142
H	-3.26303	5.83077	3.95443
H	-2.99916	5.73187	1.45627
H	-2.01206	3.71596	0.37929
H	-1.57025	1.85088	4.28760
H	-2.54377	3.87311	5.35640
C	4.22546	3.16191	-4.37998
C	2.86349	3.35320	-4.66083
C	1.87924	2.72040	-3.87902
C	3.62517	1.71179	-2.51688
C	4.60432	2.33354	-3.30785
H	4.99392	3.65618	-4.99632
H	2.55671	3.99680	-5.50151
H	0.81700	2.87343	-4.12346
H	3.93527	1.06367	-1.68083
H	5.67160	2.17168	-3.08355
C	-2.92425	2.21123	-3.99458
C	-2.43215	3.02231	-2.95760
C	-1.27857	2.63887	-2.25455
C	-1.08902	0.64667	-3.64122
C	-2.25214	1.02418	-4.33255
H	-3.83467	2.50560	-4.54178
H	-2.95311	3.95684	-2.69205
H	-0.88832	3.27112	-1.43952
H	-0.56818	-0.28052	-3.92760
H	-2.63384	0.38438	-5.14488
C	-2.40272	-5.00809	0.82236
C	-1.19052	-7.15678	0.27621
C	-2.47003	-5.93686	-1.53620
H	-3.29260	-5.60591	1.12089
H	-2.77178	-4.02724	0.45283
H	-1.78751	-4.83833	1.73375
H	-0.61042	-7.72700	-0.47949
H	-2.09706	-7.74470	0.53952

H	-0.55422	-7.06689	1.18177
H	-2.83204	-4.96056	-1.92497
H	-3.36323	-6.55798	-1.30197
H	-1.90552	-6.45198	-2.34453
C	-7.14078	0.24912	-0.66315
H	-6.29556	1.78549	0.61902
H	-5.37164	-2.30050	-2.16003
C	-6.89104	-0.90186	-1.44921
H	-8.16821	0.63909	-0.57574
H	-7.72377	-1.40165	-1.96996
C	3.92264	-2.37029	1.66610
C	6.69378	-1.84293	1.89837
C	5.84155	-1.63809	2.99744
C	4.46652	-1.90120	2.88028
C	4.78739	-2.57676	0.57140
C	6.16323	-2.31464	0.68545
H	7.77452	-1.64662	1.99162
H	6.25282	-1.28335	3.95694
H	3.80654	-1.75388	3.75279
H	4.37877	-2.96088	-0.37861
H	6.82801	-2.49235	-0.17598

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	3.10	0.53882	YES	YES
8	a	10.75	0.04342	YES	YES
9	a	15.03	0.16149	YES	YES
10	a	19.28	0.05407	YES	YES
11	a	20.21	0.10899	YES	YES
12	a	24.80	0.07246	YES	YES
13	a	26.09	0.07971	YES	YES
14	a	29.53	0.00722	YES	YES
15	a	33.23	0.21762	YES	YES
16	a	37.44	0.23408	YES	YES
17	a	40.32	0.04167	YES	YES
18	a	43.61	0.10116	YES	YES
19	a	45.63	0.46519	YES	YES
20	a	47.38	0.20154	YES	YES
21	a	52.29	0.84368	YES	YES
22	a	54.65	1.51323	YES	YES
23	a	58.03	0.27053	YES	YES
24	a	60.85	0.24269	YES	YES
25	a	66.56	0.26864	YES	YES
26	a	67.92	0.09104	YES	YES
27	a	73.66	0.36157	YES	YES
28	a	80.33	1.12120	YES	YES
29	a	82.18	0.58864	YES	YES

30	a	84.72	2.25876	YES	YES
31	a	85.05	0.16973	YES	YES
32	a	90.08	0.20258	YES	YES
33	a	96.90	0.47710	YES	YES
34	a	101.91	0.31551	YES	YES
35	a	114.69	0.72883	YES	YES
36	a	122.43	2.89656	YES	YES
37	a	131.13	0.47377	YES	YES
38	a	140.22	3.12911	YES	YES
39	a	159.14	0.32251	YES	YES
40	a	162.09	2.29371	YES	YES
41	a	168.23	0.25259	YES	YES
42	a	177.53	0.39451	YES	YES
43	a	183.71	1.28705	YES	YES
44	a	188.73	0.28989	YES	YES
45	a	192.91	0.10422	YES	YES
46	a	199.91	0.86904	YES	YES
47	a	204.28	0.11244	YES	YES
48	a	208.85	1.40501	YES	YES
49	a	211.82	2.33003	YES	YES
50	a	217.71	1.68761	YES	YES

./acetonitrile

BP86/SV(P) energy (au): -132.6525337369

PBE0/def2-TZVPP energy (au): -132.6404830920
cosmo_dcm Total energy + OC corr. = -132.6498470987 Total energy + OC corr. = -132.6498470987
cosmo_acetone Total energy + OC corr. = -132.6511082705 Total energy + OC corr. = -132.6511082705

Zero point energy (au): 0.0438597
Entropy (kJ mol^-1): 0.25271
Chemical potential (kJ mol^-1): 51.86

XYZ coordinates:

6

C	0.00019	-0.00041	-0.16472
C	-0.00006	0.00010	1.29743
H	-0.94634	-0.43336	1.68734
H	0.09729	1.03651	1.68681
H	0.84865	-0.60207	1.68788
N	-0.00008	0.00018	-1.33561

Vibrational Spectrum:

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	371.50	0.02558	YES	YES
8	a	371.64	0.02647	YES	YES
9	a	928.92	0.72143	YES	YES
10	a	1024.62	5.09825	YES	YES
11	a	1024.95	5.07499	YES	YES
12	a	1356.97	3.38774	YES	YES
13	a	1410.67	13.41487	YES	YES
14	a	1411.06	13.46100	YES	YES
15	a	2299.66	9.64529	YES	YES
16	a	2956.45	2.55349	YES	YES
17	a	3047.79	0.11487	YES	YES

./TS34

BP86/SV(P) energy (au): -3254.4977373230

PBE0/def2-TZVPP energy (au): -3253.995627227
cosmo_dcm Total energy + OC corr. = -3254.0429448485
cosmo_acetone Total energy + OC corr. = -3254.0481943855

Zero point energy (au): 0.8837293
Entropy (kJ mol^-1): 1.39338
Chemical potential (kJ mol^-1): 2069.06

XYZ coordinates:

114

C	0.40752	2.50560	3.73793
C	1.79286	2.66749	3.37916
C	-0.36971	3.44099	2.98531
C	1.85760	3.71201	2.38639
C	0.53169	4.19175	2.13509
H	0.02050	1.79204	4.47768
H	2.64231	2.14511	3.83354
H	-1.45191	3.60425	3.07074
H	2.77665	4.09916	1.92672
H	0.25138	5.01760	1.46924
Ru	0.64250	2.01562	1.53812
C	-0.00149	-0.86906	2.83321
C	0.34808	0.01590	1.99766
C	-1.97878	3.73494	-0.15282
P	-1.30569	2.04796	0.23543
C	-2.79819	1.20512	0.98697
C	-1.33435	1.19720	-1.41451
C	-1.72364	1.70621	-2.62865
N	-0.98556	-0.13978	-1.32118
C	-1.77505	0.84317	-3.78625
C	-1.43401	-0.54241	-3.65401
C	-1.02271	-1.07596	-2.34727
O	-0.72029	-2.26305	-2.11407
C	2.18273	2.02161	-1.77850
P	2.33052	1.50979	-0.00151
C	4.01406	2.15621	0.48741
C	2.78602	-0.30927	-0.15894
C	4.08819	-0.75371	-0.42179
N	1.77611	-1.18853	0.04894
C	4.33477	-2.14197	-0.41237
C	3.29015	-3.04395	-0.20993
C	1.97867	-2.53404	-0.03669
N	0.83495	-3.32218	-0.00589
C	0.80952	-4.68819	0.33835
C	-0.48645	-5.44601	-0.03491
O	1.77374	-5.22638	0.86733
H	-2.02411	2.75924	-2.71890
H	-0.68467	-0.50598	-0.40834

H	4.89902	-0.03609	-0.61014
H	5.35533	-2.52026	-0.58712
H	3.44819	-4.12935	-0.20569
H	0.04020	-2.92273	-0.55468
C	-1.50063	-1.40484	-4.77254
C	-2.18148	1.31887	-5.06223
H	0.89112	-0.63829	1.00210
C	6.56006	3.04181	1.35789
C	6.02751	3.50116	0.14348
C	4.76481	3.05759	-0.29502
C	4.56405	1.69048	1.70564
C	5.82640	2.12673	2.13538
H	7.55004	3.38807	1.69628
H	6.60024	4.20624	-0.48098
H	4.38092	3.41292	-1.26304
H	4.00567	0.96072	2.31457
H	6.24239	1.74648	3.08271
C	1.95959	2.92536	-4.44985
C	1.92060	3.84721	-3.38842
C	2.01724	3.39735	-2.06151
C	2.22532	1.10462	-2.85016
C	2.10562	1.55590	-4.17664
H	1.87767	3.27617	-5.49130
H	1.81243	4.92481	-3.59527
H	1.97880	4.12560	-1.23388
H	2.35721	0.02776	-2.66048
H	2.13412	0.82658	-5.00240
C	-2.91886	6.34965	-0.69142
C	-3.65014	5.49503	0.14856
C	-3.18863	4.19298	0.41362
C	-1.24110	4.60657	-0.98612
C	-1.71424	5.89981	-1.26160
H	-3.28571	7.36724	-0.90264
H	-4.59497	5.83815	0.60086
H	-3.78336	3.53331	1.06408
H	-0.29324	4.26620	-1.43050
H	-1.13552	6.56356	-1.92503
C	-5.11035	0.04964	2.14032
C	-4.01923	0.40617	2.95039
C	-2.86647	0.97044	2.37547
C	-3.90105	0.84260	0.17947
C	-5.04529	0.26429	0.75236
H	-6.01149	-0.39932	2.58948
H	-4.05823	0.23743	4.03908
H	-2.00545	1.21889	3.01138
H	-3.87304	1.01660	-0.90855
H	-5.89417	-0.01658	0.10802
C	-1.75793	-4.63238	0.30262
C	-0.49845	-6.77956	0.73748
C	-0.42851	-5.72067	-1.56315
H	0.47901	-6.30616	-1.82868
H	-0.43281	-4.77762	-2.15015
H	-1.31788	-6.31697	-1.86617
H	-2.65633	-5.25819	0.10617
H	-1.85840	-3.72057	-0.32485
H	-1.77892	-4.33634	1.37479
H	-1.38536	-7.37949	0.43793
H	-0.54663	-6.60911	1.83468

H	0.41651	-7.37136	0.53129
H	-2.45295	2.38125	-5.17649
C	-2.24343	0.45492	-6.15665
C	-1.90154	-0.91146	-6.01571
H	-1.23520	-2.46435	-4.63417
H	-2.56479	0.83953	-7.13855
H	-1.95701	-1.58453	-6.88630
C	-0.32620	-1.89101	3.76313
C	-0.97168	-3.88728	5.66213
C	0.30754	-3.30074	5.66812
C	0.63366	-2.31529	4.72969
C	-1.61652	-2.49612	3.77063
C	-1.93111	-3.48219	4.71333
H	-1.22437	-4.66353	6.40286
H	1.05747	-3.61997	6.41050
H	1.63319	-1.85371	4.72741
H	-2.36311	-2.16913	3.03053
H	-2.93235	-3.94263	4.71210

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-417.30	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	12.47	0.22322	YES	YES
9	a	15.98	0.09939	YES	YES
10	a	19.45	0.09420	YES	YES
11	a	24.06	0.06240	YES	YES
12	a	24.35	0.76018	YES	YES
13	a	30.48	0.05601	YES	YES
14	a	31.57	0.32064	YES	YES
15	a	37.33	0.26413	YES	YES
16	a	41.66	0.27593	YES	YES
17	a	42.49	0.01817	YES	YES
18	a	45.40	0.22425	YES	YES
19	a	47.61	0.70052	YES	YES
20	a	48.96	0.40420	YES	YES
21	a	52.09	0.50230	YES	YES
22	a	54.14	0.01644	YES	YES
23	a	57.68	0.11347	YES	YES
24	a	59.65	0.37294	YES	YES
25	a	63.46	1.75314	YES	YES
26	a	65.66	1.17526	YES	YES
27	a	72.22	2.01072	YES	YES
28	a	73.80	0.85624	YES	YES
29	a	80.59	0.43226	YES	YES
30	a	83.95	0.44208	YES	YES
31	a	90.23	0.37474	YES	YES
32	a	96.36	0.65459	YES	YES

33	a	101.94	1.36139	YES	YES
34	a	102.33	0.71248	YES	YES
35	a	115.67	2.35425	YES	YES
36	a	123.38	3.35700	YES	YES
37	a	129.10	0.50386	YES	YES
38	a	133.96	1.65384	YES	YES
39	a	148.29	15.38598	YES	YES
40	a	156.87	2.94003	YES	YES
41	a	164.90	7.03085	YES	YES
42	a	169.96	2.33155	YES	YES
43	a	175.23	10.72099	YES	YES
44	a	185.36	3.66129	YES	YES
45	a	194.02	1.05632	YES	YES
46	a	200.33	0.45987	YES	YES
47	a	202.94	1.07098	YES	YES
48	a	208.65	2.49262	YES	YES
49	a	216.60	7.20320	YES	YES
50	a	220.62	0.77112	YES	YES

./TS35

BP86/SV(P) energy (au): -3254.4897504080

PBE0/def2-TZVPP energy (au): -3253.992168418
cosmo_dcm Total energy + OC corr. = -3254.0395647858
cosmo_acetone Total energy + OC corr. = -3254.0448781805

Zero point energy (au): 0.8867127
Entropy (kJ mol^-1): 1.39218
Chemical potential (kJ mol^-1): 2071.94

XYZ coordinates:

114

C	0.10857	3.19658	3.59586
C	1.52543	3.26971	3.33604
C	-0.57543	3.90401	2.56031
C	1.70167	4.03351	2.12781
C	0.41562	4.43002	1.64408
H	-0.36132	2.69903	4.45500
H	2.32106	2.88674	3.98574
H	-1.65891	4.06682	2.49453
H	2.66677	4.29127	1.67169
H	0.21613	5.08453	0.78834
Ru	0.52956	2.14256	1.63611
C	-0.05852	-0.67907	3.15633
C	0.26998	0.37326	2.50491
C	-2.30533	3.27586	-0.10682
P	-1.31841	1.72320	0.21462
C	-2.61015	0.59421	0.94398
C	-1.21768	1.04355	-1.52759
C	-1.91902	1.58775	-2.58157
N	-0.50607	-0.12941	-1.71430
C	-1.89843	0.95988	-3.87840
C	-1.17722	-0.26088	-4.04725
C	-0.46969	-0.85329	-2.90436
O	0.13609	-1.94526	-2.95768
C	2.33556	1.56960	-1.49738
P	2.29973	1.27992	0.32824
C	3.95795	1.95422	0.85684
C	2.55734	-0.57507	0.48208
C	3.63117	-1.13508	1.19352
N	1.57813	-1.33132	-0.05975
C	3.64709	-2.53333	1.37742
C	2.63966	-3.32138	0.82710
C	1.62797	-2.67905	0.06195
N	0.66054	-3.38900	-0.64840
C	0.19231	-4.66294	-0.32269
C	-0.70546	-5.34245	-1.38501
O	0.48002	-5.19894	0.74812
H	-2.52310	2.49274	-2.44169
H	0.13506	-0.51845	-0.96858

H	4.44494	-0.51205	1.58738
H	4.46971	-3.00591	1.93929
H	2.62234	-4.41142	0.94783
H	0.34682	-2.90189	-1.52751
C	-1.15239	-0.90898	-5.30339
C	-2.58852	1.50299	-4.99644
H	1.28183	-0.19193	2.86413
C	6.45338	2.98942	1.71650
C	6.06878	3.09349	0.37067
C	4.83327	2.57575	-0.06010
C	4.35353	1.86047	2.21271
C	5.59266	2.36509	2.63750
H	7.42280	3.39346	2.05050
H	6.73653	3.57857	-0.35992
H	4.55580	2.66022	-1.12145
H	3.68863	1.37870	2.94723
H	5.88662	2.27374	3.69606
C	2.49517	2.17770	-4.24898
C	1.93010	3.10484	-3.35602
C	1.84400	2.79758	-1.98830
C	2.91445	0.64824	-2.39717
C	2.98475	0.95120	-3.76735
H	2.55350	2.41144	-5.32447
H	1.54866	4.06961	-3.72814
H	1.39887	3.51953	-1.28321
H	3.31036	-0.31352	-2.03631
H	3.42706	0.22011	-4.46332
C	-3.73642	5.67345	-0.58903
C	-4.31799	4.64021	0.16208
C	-3.61205	3.44548	0.39745
C	-1.72931	4.32148	-0.86540
C	-2.44028	5.50695	-1.10953
H	-4.29346	6.60611	-0.77511
H	-5.33715	4.75530	0.56611
H	-4.09344	2.64210	0.97574
H	-0.72176	4.19836	-1.29343
H	-1.97903	6.30653	-1.71229
C	-4.65361	-0.97994	2.10988
C	-3.88744	-0.11413	2.90912
C	-2.86809	0.66082	2.33163
C	-3.39166	-0.27101	0.14772
C	-4.40108	-1.05714	0.73033
H	-5.44866	-1.59405	2.56334
H	-4.08075	-0.04406	3.99207
H	-2.26674	1.33178	2.96644
H	-3.22452	-0.33288	-0.93857
H	-4.99907	-1.73079	0.09500
C	-1.97413	-4.48660	-1.62675
C	-1.11015	-6.73178	-0.85657
C	0.09002	-5.49076	-2.70736
H	1.02634	-6.07162	-2.55231
H	0.35374	-4.50596	-3.14917
H	-0.52712	-6.04049	-3.45240
H	-2.65116	-5.01618	-2.33341
H	-1.73088	-3.50062	-2.07772
H	-2.53539	-4.31856	-0.68076
H	-1.74857	-7.24753	-1.60690
H	-1.67930	-6.65500	0.09406

H	-0.21966	-7.36525	-0.65946
H	-3.15400	2.44171	-4.87590
C	-2.55227	0.85509	-6.23173
C	-1.83188	-0.35398	-6.38946
H	-0.58924	-1.85024	-5.39575
H	-3.09091	1.28628	-7.09156
H	-1.81283	-0.85731	-7.36963
C	-0.36177	-1.83895	3.93226
C	-0.98414	-4.11468	5.47545
C	-1.02791	-2.83584	6.06461
C	-0.71280	-1.70312	5.30596
C	-0.32288	-3.13562	3.34982
C	-0.62765	-4.26217	4.12225
H	-1.22768	-5.00400	6.07967
H	-1.30481	-2.72582	7.12546
H	-0.73729	-0.70013	5.76091
H	-0.04118	-3.26386	2.29408
H	-0.58243	-5.25833	3.65435

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-593.20	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	8.00	0.35152	YES	YES
9	a	17.89	0.17018	YES	YES
10	a	19.81	0.11954	YES	YES
11	a	22.77	0.18847	YES	YES
12	a	23.83	0.16605	YES	YES
13	a	27.25	0.09222	YES	YES
14	a	29.69	0.20507	YES	YES
15	a	33.48	0.19457	YES	YES
16	a	37.52	0.14968	YES	YES
17	a	41.98	0.09048	YES	YES
18	a	43.42	0.02607	YES	YES
19	a	47.70	0.06027	YES	YES
20	a	49.81	0.08448	YES	YES
21	a	54.64	0.22860	YES	YES
22	a	57.20	0.34005	YES	YES
23	a	60.49	1.59946	YES	YES
24	a	60.98	0.53597	YES	YES
25	a	65.28	1.01577	YES	YES
26	a	67.87	0.99262	YES	YES
27	a	69.66	0.11875	YES	YES
28	a	80.35	0.62361	YES	YES
29	a	85.69	0.79402	YES	YES
30	a	88.08	1.26567	YES	YES
31	a	88.94	0.25341	YES	YES
32	a	95.35	0.64159	YES	YES

33	a	100.11	0.85580	YES	YES
34	a	103.14	0.68727	YES	YES
35	a	114.86	0.42817	YES	YES
36	a	116.29	0.73480	YES	YES
37	a	125.30	0.87023	YES	YES
38	a	126.87	1.51240	YES	YES
39	a	140.01	3.30517	YES	YES
40	a	163.84	1.59825	YES	YES
41	a	168.31	0.60281	YES	YES
42	a	171.34	0.98358	YES	YES
43	a	182.92	2.04602	YES	YES
44	a	191.29	1.13286	YES	YES
45	a	198.26	0.75550	YES	YES
46	a	203.13	0.60110	YES	YES
47	a	211.97	2.79423	YES	YES
48	a	214.30	0.32871	YES	YES
49	a	219.10	1.46895	YES	YES
50	a	225.78	1.60100	YES	YES

./TS45

BP86/SV(P) energy (au): -3254.4988968980

PBE0/def2-TZVPP energy (au): -3253.996018670
cosmo_dcm Total energy + OC corr. = -3254.0443307801
cosmo_acetone Total energy + OC corr. = -3254.0497258875

Zero point energy (au): 0.8868771
Entropy (kJ mol^-1): 1.37925
Chemical potential (kJ mol^-1): 2073.71

XYZ coordinates:

114

C	2.29946	3.30701	1.62449
C	2.90718	3.34242	0.33246
C	1.07139	4.04873	1.56845
C	2.06080	4.14070	-0.53511
C	0.94575	4.58509	0.22827
H	2.69517	2.78833	2.50803
H	3.88396	2.91965	0.07514
H	0.39161	4.22957	2.41055
H	2.27021	4.38750	-1.58420
H	0.14070	5.24272	-0.12570
Ru	0.88255	2.27243	0.17419
C	1.17466	-0.27382	2.04457
C	0.91269	0.77943	1.35976
C	-2.38643	3.45611	-0.85880
P	-1.46440	2.19925	0.15319
C	-2.17097	2.49668	1.85050
C	-2.28071	0.58814	-0.31256
C	-3.45823	0.45689	-1.00829
N	-1.60688	-0.54991	0.10125
C	-3.98980	-0.85457	-1.28820
C	-3.27200	-2.01484	-0.85541
C	-1.99888	-1.86545	-0.13385
O	-1.29271	-2.81192	0.26440
C	0.24776	0.13915	-2.85512
P	1.48277	0.85816	-1.65262
C	2.66932	1.71909	-2.80795
C	2.41779	-0.72303	-1.23452
C	3.53893	-1.17287	-1.94136
N	1.83115	-1.52181	-0.29262
C	4.04996	-2.45880	-1.65664
C	3.40362	-3.29819	-0.75197
C	2.23862	-2.81182	-0.10272
N	1.42276	-3.56498	0.72086
C	1.79251	-4.77027	1.35884
C	0.64032	-5.56172	2.01758
O	2.95415	-5.15704	1.34544
H	-3.99792	1.34438	-1.36555
H	-0.72163	-0.43544	0.62756

H	3.99503	-0.55764	-2.72839
H	4.94258	-2.82213	-2.19210
H	3.75213	-4.31598	-0.54102
H	0.43277	-3.23475	0.76601
C	-3.78023	-3.30668	-1.12077
C	-5.21484	-1.03638	-1.98566
H	1.41604	-0.92073	0.83558
C	-3.13640	2.99807	4.46333
C	-2.78088	4.06891	3.62450
C	-2.30158	3.82150	2.32794
C	-2.53521	1.42770	2.69701
C	-3.01533	1.67988	3.99449
H	-3.51710	3.19304	5.47907
H	-2.88590	5.10785	3.97781
H	-2.05009	4.67476	1.67669
H	-2.45920	0.38588	2.34956
H	-3.30627	0.83397	4.63862
C	-3.78169	5.36281	-2.41627
C	-2.43023	5.08800	-2.68388
C	-1.73716	4.14274	-1.90747
C	-3.74405	3.75025	-0.58778
C	-4.43504	4.69423	-1.36574
H	-4.32554	6.10708	-3.02042
H	-1.90741	5.61692	-3.49724
H	-0.67139	3.94361	-2.10754
H	-4.26475	3.25091	0.24476
H	-5.49166	4.91474	-1.14193
C	4.43149	3.16176	-4.49774
C	3.09437	2.95894	-4.87559
C	2.22025	2.23873	-4.04183
C	4.01895	1.92883	-2.43682
C	4.89264	2.63828	-3.27713
H	5.11688	3.72009	-5.15579
H	2.72420	3.35368	-5.83585
H	1.18189	2.07472	-4.36855
H	4.40706	1.51515	-1.49243
H	5.94334	2.77966	-2.97517
C	-1.55290	-0.78014	-4.83964
C	-1.73128	0.48341	-4.25513
C	-0.84392	0.93298	-3.26283
C	0.42006	-1.13161	-3.45115
C	-0.47858	-1.58726	-4.42909
H	-2.25170	-1.13809	-5.61309
H	-2.57063	1.12694	-4.56530
H	-1.00375	1.92227	-2.81042
H	1.26294	-1.77929	-3.16723
H	-0.33052	-2.58284	-4.87836
C	-0.19331	-4.66885	2.96887
C	1.25922	-6.73139	2.80696
C	-0.26401	-6.11126	0.88114
H	-0.95871	-5.29570	3.47752
H	-0.73624	-3.86456	2.42845
H	0.44250	-4.20397	3.75338
H	0.45065	-7.34311	3.26321
H	1.92047	-6.36476	3.62122
H	1.87041	-7.38552	2.15129
H	0.31704	-6.74293	0.17322
H	-0.75331	-5.29043	0.31392

H	-1.06501	-6.74586	1.32198
C	-5.70555	-2.31843	-2.23639
H	-5.77777	-0.15019	-2.32251
H	-3.20495	-4.17853	-0.77336
C	-4.98848	-3.45944	-1.80379
H	-6.65999	-2.44311	-2.77368
H	-5.38612	-4.46712	-2.00516
C	1.36731	-0.91339	3.33998
C	1.78863	-2.07208	5.89435
C	2.61418	-2.42424	4.81228
C	2.40613	-1.85519	3.54643
C	0.54233	-0.56390	4.44066
C	0.75387	-1.13877	5.70188
H	1.95390	-2.52040	6.88755
H	3.43344	-3.14810	4.95337
H	3.07259	-2.12952	2.71331
H	-0.26622	0.17015	4.29308
H	0.10487	-0.85251	6.54603

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-934.80	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	12.97	0.02853	YES	YES
9	a	19.40	0.25151	YES	YES
10	a	20.59	0.13481	YES	YES
11	a	22.81	0.06171	YES	YES
12	a	26.33	0.13345	YES	YES
13	a	31.50	0.13499	YES	YES
14	a	33.14	0.17141	YES	YES
15	a	35.58	0.70636	YES	YES
16	a	41.97	0.19714	YES	YES
17	a	43.21	0.21690	YES	YES
18	a	47.59	0.68739	YES	YES
19	a	48.58	0.18251	YES	YES
20	a	52.71	0.50892	YES	YES
21	a	56.17	0.50385	YES	YES
22	a	57.93	0.18469	YES	YES
23	a	59.67	0.26198	YES	YES
24	a	62.27	0.50503	YES	YES
25	a	69.00	0.13660	YES	YES
26	a	71.60	0.31675	YES	YES
27	a	76.21	0.02624	YES	YES
28	a	78.37	1.24902	YES	YES
29	a	82.71	1.05906	YES	YES
30	a	87.56	0.62317	YES	YES
31	a	94.80	0.97073	YES	YES
32	a	95.28	0.97032	YES	YES

33	a	106.96	0.55488	YES	YES
34	a	110.45	0.50138	YES	YES
35	a	119.94	1.23890	YES	YES
36	a	122.89	1.36536	YES	YES
37	a	127.17	2.21030	YES	YES
38	a	138.03	2.19479	YES	YES
39	a	161.22	0.62884	YES	YES
40	a	164.55	0.75982	YES	YES
41	a	166.98	1.99571	YES	YES
42	a	170.26	2.37404	YES	YES
43	a	180.80	0.78559	YES	YES
44	a	193.82	4.90737	YES	YES
45	a	198.75	0.48944	YES	YES
46	a	205.48	6.29101	YES	YES
47	a	211.44	2.19027	YES	YES
48	a	213.13	1.08583	YES	YES
49	a	214.62	1.56544	YES	YES
50	a	216.14	2.21445	YES	YES

./TS67

BP86/SV(P) energy (au): -3330.8808892680

PBE0/def2-TZVPP energy (au): -3330.388550597
cosmo_dcm Total energy + OC corr. = -3330.4371526455
cosmo_acetone Total energy + OC corr. = -3330.4426033546

Zero point energy (au): 0.9126460
Entropy (kJ mol^-1): 1.40202
Chemical potential (kJ mol^-1): 2139.54

XYZ coordinates:

117

C	1.57246	4.43949	0.83377
C	2.16869	4.32473	-0.47276
C	0.17232	4.67270	0.66651
C	1.12000	4.52665	-1.44447
C	-0.10473	4.74210	-0.75501
H	2.10357	4.36801	1.79262
H	3.23636	4.20924	-0.69397
H	-0.55637	4.84453	1.47004
H	1.25907	4.53140	-2.53365
H	-1.08110	4.95459	-1.20728
Ru	0.69341	2.62001	-0.19539
C	2.95239	1.35491	1.57443
C	1.78571	1.48745	0.90933
P	-1.42266	1.83407	0.62603
C	-2.27632	0.27337	0.04184
C	-3.51864	0.18222	-0.54350
N	-1.55462	-0.87719	0.28122
C	-4.04428	-1.11422	-0.90211
C	-3.25989	-2.28995	-0.66902
C	-1.92860	-2.16704	-0.05668
O	-1.15316	-3.12174	0.17015
P	1.07644	1.21672	-2.05824
C	1.95132	-0.46871	-1.99903
C	2.81241	-0.86268	-3.03310
N	1.67171	-1.31755	-0.97967
C	3.40019	-2.14324	-2.97329
C	3.08930	-3.01981	-1.93544
C	2.16754	-2.58604	-0.94893
N	1.68902	-3.38756	0.07925
C	2.35522	-4.51578	0.60160
O	3.47649	-4.82521	0.21898
H	3.65896	2.16809	1.30255
C	-2.78146	3.08480	0.39585
C	-1.45929	1.54968	2.46602
H	-4.12669	1.07845	-0.72254
H	-0.63246	-0.77487	0.77512
C	-5.33378	-1.26718	-1.48141
C	-3.76374	-3.56489	-1.01514

C	-0.40157	0.79908	-3.10052
C	2.23848	2.05405	-3.25387
H	3.03076	-0.19099	-3.87334
H	4.09374	-2.46331	-3.76832
H	3.52009	-4.02549	-1.86584
H	0.69589	-3.20347	0.35385
C	1.56858	-5.32021	1.66211
O	0.90071	-0.32955	1.19133
H	1.37389	-0.76018	1.94859
H	1.26071	-0.81855	0.20933
C	-4.81330	5.01645	-0.00817
C	-4.23503	4.35754	-1.10801
C	-3.22063	3.40672	-0.90967
C	-3.36913	3.74918	1.49423
C	-4.37433	4.71230	1.28991
H	-5.60578	5.76596	-0.16485
H	-4.57577	4.58695	-2.13121
H	-2.77209	2.90166	-1.77978
H	-3.04890	3.51564	2.52131
H	-4.82023	5.22227	2.15946
C	-1.57462	1.23196	5.27299
C	-0.53142	1.97012	4.68899
C	-0.47188	2.12384	3.29263
C	-2.50763	0.81126	3.06070
C	-2.56042	0.65170	4.45519
H	-1.61998	1.10722	6.36728
H	0.24880	2.42482	5.32151
H	0.36101	2.68000	2.83691
H	-3.29467	0.35986	2.43482
H	-3.38129	0.06992	4.90576
C	4.11661	3.30795	-4.95920
C	4.47810	2.96154	-3.64363
C	3.54585	2.34350	-2.79600
C	1.88980	2.38531	-4.57948
C	2.82429	3.01637	-5.42335
H	4.84718	3.79729	-5.62364
H	5.49619	3.17191	-3.27677
H	3.84303	2.06088	-1.77214
H	0.89073	2.14251	-4.97164
H	2.53607	3.27059	-6.45644
C	-2.68283	0.28582	-4.69396
C	-2.32458	1.60944	-4.38111
C	-1.20163	1.86347	-3.57745
C	-0.76586	-0.52486	-3.42359
C	-1.90551	-0.77739	-4.20796
H	-3.56889	0.08418	-5.31780
H	-2.92587	2.45058	-4.76416
H	-0.93440	2.90410	-3.32938
H	-0.16566	-1.37542	-3.06771
H	-2.18147	-1.81803	-4.44335
C	0.93990	-4.38898	2.72710
C	2.54875	-6.29958	2.33590
C	0.45263	-6.10977	0.92601
H	0.47461	-5.00592	3.52722
H	0.13496	-3.74702	2.30705
H	1.70768	-3.74005	3.20540
H	0.88315	-6.78066	0.15019
H	-0.28374	-5.43016	0.44607

H	-0.09516	-6.74517	1.65718
H	2.00377	-6.92665	3.07476
H	3.36075	-5.75820	2.86763
H	3.02832	-6.96718	1.59053
H	-3.13492	-4.44725	-0.81908
C	-5.03416	-3.68803	-1.58139
C	-5.81920	-2.53267	-1.81298
H	-5.95009	-0.37091	-1.66208
H	-6.82346	-2.63390	-2.25635
H	-5.42901	-4.68274	-1.84440
C	3.46787	0.37761	2.55615
C	4.53696	-1.47776	4.42793
C	5.34855	-0.95083	3.40715
C	4.82222	-0.03366	2.48601
C	2.66928	-0.13776	3.61100
C	3.19837	-1.06232	4.52837
H	4.95234	-2.19619	5.15297
H	6.40371	-1.25962	3.32676
H	5.46779	0.36952	1.68754
H	1.64065	0.23628	3.75093
H	2.56213	-1.44083	5.34570

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-308.91	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	15.20	0.06657	YES	YES
9	a	17.72	0.07422	YES	YES
10	a	21.67	0.02947	YES	YES
11	a	26.38	0.00378	YES	YES
12	a	29.03	0.20459	YES	YES
13	a	31.71	0.21225	YES	YES
14	a	34.07	0.12647	YES	YES
15	a	35.17	0.12385	YES	YES
16	a	41.01	0.04104	YES	YES
17	a	47.25	0.04403	YES	YES
18	a	47.53	0.81485	YES	YES
19	a	48.71	0.42542	YES	YES
20	a	51.98	0.20503	YES	YES
21	a	54.17	0.19151	YES	YES
22	a	58.22	0.71934	YES	YES
23	a	60.00	0.07022	YES	YES
24	a	64.07	0.18429	YES	YES
25	a	69.63	0.58239	YES	YES
26	a	70.23	1.52573	YES	YES
27	a	71.16	1.89974	YES	YES
28	a	75.42	1.25835	YES	YES
29	a	81.53	0.34466	YES	YES

30	a	85.38	0.07600	YES	YES
31	a	89.50	0.94360	YES	YES
32	a	94.84	0.69850	YES	YES
33	a	99.07	0.72643	YES	YES
34	a	108.20	0.88554	YES	YES
35	a	112.19	1.29551	YES	YES
36	a	119.80	0.18723	YES	YES
37	a	127.56	3.32531	YES	YES
38	a	129.99	0.42463	YES	YES
39	a	140.18	2.37827	YES	YES
40	a	155.51	0.41490	YES	YES
41	a	165.39	1.00449	YES	YES
42	a	171.17	0.24431	YES	YES
43	a	180.16	0.45591	YES	YES
44	a	187.91	3.43719	YES	YES
45	a	193.39	0.47411	YES	YES
46	a	198.73	1.21802	YES	YES
47	a	205.00	0.87540	YES	YES
48	a	208.39	2.09300	YES	YES
49	a	212.83	2.07671	YES	YES
50	a	215.06	0.55455	YES	YES

./TS78

BP86/SV(P) energy (au): -3330.8802158220

PBE0/def2-TZVPP energy (au): -3330.393145860
cosmo_dcm Total energy + OC corr. = -3330.4429229956
cosmo_acetone Total energy + OC corr. = -3330.4484877664

Zero point energy (au): 0.9132646
Entropy (kJ mol^-1): 1.38774
Chemical potential (kJ mol^-1): 2145.41

XYZ coordinates:

117

C	-1.52432	0.41953	4.07022
C	-0.17028	-0.01822	4.27953
C	-1.49839	1.81104	3.72585
C	0.68364	1.12971	4.07422
C	-0.11970	2.25673	3.74368
H	-2.43031	-0.18983	4.18934
H	0.14949	-1.00416	4.63236
H	-2.37272	2.45443	3.56458
H	1.77529	1.13091	4.19189
H	0.22786	3.28167	3.56446
Ru	-0.40598	0.64719	2.11479
C	-1.16689	-2.29301	1.14404
C	-1.38185	-0.89015	1.19095
P	-1.28591	2.23810	0.57969
C	-0.80387	2.14392	-1.22148
C	-0.31560	3.14494	-2.02757
N	-1.00931	0.88590	-1.76050
C	-0.03201	2.87114	-3.41714
C	-0.25528	1.55690	-3.94540
C	-0.77641	0.49720	-3.06958
O	-1.01231	-0.68009	-3.42002
P	1.68609	0.04584	1.17475
C	1.92766	-1.39126	-0.03134
C	3.19008	-1.94323	-0.27802
N	0.82991	-1.88489	-0.67283
C	3.30447	-3.00623	-1.19682
C	2.18208	-3.46989	-1.88800
C	0.93508	-2.85784	-1.63026
N	-0.24490	-3.14700	-2.29936
C	-0.55054	-4.40109	-2.86814
O	0.16778	-5.37188	-2.66879
H	-1.90258	-2.84960	0.51038
C	-0.92831	4.00837	1.02270
C	-3.14851	2.32078	0.37812
H	-0.15234	4.15581	-1.62894
H	-1.45046	0.17544	-1.14959
C	0.46114	3.87525	-4.29482
C	0.01326	1.27889	-5.30550

C	2.61560	1.36579	0.24567
C	2.95598	-0.53477	2.42997
H	4.07701	-1.55066	0.23973
H	4.29133	-3.45539	-1.39516
H	2.24545	-4.27687	-2.62810
H	-0.80341	-2.30189	-2.55995
C	-1.82222	-4.43559	-3.74484
O	-2.35801	-0.51084	0.28620
H	-2.88599	-1.29670	-0.01726
H	-0.17293	-1.95903	0.06285
C	-0.33236	6.66076	1.82383
C	0.67000	5.84503	1.26964
C	0.37779	4.52713	0.88276
C	-1.93058	4.83526	1.57911
C	-1.63026	6.14887	1.98161
H	-0.10120	7.69355	2.13179
H	1.69265	6.23617	1.13873
H	1.17904	3.89784	0.46888
H	-2.95934	4.46185	1.69568
H	-2.42492	6.77776	2.41523
C	-5.95461	2.58109	0.11710
C	-5.09844	3.20218	-0.80822
C	-3.70529	3.07616	-0.67766
C	-4.01572	1.69220	1.29452
C	-5.40919	1.82598	1.16916
H	-7.04754	2.68275	0.01622
H	-5.51582	3.79271	-1.64029
H	-3.04871	3.57638	-1.40822
H	-3.59828	1.07375	2.10304
H	-6.07316	1.32900	1.89555
C	4.79198	-1.58731	4.31631
C	3.51040	-2.14988	4.18452
C	2.59943	-1.62829	3.25243
C	4.25434	0.00807	2.55108
C	5.16074	-0.51169	3.49398
H	5.50418	-1.99265	5.05339
H	3.21188	-3.00652	4.81023
H	1.60577	-2.09251	3.15340
H	4.58147	0.83469	1.90342
H	6.16712	-0.06929	3.57636
C	4.07300	3.40796	-1.07147
C	3.83827	3.48735	0.31262
C	3.09781	2.48600	0.96260
C	2.84561	1.30317	-1.14560
C	3.56103	2.32181	-1.79942
H	4.65248	4.19440	-1.58178
H	4.23109	4.33816	0.89361
H	2.90207	2.57879	2.04372
H	2.47268	0.45289	-1.73781
H	3.72630	2.25572	-2.88696
C	-1.49026	-3.71602	-5.08038
C	-3.00779	-3.72423	-3.04739
C	-2.17867	-5.91014	-4.01327
H	-3.06343	-5.96755	-4.68419
H	-2.42020	-6.44737	-3.07034
H	-1.33437	-6.44591	-4.49421
H	-1.23585	-2.64599	-4.92080
H	-2.37397	-3.76107	-5.75439

H	-0.64221	-4.21373	-5.59961
H	-3.21537	-4.16344	-2.04597
H	-3.92473	-3.84805	-3.66289
H	-2.84096	-2.63022	-2.93826
H	0.63391	4.89106	-3.90315
C	0.71879	3.58507	-5.63521
C	0.49637	2.28342	-6.14594
H	-0.17327	0.26022	-5.67916
H	1.09629	4.37687	-6.30298
H	0.70111	2.06673	-7.20677
C	-0.55549	-3.19228	2.17051
C	0.44947	-5.04869	4.07936
C	-0.46337	-4.05326	4.47060
C	-0.96380	-3.14386	3.52422
C	0.33975	-4.22133	1.79027
C	0.83997	-5.13549	2.73211
H	0.83485	-5.77030	4.81810
H	-0.80639	-3.99833	5.51717
H	-1.71872	-2.40177	3.82553
H	0.64081	-4.32857	0.73492
H	1.53420	-5.92737	2.40715

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-891.86	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	14.55	0.10878	YES	YES
9	a	16.43	0.01800	YES	YES
10	a	22.50	0.04461	YES	YES
11	a	26.16	0.07189	YES	YES
12	a	26.89	0.04652	YES	YES
13	a	32.32	0.45130	YES	YES
14	a	36.50	0.24107	YES	YES
15	a	38.62	0.34468	YES	YES
16	a	41.79	0.17786	YES	YES
17	a	46.75	0.52432	YES	YES
18	a	51.05	0.11276	YES	YES
19	a	52.14	0.55349	YES	YES
20	a	56.62	0.45134	YES	YES
21	a	58.09	0.38947	YES	YES
22	a	59.81	0.12359	YES	YES
23	a	63.56	0.65504	YES	YES
24	a	65.17	0.41657	YES	YES
25	a	67.23	0.17965	YES	YES
26	a	71.32	0.59435	YES	YES
27	a	75.43	0.74807	YES	YES
28	a	83.30	0.26883	YES	YES
29	a	87.50	2.16624	YES	YES

30	a	89.13	2.78082	YES	YES
31	a	96.75	0.12205	YES	YES
32	a	105.88	0.40008	YES	YES
33	a	109.04	1.60402	YES	YES
34	a	112.33	0.06101	YES	YES
35	a	117.92	2.65962	YES	YES
36	a	129.39	1.83581	YES	YES
37	a	133.44	1.06792	YES	YES
38	a	141.95	0.87181	YES	YES
39	a	156.87	0.72190	YES	YES
40	a	165.12	0.59553	YES	YES
41	a	172.83	2.45699	YES	YES
42	a	174.54	3.13635	YES	YES
43	a	177.29	2.81741	YES	YES
44	a	182.88	0.97408	YES	YES
45	a	187.73	4.96148	YES	YES
46	a	189.18	3.76050	YES	YES
47	a	198.23	0.93156	YES	YES
48	a	202.50	3.06563	YES	YES
49	a	206.90	2.47268	YES	YES
50	a	211.33	0.33752	YES	YES

./TS810

BP86/SV(P) energy (au): -3330.8731180040

PBE0/def2-TZVPP energy (au): -3330.378632471
cosmo_dcm Total energy + OC corr. = -3330.4323994007
cosmo_acetone Total energy + OC corr. = -3330.4386240770

Zero point energy (au): 0.9112737
Entropy (kJ mol^-1): 1.42425
Chemical potential (kJ mol^-1): 2132.32

XYZ coordinates:

117

C	2.47537	3.02547	-2.37279
C	1.24813	3.76962	-2.52225
C	2.98908	3.29604	-1.05121
C	0.97719	4.44860	-1.30771
C	2.04269	4.13391	-0.38184
H	2.97866	2.45820	-3.16635
H	0.63199	3.81570	-3.42988
H	3.95104	2.95792	-0.64288
H	0.12416	5.10720	-1.10069
H	2.15377	4.54737	0.62901
Ru	1.07345	2.08568	-0.85333
C	3.24387	-0.14363	-1.50734
C	2.18574	0.43480	-0.57880
P	-0.25318	2.26912	1.14949
C	-1.27060	0.89014	1.89170
C	-2.52300	1.07302	2.43450
N	-0.61648	-0.31581	2.08000
C	-3.14894	0.01576	3.19488
C	-2.44810	-1.21147	3.40084
C	-1.09967	-1.40879	2.83083
O	-0.40962	-2.41984	2.95664
P	-0.40591	0.78200	-2.17520
C	-1.31986	-0.62108	-1.35620
C	-2.71815	-0.61935	-1.21374
N	-0.53351	-1.61495	-0.90727
C	-3.30525	-1.73827	-0.58987
C	-2.51205	-2.79834	-0.15072
C	-1.10490	-2.69473	-0.32714
N	-0.20547	-3.67608	0.07666
C	-0.47530	-4.87281	0.75828
O	-1.61872	-5.24279	0.99342
O	2.08276	-0.05781	0.60560
H	2.76775	-0.32192	-2.49572
C	-1.46452	3.66790	1.02138
C	0.74863	2.69211	2.66836
H	-3.04861	2.03072	2.32675
H	0.31128	-0.48552	1.66586
C	-4.44167	0.16310	3.76569

C	-3.03468	-2.25186	4.15246
C	-1.75218	1.68786	-3.08619
C	0.44097	-0.01997	-3.63559
H	-3.33486	0.20982	-1.58884
H	3.97042	0.68396	-1.68601
H	-4.39829	-1.78391	-0.45444
H	-2.92548	-3.69425	0.32891
H	0.77614	-3.39804	-0.03241
C	0.77875	-5.69968	1.13598
H	1.26576	0.99819	0.65879
C	1.69421	-1.09827	-5.93823
C	1.26077	-1.94309	-4.90442
C	0.64271	-1.41158	-3.75695
C	0.87263	0.82235	-4.68717
C	1.49658	0.28952	-5.82581
H	2.17785	-1.51886	-6.83476
H	1.39861	-3.03367	-4.98775
H	0.32274	-2.08330	-2.94759
H	0.69365	1.90811	-4.63825
H	1.81846	0.96326	-6.63663
C	-3.78588	3.00533	-4.54621
C	-3.48094	1.65864	-4.81801
C	-2.46947	1.00448	-4.09881
C	-2.06771	3.03352	-2.81967
C	-3.07816	3.69067	-3.54629
H	-4.57390	3.52037	-5.11939
H	-4.02958	1.11366	-5.60328
H	-2.23327	-0.04600	-4.33365
H	-1.52128	3.57584	-2.03507
H	-3.30839	4.74622	-3.32753
C	-3.28336	5.81521	0.75019
C	-2.05538	6.00872	1.40556
C	-1.15094	4.94216	1.54576
C	-2.69120	3.48602	0.34393
C	-3.59856	4.55140	0.22164
H	-3.99674	6.64975	0.65325
H	-1.80009	6.99575	1.82432
H	-0.20272	5.10643	2.08127
H	-2.95029	2.50470	-0.08348
H	-4.55932	4.38946	-0.29369
C	2.20651	3.24823	5.02716
C	2.88218	2.90778	3.84522
C	2.15756	2.63158	2.67186
C	0.07557	3.01897	3.86936
C	0.80058	3.30208	5.03616
H	2.77403	3.46367	5.94705
H	3.98254	2.84947	3.83256
H	2.70146	2.35137	1.75672
H	-1.02576	3.04797	3.89932
H	0.26181	3.55878	5.96272
C	0.32510	-6.85042	2.05530
C	1.82287	-4.82298	1.87008
C	1.38601	-6.28348	-0.16664
H	1.73721	-5.48593	-0.85846
H	0.64776	-6.91308	-0.70954
H	2.26327	-6.92135	0.08133
H	2.30561	-4.07318	1.20206
H	2.63976	-5.46956	2.25975

H	1.36472	-4.27578	2.72102
H	-0.45023	-7.47561	1.56549
H	-0.10827	-6.45961	3.00053
H	1.19437	-7.49596	2.30839
C	-5.01043	-0.87400	4.50842
H	-4.99208	1.10731	3.61866
H	-2.46329	-3.18380	4.28375
C	-4.30860	-2.08638	4.70316
H	-6.01389	-0.74593	4.94659
H	-4.76693	-2.89897	5.28961
C	3.97507	-1.38032	-1.02029
C	5.40001	-3.67854	-0.17934
C	4.51815	-3.75474	-1.27024
C	3.80860	-2.61339	-1.68409
C	4.86515	-1.31602	0.07329
C	5.57042	-2.45498	0.49237
H	5.96078	-4.57057	0.14411
H	4.38857	-4.70657	-1.81104
H	3.12977	-2.67421	-2.55148
H	5.01595	-0.36024	0.60254
H	6.26442	-2.38544	1.34593

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-1327.36	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	10.51	0.02283	YES	YES
9	a	11.61	0.06538	YES	YES
10	a	17.44	0.12990	YES	YES
11	a	19.03	0.21824	YES	YES
12	a	26.05	0.13235	YES	YES
13	a	30.33	0.17226	YES	YES
14	a	32.92	0.16118	YES	YES
15	a	37.52	0.15687	YES	YES
16	a	39.36	0.21679	YES	YES
17	a	43.52	0.08961	YES	YES
18	a	48.58	0.21123	YES	YES
19	a	50.75	0.10778	YES	YES
20	a	52.51	0.17047	YES	YES
21	a	54.84	0.13917	YES	YES
22	a	56.21	0.23656	YES	YES
23	a	58.71	0.09460	YES	YES
24	a	63.14	0.26439	YES	YES
25	a	64.50	0.61685	YES	YES
26	a	64.85	0.10055	YES	YES
27	a	70.56	2.88117	YES	YES
28	a	76.96	0.33100	YES	YES
29	a	80.90	0.26503	YES	YES

30	a	91.40	0.45322	YES	YES
31	a	93.13	0.17008	YES	YES
32	a	97.18	0.44017	YES	YES
33	a	106.91	0.85934	YES	YES
34	a	108.09	0.09274	YES	YES
35	a	111.04	0.32812	YES	YES
36	a	123.62	0.59705	YES	YES
37	a	126.35	0.93012	YES	YES
38	a	128.69	0.87508	YES	YES
39	a	130.77	0.44380	YES	YES
40	a	140.69	1.18335	YES	YES
41	a	146.10	2.29917	YES	YES
42	a	157.75	0.04851	YES	YES
43	a	167.88	0.92387	YES	YES
44	a	171.85	2.54964	YES	YES
45	a	181.36	0.31394	YES	YES
46	a	184.49	0.63730	YES	YES
47	a	192.63	0.41674	YES	YES
48	a	201.46	0.92164	YES	YES
49	a	212.42	1.97932	YES	YES
50	a	214.01	1.75364	YES	YES

./TS911

BP86/SV(P) energy (au): -3330.8886793980

PBE0/def2-TZVPP energy (au): -3330.389895857
cosmo_dcm Total energy + OC corr. = -3330.4410915067
cosmo_acetone Total energy + OC corr. = -3330.4469291974

Zero point energy (au): 0.9121826
Entropy (kJ mol^-1): 1.38443
Chemical potential (kJ mol^-1): 2144.84

XYZ coordinates:

117

C	2.23707	3.62744	-0.91058
C	1.48720	3.62280	-2.12347
C	1.36071	4.08450	0.13933
C	0.14826	4.09413	-1.84283
C	0.08167	4.37619	-0.44264
H	3.30355	3.39017	-0.81985
H	1.89645	3.36747	-3.10892
H	1.64292	4.27837	1.18213
H	-0.66540	4.27750	-2.55532
H	-0.78870	4.78790	0.08606
Ru	0.48022	2.13329	-0.68736
C	2.87299	1.49511	1.28331
C	1.37518	1.16172	1.00824
P	-1.65979	1.78436	0.24549
C	-2.29583	0.04418	0.31759
C	-3.51759	-0.43181	-0.09534
N	-1.37527	-0.81202	0.88373
C	-3.83523	-1.82658	0.11237
C	-2.84497	-2.70563	0.66266
C	-1.50941	-2.18499	0.99886
O	-0.53032	-2.87009	1.35992
P	0.40259	0.53556	-2.48340
C	1.92219	-0.50978	-2.11535
C	2.98244	-0.89106	-2.93130
N	1.85522	-0.88258	-0.81260
C	3.99986	-1.68092	-2.34144
C	3.88039	-2.14803	-1.03630
C	2.72869	-1.78283	-0.27438
N	2.41061	-2.30942	0.96230
C	3.29665	-3.05439	1.78901
O	4.47797	-3.17430	1.49330
C	3.51275	0.89471	2.52009
O	0.76489	0.54681	1.89587
H	3.45741	1.22911	0.37562
C	-2.99671	2.72142	-0.63450
C	-1.92364	2.27490	2.02483
H	-4.25644	0.23813	-0.55826
H	-0.50095	-0.39141	1.29082

C	-5.10831	-2.36659	-0.21605
C	-3.14073	-4.07178	0.87153
C	-0.87023	-0.81772	-2.75013
C	0.55917	1.01905	-4.27911
H	3.05316	-0.56728	-3.97797
H	4.88929	-1.95447	-2.93278
H	4.63666	-2.79130	-0.57249
H	1.40729	-2.25701	1.24276
C	2.66974	-3.71921	3.03240
H	2.94571	2.60049	1.36062
H	1.24565	0.23032	-0.25404
C	-4.94552	4.19277	-2.06692
C	-4.67280	4.50117	-0.72466
C	-3.70889	3.76842	-0.00825
C	-3.26790	2.42783	-1.98992
C	-4.24247	3.14986	-2.69708
H	-5.70645	4.76355	-2.62360
H	-5.21840	5.31582	-0.22132
H	-3.52009	4.01496	1.04789
H	-2.71955	1.61823	-2.49379
H	-4.45394	2.89760	-3.74938
C	-2.42785	3.07089	4.69230
C	-1.25695	3.48928	4.03986
C	-1.00576	3.08910	2.71627
C	-3.09633	1.85157	2.69186
C	-3.34495	2.24818	4.01531
H	-2.62393	3.37990	5.73199
H	-0.52692	4.12537	4.56649
H	-0.07388	3.39939	2.22352
H	-3.82421	1.20390	2.17688
H	-4.26275	1.90698	4.52152
C	0.65548	1.59588	-7.05629
C	0.97112	0.30761	-6.58941
C	0.90523	0.01507	-5.21879
C	0.19947	2.29234	-4.76646
C	0.25001	2.58028	-6.14283
H	0.70295	1.82259	-8.13370
H	1.25358	-0.48601	-7.30035
H	1.08967	-1.01857	-4.88872
H	-0.16032	3.06554	-4.07779
H	-0.03755	3.58293	-6.49835
C	-2.73740	-2.85425	-3.38052
C	-2.85764	-1.58103	-3.96334
C	-1.92717	-0.57540	-3.66003
C	-0.76592	-2.09528	-2.16027
C	-1.68874	-3.10606	-2.48299
H	-3.45618	-3.65061	-3.63132
H	-3.66965	-1.37161	-4.67880
H	-2.00421	0.39304	-4.17893
H	0.04029	-2.32647	-1.45091
H	-1.57912	-4.10054	-2.02244
C	1.79782	-2.72350	3.83520
C	3.82123	-4.23531	3.91862
C	1.81146	-4.91946	2.54534
H	0.88545	-2.41567	3.28229
H	2.37221	-1.81416	4.11604
H	1.45770	-3.21677	4.77247
H	2.42395	-5.63585	1.95422

H	0.94444	-4.58875	1.93634
H	1.41485	-5.46392	3.43098
H	3.40020	-4.76014	4.80361
H	4.45704	-3.39848	4.27895
H	4.47420	-4.94212	3.36595
C	-5.38705	-3.71666	0.00327
H	-5.87872	-1.70244	-0.64125
C	-4.40356	-4.57507	0.55079
H	-2.35741	-4.71748	1.29850
H	-6.38291	-4.11667	-0.24886
H	-4.63709	-5.63771	0.72565
C	4.84001	-0.07978	4.82707
C	5.32772	-0.39218	3.54787
C	4.66618	0.09264	2.40597
C	3.02937	1.19798	3.81264
C	3.68547	0.71412	4.95498
H	5.35892	-0.45277	5.72538
H	6.22756	-1.01733	3.43115
H	5.06421	-0.15484	1.40733
H	2.12867	1.82216	3.92832
H	3.29590	0.96312	5.95593

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-1157.36	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	14.52	0.02608	YES	YES
9	a	18.46	0.02961	YES	YES
10	a	21.25	0.00998	YES	YES
11	a	27.03	0.05626	YES	YES
12	a	31.43	0.01676	YES	YES
13	a	33.07	0.25529	YES	YES
14	a	36.69	0.25306	YES	YES
15	a	42.44	0.04678	YES	YES
16	a	46.22	0.63462	YES	YES
17	a	50.15	0.44033	YES	YES
18	a	50.70	0.47364	YES	YES
19	a	55.90	0.61278	YES	YES
20	a	57.12	0.22999	YES	YES
21	a	59.76	1.77166	YES	YES
22	a	62.79	0.77008	YES	YES
23	a	67.02	0.08757	YES	YES
24	a	68.24	1.70680	YES	YES
25	a	69.67	0.08846	YES	YES
26	a	76.63	1.14715	YES	YES
27	a	80.30	0.17269	YES	YES
28	a	85.84	0.86167	YES	YES
29	a	89.80	1.17795	YES	YES

30	a	92.27	0.18719	YES	YES
31	a	97.87	1.20445	YES	YES
32	a	102.45	0.76705	YES	YES
33	a	108.73	1.42016	YES	YES
34	a	118.59	0.94357	YES	YES
35	a	125.77	1.58221	YES	YES
36	a	128.95	0.27092	YES	YES
37	a	136.22	1.62822	YES	YES
38	a	144.86	0.70441	YES	YES
39	a	149.95	1.57280	YES	YES
40	a	154.77	1.75432	YES	YES
41	a	159.01	3.61403	YES	YES
42	a	170.05	3.27191	YES	YES
43	a	172.50	0.86248	YES	YES
44	a	180.21	0.71995	YES	YES
45	a	187.03	1.67361	YES	YES
46	a	191.39	0.23873	YES	YES
47	a	193.70	4.71921	YES	YES
48	a	203.46	2.37822	YES	YES
49	a	209.05	1.33633	YES	YES
50	a	212.36	0.73587	YES	YES

./phenylacetaldehyde

BP86_SV(P) energy (au): -384.6020695526

PBE0/def2-TZVPP energy (au): -384.5692095835
cosmo_dcm Total energy + OC corr. = -384.5769471283
cosmo_acetone Total energy + OC corr. = -384.5779097746

Zero point energy (au): 0.1335420
Entropy (kJ mol^-1): 0.38258
Chemical potential (kJ mol^-1): 260.28

XYZ coordinates:

17

C	0.28950	0.40090	2.38092
C	0.32998	-0.82580	1.46674
C	0.14941	-0.44224	0.00968
H	1.32881	-1.30258	1.61087
H	-0.44586	-1.53834	1.81678
C	-0.21070	0.37878	-2.67807
C	-1.32405	0.06408	-1.87906
C	-1.14470	-0.33844	-0.54564
C	1.25850	-0.11864	-0.80068
C	1.08174	0.28766	-2.13399
H	-0.35075	0.69384	-3.72544
H	-2.34187	0.13047	-2.29846
H	-2.02316	-0.58320	0.07555
H	2.27800	-0.19864	-0.38578
H	1.96115	0.53052	-2.75339
O	-0.41027	0.51064	3.36501
H	0.98570	1.23739	2.05810

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	28.07	1.20413	YES	YES
8	a	53.17	3.69292	YES	YES
9	a	135.70	2.18436	YES	YES
10	a	276.69	2.23294	YES	YES
11	a	325.44	1.85301	YES	YES
12	a	403.48	0.01967	YES	YES
13	a	427.68	4.82544	YES	YES
14	a	504.60	27.69765	YES	YES

15	a	565.59	0.95174	YES	YES
16	a	613.72	0.04099	YES	YES
17	a	699.31	33.70485	YES	YES
18	a	739.50	0.21197	YES	YES
19	a	751.12	12.64985	YES	YES
20	a	828.31	1.92166	YES	YES
21	a	832.09	0.95271	YES	YES
22	a	896.14	0.94354	YES	YES
23	a	953.36	0.04605	YES	YES
24	a	976.79	1.69581	YES	YES
25	a	980.82	0.75921	YES	YES
26	a	985.61	1.06085	YES	YES
27	a	1020.97	48.18083	YES	YES
28	a	1027.84	1.90814	YES	YES
29	a	1078.38	8.46858	YES	YES
30	a	1141.44	0.03362	YES	YES
31	a	1151.23	16.01845	YES	YES
32	a	1162.48	0.15504	YES	YES
33	a	1190.05	0.43912	YES	YES
34	a	1251.46	7.58204	YES	YES
35	a	1308.48	0.72042	YES	YES
36	a	1366.25	4.68092	YES	YES
37	a	1371.64	0.30372	YES	YES
38	a	1397.15	8.16094	YES	YES
39	a	1447.21	5.04175	YES	YES
40	a	1489.59	16.29532	YES	YES
41	a	1598.85	1.91258	YES	YES
42	a	1617.69	8.11997	YES	YES
43	a	1792.33	228.19820	YES	YES
44	a	2770.39	110.93430	YES	YES
45	a	2940.00	11.74348	YES	YES
46	a	3029.73	6.69892	YES	YES
47	a	3083.05	6.49326	YES	YES
48	a	3086.94	2.02734	YES	YES
49	a	3096.89	5.99723	YES	YES
50	a	3105.37	26.10191	YES	YES

./phenylacetylene

BP86_SV(P) energy (au): -308.1699045398

PBE0/def2-TZVPP energy (au): -308.1232271529
cosmo_dcm Total energy + OC corr. = -308.1293138768 Total energy + OC corr. = -308.1293138768
cosmo_acetone Total energy + OC corr. = -308.1300548063 Total energy + OC corr. = -308.1300548063

Zero point energy (au): 0.1064970
Entropy (kJ mol^-1): 0.33588
Chemical potential (kJ mol^-1): 199.28

XYZ coordinates:

14

C	0.00005	-0.00028	3.23756
C	-0.00009	-0.00014	2.01158
C	-0.00009	0.00017	0.57921
C	0.00008	-0.00030	-2.25084
C	-1.21648	-0.00022	-1.54507
C	-1.22154	0.00055	-0.14333
C	1.22149	0.00036	-0.14319
C	1.21657	-0.00004	-1.54489
H	0.00021	-0.00080	-3.35338
H	-2.17324	-0.00044	-2.09328
H	-2.17286	0.00052	0.41203
H	2.17269	0.00041	0.41234
H	2.17336	-0.00029	-2.09305
H	0.00000	-0.00063	4.31970

Vibrational Spectrum:

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	138.60	1.56272	YES	YES
8	a	153.35	1.02814	YES	YES
9	a	360.75	2.76719	YES	YES
10	a	399.53	0.00000	YES	YES
11	a	458.67	0.36366	YES	YES
12	a	517.40	2.58701	YES	YES
13	a	545.30	5.40493	YES	YES
14	a	599.98	35.57629	YES	YES

15	a	614.17	0.56225	YES	YES
16	a	644.35	35.24612	YES	YES
17	a	691.72	31.09793	YES	YES
18	a	758.33	2.36982	YES	YES
19	a	760.59	32.35929	YES	YES
20	a	830.63	0.00000	YES	YES
21	a	909.83	3.35487	YES	YES
22	a	956.95	0.00003	YES	YES
23	a	982.16	0.08978	YES	YES
24	a	984.04	0.15648	YES	YES
25	a	1025.34	3.72379	YES	YES
26	a	1071.47	5.60100	YES	YES
27	a	1142.05	0.00025	YES	YES
28	a	1158.82	0.00066	YES	YES
29	a	1204.71	0.88037	YES	YES
30	a	1290.64	0.07689	YES	YES
31	a	1357.27	0.05300	YES	YES
32	a	1438.18	4.75514	YES	YES
33	a	1482.79	13.38073	YES	YES
34	a	1581.92	1.09556	YES	YES
35	a	1614.46	1.69330	YES	YES
36	a	2144.66	3.15957	YES	YES
37	a	3091.46	0.45532	YES	YES
38	a	3100.05	5.04432	YES	YES
39	a	3110.63	14.91804	YES	YES
40	a	3118.10	16.69175	YES	YES
41	a	3121.74	4.08489	YES	YES

./water

BP86/SV(P) energy (au): -76.3451982257

PBE0/def2-TZVPP energy (au): -76.379977474
cosmo_dcm Total energy + OC corr. = -76.3884032920
cosmo_acetone Total energy + OC corr. = -76.3894169945

Zero point energy (au): 0.0199819
Entropy (kJ mol^-1): 0.19525
Chemical potential (kJ mol^-1): 4.17

XYZ coordinates:

3

O	0.00000	-0.06795	0.00000
H	0.77073	0.53925	0.00000
H	-0.77073	0.53925	0.00000

Vibrational Spectrum:

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a'	1604.14	62.02422	YES	YES
8	a'	3526.31	0.10492	YES	YES

./5/a

BP86_SV(P) energy (au): -3254.5242183060

PBE0/def2-TZVPP energy (au): -3254.021085297
cosmo_dcm Total energy + OC corr. = -3254.0721951040

Zero point energy (au): 0.8907793
Entropy (kJ mol^-1): 1.40305
Chemical potential (kJ mol^-1): 2079.11

XYZ coordinates:

114

C	2.12817	-2.84996	-2.72663
C	2.84461	-3.21073	-1.53450
C	0.80081	-3.37149	-2.61239
C	1.95954	-3.98958	-0.70366
C	0.70508	-4.09898	-1.36391
H	2.53462	-2.27817	-3.57169
H	3.90108	-2.99960	-1.33139
H	0.01221	-3.30109	-3.37266
H	2.22540	-4.43548	0.26410
H	-0.16965	-4.65990	-1.01427
Ru	1.12278	-1.82021	-0.94386
C	2.84955	0.75609	-1.55912
C	-2.22824	-2.53725	-1.73924
P	-1.13363	-1.10706	-1.26333
C	-1.33614	0.04343	-2.70851
C	-2.18684	-0.27453	0.02792
C	-3.50734	-0.62033	0.21978
N	-1.66129	0.82842	0.67772
C	-4.34885	0.15353	1.09674
C	-3.80418	1.30798	1.73518
C	-2.40096	1.67970	1.50201
O	-1.86471	2.68769	1.99883
C	-0.03232	-1.64256	2.49731
P	1.38243	-1.30118	1.36033
C	2.75339	-2.32890	2.09275
C	1.94544	0.44323	1.77627
C	3.19269	0.65379	2.38526
N	1.13708	1.45561	1.39319
C	3.64075	1.98193	2.52785
C	2.83828	3.03612	2.10827
C	1.54695	2.73655	1.58915
N	0.62019	3.72728	1.28391
C	0.88002	5.09734	1.12691
C	-0.37203	5.99218	0.93319
O	2.01678	5.55691	1.15497
H	-3.94536	-1.46863	-0.32059
H	-0.62391	1.03385	0.69102
H	3.81232	-0.18071	2.73502
H	4.62548	2.18602	2.98010

H	3.14920	4.08511	2.18145
H	-0.36930	3.39814	1.34771
C	-4.60891	2.09997	2.58493
C	-5.71089	-0.17751	1.33046
C	4.90112	-3.82934	3.16967
C	3.64734	-3.83512	3.80051
C	2.58000	-3.08505	3.27186
C	4.02353	-2.32370	1.46872
C	5.08896	-3.06373	2.00411
H	5.73570	-4.41494	3.58802
H	3.49325	-4.42228	4.72044
H	1.60949	-3.09306	3.79015
H	4.18791	-1.71320	0.56674
H	6.07410	-3.04049	1.50991
C	-2.11972	-2.31356	4.27567
C	-1.68953	-3.24580	3.31477
C	-0.65710	-2.90856	2.42498
C	-0.46350	-0.71485	3.46852
C	-1.50869	-1.05086	4.34767
H	-2.93394	-2.57315	4.97164
H	-2.15859	-4.24200	3.26065
H	-0.31516	-3.64582	1.67899
H	0.00960	0.27582	3.54460
H	-1.84215	-0.31659	5.09827
C	-3.84778	-4.74933	-2.44069
C	-3.53705	-3.76958	-3.39677
C	-2.73669	-2.66520	-3.04969
C	-2.54412	-3.52961	-0.78192
C	-3.35332	-4.62302	-1.12957
H	-4.47971	-5.60981	-2.71404
H	-3.92485	-3.85560	-4.42487
H	-2.51513	-1.89973	-3.80910
H	-2.17343	-3.43451	0.25099
H	-3.60145	-5.38176	-0.36936
C	-1.73849	1.63053	-5.01210
C	-0.59754	0.81847	-4.90606
C	-0.39248	0.03569	-3.75779
C	-2.48161	0.86362	-2.82111
C	-2.67474	1.65662	-3.96413
H	-1.89498	2.25074	-5.90969
H	0.14967	0.80376	-5.71589
H	0.52088	-0.57262	-3.67048
H	-3.23417	0.88447	-2.01702
H	-3.56862	2.29780	-4.03465
C	-1.13605	6.05656	2.28243
C	-1.29764	5.43271	-0.17314
C	0.10978	7.40235	0.54108
H	-2.13600	6.14252	-0.35031
H	-1.74958	4.45691	0.10686
H	-0.74924	5.30789	-1.13317
H	0.78670	7.82522	1.31188
H	-0.76436	8.08047	0.42642
H	0.67018	7.38650	-0.41814
H	-2.00338	6.74801	2.18773
H	-0.48071	6.44492	3.09298
H	-1.52619	5.06181	2.58653
C	-5.94386	1.75335	2.80575
H	-4.15864	2.98578	3.05859

H	-6.14303	-1.06336	0.83651
C	-6.49383	0.61206	2.17395
H	-7.54968	0.34682	2.34727
H	-6.57254	2.37026	3.46791
C	2.71861	2.04278	-2.26816
C	2.56966	4.51642	-3.64799
C	3.81840	3.92425	-3.39235
C	3.89290	2.70189	-2.70922
C	1.46735	2.65786	-2.51595
C	1.39767	3.87789	-3.20371
H	2.51061	5.47846	-4.18235
H	4.74503	4.42056	-3.72433
H	4.87767	2.24489	-2.51366
H	0.54490	2.18220	-2.14938
H	0.41411	4.33975	-3.38857
C	1.97978	-0.22006	-1.29579
H	3.86527	0.53096	-1.16400

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	6.66	0.19021	YES	YES
8	a	14.86	0.09991	YES	YES
9	a	19.90	0.01182	YES	YES
10	a	20.99	0.06633	YES	YES
11	a	26.78	0.00828	YES	YES
12	a	28.21	0.15919	YES	YES
13	a	31.64	0.05636	YES	YES
14	a	34.00	0.49782	YES	YES
15	a	35.91	0.06688	YES	YES
16	a	41.47	0.82398	YES	YES
17	a	44.58	0.13603	YES	YES
18	a	48.26	0.00200	YES	YES
19	a	51.51	0.22008	YES	YES
20	a	52.76	0.11556	YES	YES
21	a	57.46	0.31709	YES	YES
22	a	57.85	0.46078	YES	YES
23	a	63.42	0.12958	YES	YES
24	a	66.86	0.58942	YES	YES
25	a	69.63	0.33684	YES	YES
26	a	76.25	0.18497	YES	YES
27	a	77.02	0.38628	YES	YES
28	a	78.15	0.45275	YES	YES
29	a	86.51	1.41022	YES	YES
30	a	90.76	0.37177	YES	YES
31	a	93.39	1.36930	YES	YES
32	a	95.53	0.03274	YES	YES
33	a	104.24	0.58463	YES	YES

34	a	107.53	1.12602	YES	YES
35	a	115.38	0.65491	YES	YES
36	a	125.29	1.63500	YES	YES
37	a	127.85	0.50389	YES	YES
38	a	135.72	1.90139	YES	YES
39	a	162.93	0.50496	YES	YES
40	a	166.12	1.11057	YES	YES
41	a	168.64	1.49090	YES	YES
42	a	183.06	0.88822	YES	YES
43	a	189.20	0.90102	YES	YES
44	a	197.19	0.84349	YES	YES
45	a	206.37	0.11562	YES	YES
46	a	211.07	1.21679	YES	YES
47	a	213.39	2.21905	YES	YES
48	a	217.09	2.80914	YES	YES
49	a	223.22	1.89346	YES	YES
50	a	228.36	1.49364	YES	YES

./5/b

BP86_SV(P) energy (au): -3254.5287065190

PBE0/def2-TZVPP energy (au): -3254.025901436
cosmo_dcm Total energy + OC corr. = -3254.0757090953

Zero point energy (au): 0.8902358
Entropy (kJ mol^-1): 1.41728
Chemical potential (kJ mol^-1): 2073.64

XYZ coordinates:

114

C	2.15607	-2.97843	-2.38153
C	2.76982	-3.21463	-1.10099
C	0.82752	-3.50526	-2.33251
C	1.82418	-3.93296	-0.28134
C	0.63361	-4.11501	-1.03096
H	2.62974	-2.48552	-3.24122
H	3.80239	-2.97494	-0.82258
H	0.10531	-3.52132	-3.15915
H	2.00854	-4.28092	0.74397
H	-0.26587	-4.64956	-0.70379
Ru	1.00873	-1.79056	-0.81206
C	2.23308	0.94559	-1.84976
C	-2.29608	-2.62416	-1.73571
P	-1.25819	-1.15821	-1.24935
C	-1.41726	-0.03676	-2.72459
C	-2.38398	-0.30652	-0.03045
C	-3.68880	-0.70381	0.16799
N	-1.92145	0.86172	0.54840
C	-4.57378	0.07985	0.99309
C	-4.09412	1.29958	1.55876
C	-2.71236	1.73278	1.30030
O	-2.24067	2.81076	1.71157
C	-0.15886	-1.22758	2.58339
P	1.24514	-0.98312	1.40923
C	2.65076	-1.85229	2.26349
C	1.70236	0.82375	1.58417
C	2.93546	1.22406	2.11939
N	0.80564	1.70190	1.08321
C	3.26561	2.59302	2.07016
C	2.36761	3.50315	1.52166
C	1.10851	3.02099	1.07212
N	0.09944	3.87995	0.63755
C	0.30244	5.12043	0.02876
C	-0.97620	5.96570	-0.19733
O	1.42326	5.50391	-0.29991
H	-4.08149	-1.60285	-0.32289
H	-0.89395	1.12900	0.54103
H	3.63203	0.50009	2.56071
H	4.23178	2.94203	2.46903

H	2.59536	4.57366	1.45035
H	-0.86318	3.55326	0.88882
C	-4.94316	2.09988	2.35577
C	-5.91825	-0.30636	1.24482
C	4.82732	-3.16554	3.50916
C	3.54702	-3.21952	4.08214
C	2.46417	-2.56327	3.46857
C	3.94514	-1.80248	1.69275
C	5.02492	-2.44839	2.31508
H	5.67426	-3.67702	3.99477
H	3.38397	-3.77064	5.02262
H	1.47140	-2.60599	3.94165
H	4.11795	-1.22976	0.76691
H	6.02958	-2.38850	1.86511
C	-2.20923	-1.75085	4.45205
C	-1.87917	-2.71456	3.48256
C	-0.86577	-2.44963	2.54699
C	-0.48891	-0.26781	3.56425
C	-1.51565	-0.52918	4.48820
H	-3.00973	-1.95340	5.18197
H	-2.41537	-3.67741	3.45492
H	-0.60323	-3.20747	1.78984
H	0.04950	0.69130	3.61041
H	-1.77090	0.23053	5.24452
C	-3.83986	-4.88426	-2.45682
C	-3.50235	-3.92157	-3.42102
C	-2.74007	-2.79345	-3.06462
C	-2.63886	-3.59981	-0.76987
C	-3.41065	-4.71681	-1.12740
H	-4.44190	-5.76350	-2.73776
H	-3.83981	-4.03959	-4.46364
H	-2.49784	-2.04177	-3.83151
H	-2.31991	-3.47473	0.27702
H	-3.68019	-5.46197	-0.36099
C	-1.72436	1.54768	-5.04671
C	-0.61913	0.69007	-4.91923
C	-0.46253	-0.09324	-3.76329
C	-2.53145	0.82129	-2.86432
C	-2.67742	1.61180	-4.01617
H	-1.84215	2.16851	-5.94982
H	0.13467	0.63334	-5.72151
H	0.41764	-0.74740	-3.66657
H	-3.29739	0.87579	-2.07490
H	-3.54726	2.28276	-4.10659
C	-1.99219	5.17917	-1.06253
C	-0.57245	7.26227	-0.92379
C	-1.60613	6.30348	1.17846
H	-1.47002	7.89798	-1.08928
H	-0.10857	7.04659	-1.90992
H	0.16539	7.84304	-0.33190
H	-1.95146	5.39362	1.71565
H	-2.48937	6.96477	1.03280
H	-0.88330	6.84427	1.82868
H	-2.87444	5.82274	-1.27652
H	-2.36561	4.26797	-0.54763
H	-1.54711	4.87812	-2.03670
C	-6.25858	1.69712	2.59737
H	-4.54117	3.03586	2.77293

H	-6.30160	-1.24246	0.80614
C	-6.74508	0.49135	2.03729
H	-7.78608	0.18204	2.22628
H	-6.92137	2.31944	3.22014
C	3.62767	1.42171	-1.73292
C	6.28629	2.38715	-1.52148
C	5.21670	3.28421	-1.68803
C	3.89984	2.81027	-1.79401
C	4.71517	0.52633	-1.57628
C	6.02930	1.00511	-1.46847
H	7.31983	2.76227	-1.44647
H	5.40629	4.36910	-1.73749
H	3.07061	3.52915	-1.90161
H	4.52424	-0.55988	-1.58050
H	6.86403	0.29268	-1.35985
C	1.69619	-0.18292	-1.39103
H	1.50886	1.62335	-2.35022

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	5.90	0.06353	YES	YES
8	a	11.33	0.30193	YES	YES
9	a	13.78	0.57558	YES	YES
10	a	19.37	0.02919	YES	YES
11	a	20.56	0.05267	YES	YES
12	a	24.36	0.01907	YES	YES
13	a	27.83	0.07910	YES	YES
14	a	30.73	0.15983	YES	YES
15	a	35.77	0.05028	YES	YES
16	a	42.93	0.07916	YES	YES
17	a	44.13	0.20305	YES	YES
18	a	47.46	0.54543	YES	YES
19	a	48.88	1.18878	YES	YES
20	a	50.35	0.13820	YES	YES
21	a	52.96	0.14927	YES	YES
22	a	58.91	0.11684	YES	YES
23	a	62.87	0.58831	YES	YES
24	a	65.01	0.39929	YES	YES
25	a	67.50	0.25586	YES	YES
26	a	69.87	0.64518	YES	YES
27	a	75.72	0.32887	YES	YES
28	a	84.24	0.38760	YES	YES
29	a	86.79	2.11661	YES	YES
30	a	88.38	0.44813	YES	YES
31	a	93.56	0.00766	YES	YES
32	a	96.92	0.95435	YES	YES
33	a	101.26	0.48227	YES	YES

34	a	107.94	0.33874	YES	YES
35	a	114.07	0.84823	YES	YES
36	a	124.59	1.33965	YES	YES
37	a	128.08	0.91455	YES	YES
38	a	141.01	2.96084	YES	YES
39	a	163.00	1.66753	YES	YES
40	a	167.68	0.16944	YES	YES
41	a	171.14	1.64963	YES	YES
42	a	182.71	2.46247	YES	YES
43	a	193.46	0.80878	YES	YES
44	a	198.54	0.56582	YES	YES
45	a	204.13	0.23580	YES	YES
46	a	209.39	0.63670	YES	YES
47	a	210.32	2.05084	YES	YES
48	a	219.49	2.18767	YES	YES
49	a	220.56	2.56807	YES	YES
50	a	226.43	1.09338	YES	YES

./15

BP86_SV(P) energy (au): -3254.5557746360

PBE0/def2-TZVPP energy (au): -3254.058835433
cosmo_dcm Total energy + OC corr. = -3254.1170981116
cosmo_acetone Total energy + OC corr. = -3254.1238437977

Zero point energy (au): 0.8934603
Entropy (kJ mol^-1): 1.36998
Chemical potential (kJ mol^-1): 2093.57

XYZ coordinates:

114

Ru	0.04918	0.07131	-1.17250
P	-1.15434	-0.53636	0.80666
P	-0.42574	2.36779	-1.08191
C	-0.46266	-2.09694	1.60159
C	0.72617	3.04936	0.18388
N	1.81351	2.19774	0.32122
O	3.92600	1.75408	1.12976
O	0.92783	-7.12275	1.53714
C	-0.37965	2.04369	3.98072
H	0.50096	2.57566	4.37550
C	-1.36505	0.56817	2.29096
C	2.96190	2.51548	1.10943
C	-2.91159	-1.05885	0.47444
C	1.91234	1.01245	-0.52538
H	2.59946	1.19452	-1.37162
C	0.43942	-6.71237	0.49169
N	0.01746	-5.38584	0.33697
H	-0.34867	-5.10189	-0.57687
C	0.03381	-4.34374	1.26772
C	0.46299	-4.50209	2.61255
H	0.82005	-5.48192	2.95406
C	4.74858	-3.43487	-0.90476
C	3.89091	5.36066	3.41074
H	4.72909	5.64676	4.06633
C	-0.25472	1.26796	2.81576
H	0.72515	1.21176	2.31912
C	-2.12263	2.99120	-0.72226
C	0.85105	-0.72486	-3.15962
H	1.84762	-0.51580	-3.56915
C	3.90687	-3.53518	0.21620
H	3.96577	-4.41528	0.87706
C	-5.62401	-1.74142	0.02260
H	-6.67823	-2.00909	-0.15560
C	1.95695	-0.27634	0.08321
H	1.67620	-0.32718	1.14750
C	0.65287	4.24846	0.84590
H	-0.21177	4.91247	0.70309
C	-2.60748	0.66916	2.95792

H	-3.48850	0.13354	2.57461
C	2.99856	-2.50630	0.50948
H	2.36313	-2.58372	1.40585
C	-3.45549	-2.24431	1.01921
H	-2.83688	-2.91428	1.63323
C	-0.34236	0.02849	-3.40364
H	-0.42244	0.92160	-4.03671
C	-3.75023	-0.21441	-0.28580
H	-3.35635	0.72684	-0.69712
C	-2.73143	1.45137	4.11917
H	-3.70787	1.51596	4.62679
C	2.77075	6.21560	3.28332
H	2.74092	7.16599	3.84103
C	2.86312	3.78849	1.85822
C	4.68235	-2.28751	-1.71663
H	5.36065	-2.18228	-2.57911
C	-4.78930	3.81180	-0.26618
H	-5.82607	4.14104	-0.08848
C	2.89951	-1.35562	-0.30976
C	-0.07080	-2.15097	2.95071
H	-0.14169	-1.27156	3.60510
C	3.77326	-1.26121	-1.42170
H	3.77316	-0.35729	-2.05078
C	-3.87797	3.74257	0.79988
H	-4.19699	4.01279	1.81944
C	-4.37334	3.45932	-1.56325
H	-5.08117	3.51173	-2.40667
C	-1.62002	2.13950	4.63485
H	-1.71895	2.74855	5.54816
C	1.72761	4.64735	1.72285
C	0.91079	-8.96045	-0.49896
H	2.00762	-8.82615	-0.38479
H	0.72847	-9.64719	-1.35383
H	0.53846	-9.44210	0.42854
C	0.20437	-7.61394	-0.74938
C	-5.09552	-0.55224	-0.50808
H	-5.73460	0.12347	-1.09970
C	-2.55176	3.32953	0.57928
H	-1.85525	3.27107	1.42887
C	-4.80092	-2.58235	0.78909
H	-5.20654	-3.51267	1.21924
C	3.93566	4.15762	2.70097
H	4.79701	3.47559	2.77395
C	0.77387	-6.95924	-2.03175
H	0.22932	-6.03365	-2.33007
H	0.68069	-7.66633	-2.88506
H	1.85045	-6.70521	-1.91783
C	-0.90503	-1.79333	-2.07711
H	-1.46666	-2.51773	-1.47504
C	0.40499	-3.38277	3.44484
H	0.72575	-3.46751	4.49616
C	-3.05096	3.04836	-1.79055
H	-2.73694	2.78522	-2.81456
C	1.70400	5.86630	2.45255
H	0.83436	6.53633	2.35184
C	-1.43661	-0.62072	-2.72047
H	-2.49371	-0.33229	-2.76065
C	-1.32204	-7.84479	-0.90176

H	-1.74916	-8.31381	0.01120
H	-1.51755	-8.52644	-1.75900
H	-1.87648	-6.89856	-1.09294
C	0.50053	-1.85052	-2.33211
H	1.19150	-2.61639	-1.95913
H	5.46888	-4.23669	-1.13478
C	0.08915	3.40425	-2.55016
C	1.05918	5.08371	-4.61422
C	-0.00110	5.50794	-3.79607
C	-0.48059	4.67998	-2.76803
C	1.16219	2.99277	-3.37068
C	1.64404	3.82601	-4.39390
H	1.43376	5.73608	-5.41965
H	-0.46210	6.49652	-3.95475
H	-1.30319	5.04109	-2.13141
H	1.63800	2.01425	-3.20585
H	2.48436	3.48804	-5.02216
N	-0.40625	-3.16388	0.78403

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	9.83	0.03435	YES	YES
8	a	17.93	0.02965	YES	YES
9	a	19.56	0.02844	YES	YES
10	a	26.88	0.12825	YES	YES
11	a	30.59	0.71377	YES	YES
12	a	32.06	0.10524	YES	YES
13	a	33.89	0.03285	YES	YES
14	a	38.66	0.35656	YES	YES
15	a	43.08	0.06666	YES	YES
16	a	44.13	0.57708	YES	YES
17	a	44.48	1.15148	YES	YES
18	a	49.48	0.55470	YES	YES
19	a	53.26	0.05913	YES	YES
20	a	54.96	0.61913	YES	YES
21	a	58.29	0.04534	YES	YES
22	a	61.11	0.29633	YES	YES
23	a	65.38	0.13103	YES	YES
24	a	66.69	0.29426	YES	YES
25	a	71.44	0.55797	YES	YES
26	a	73.00	0.40775	YES	YES
27	a	81.72	0.20403	YES	YES
28	a	84.72	1.47901	YES	YES
29	a	89.42	0.42976	YES	YES
30	a	92.62	0.07183	YES	YES
31	a	102.57	0.59341	YES	YES
32	a	105.35	0.11732	YES	YES

33	a	109.61	0.55341	YES	YES
34	a	116.58	1.64136	YES	YES
35	a	140.02	1.15108	YES	YES
36	a	142.21	0.48339	YES	YES
37	a	155.95	0.97235	YES	YES
38	a	160.80	0.42599	YES	YES
39	a	170.09	0.53638	YES	YES
40	a	174.76	3.60412	YES	YES
41	a	188.60	0.57832	YES	YES
42	a	193.23	4.56488	YES	YES
43	a	197.43	0.52396	YES	YES
44	a	198.80	0.43117	YES	YES
45	a	202.58	1.09874	YES	YES
46	a	208.53	6.04662	YES	YES
47	a	213.27	1.57916	YES	YES
48	a	214.52	2.96244	YES	YES
49	a	227.10	3.52765	YES	YES
50	a	230.70	1.99150	YES	YES

./16/a

BP86_SV(P) energy (au): -3254.4882718160

PBE0/def2-TZVPP energy (au): -3253.994803853
cosmo_dcm Total energy + OC corr. = -3254.0508261415

Zero point energy (au): 0.8888882
Entropy (kJ mol^-1): 1.42381
Chemical potential (kJ mol^-1): 2070.04

XYZ coordinates:

114

C	-1.03725	4.23427	-0.93816
C	-0.80471	3.74293	-2.25597
C	-2.24188	3.62838	-0.43306
C	-1.89922	2.85586	-2.58684
C	-2.79187	2.79379	-1.47987
H	-0.39944	4.94460	-0.39459
H	0.02604	4.01938	-2.91654
H	-2.70503	3.84193	0.53795
H	-2.02786	2.35400	-3.55502
H	-3.73914	2.23985	-1.43474
Ru	-0.72460	1.96578	-0.75160
C	1.75086	2.80569	1.03427
C	-2.73758	-0.76720	0.64023
P	-1.38899	0.47696	0.94990
C	-1.98936	1.45143	2.41473
C	-0.07098	-0.60723	1.73012
C	-0.43395	-1.65449	2.57003
N	1.21849	-0.25758	1.50167
C	0.59034	-2.37271	3.25858
C	1.96257	-1.99240	3.04154
C	2.18935	-0.90317	2.11703
O	3.43861	-0.45598	1.82896
C	-0.63792	-0.52819	-3.43196
P	0.38875	0.47159	-2.25058
C	1.47649	1.50039	-3.35372
C	1.52041	-0.87975	-1.62152
C	2.92108	-0.79430	-1.65358
N	0.85965	-1.96892	-1.19823
C	3.64720	-1.91557	-1.20879
C	2.98031	-3.06004	-0.76600
C	1.56063	-3.04285	-0.78523
N	0.76790	-4.13129	-0.40662
C	1.16811	-5.40301	0.01435
C	0.00827	-6.41767	0.20610
O	2.34627	-5.69464	0.18602
H	-1.48918	-1.92197	2.73333
H	3.43611	0.10250	-2.02533
H	4.74940	-1.89636	-1.22181
H	3.50270	-3.96297	-0.42535

H	-0.23574	-3.94414	-0.50015
C	2.99455	-2.68464	3.73592
C	0.30742	-3.43522	4.16848
C	3.14631	3.14173	-4.94750
C	2.18431	2.31527	-5.54910
C	1.35556	1.49596	-4.76055
C	2.42982	2.35780	-2.75385
C	3.26555	3.16056	-3.54604
H	3.79705	3.77899	-5.56817
H	2.07259	2.30221	-6.64569
H	0.60853	0.85781	-5.25603
H	2.50253	2.42248	-1.65607
H	4.00719	3.81640	-3.06133
C	-2.13655	-2.05248	-5.28567
C	-2.78759	-1.17713	-4.40195
C	-2.04180	-0.42183	-3.47851
C	0.00807	-1.43077	-4.31100
C	-0.73656	-2.18174	-5.23334
H	-2.71974	-2.64214	-6.01172
H	-3.88551	-1.08238	-4.42310
H	-2.56542	0.23250	-2.76536
H	1.10335	-1.54942	-4.27887
H	-0.21771	-2.87511	-5.91522
C	-4.66921	-2.76842	0.09838
C	-4.84171	-1.89470	1.18393
C	-3.88213	-0.90293	1.45848
C	-2.56107	-1.66517	-0.43769
C	-3.52016	-2.65603	-0.70536
H	-5.42557	-3.54069	-0.11747
H	-5.72917	-1.98334	1.83165
H	-4.02996	-0.24720	2.32917
H	-1.64879	-1.61182	-1.05328
H	-3.36997	-3.34144	-1.55590
C	-2.85720	3.04933	4.58747
C	-3.68293	2.88077	3.46101
C	-3.24943	2.09640	2.37950
C	-1.16774	1.63080	3.54876
C	-1.59893	2.42780	4.62430
H	-3.19693	3.66631	5.43519
H	-4.67420	3.36198	3.42389
H	-3.91098	1.97837	1.50559
H	-0.17742	1.15415	3.59766
H	-0.94079	2.55996	5.49812
C	-0.60101	-6.73761	-1.18365
C	-1.08155	-5.84334	1.14353
C	0.59650	-7.70171	0.82203
H	-1.85794	-6.61737	1.33256
H	-1.60709	-4.96032	0.71411
H	-0.65291	-5.54407	2.12521
H	1.39622	-8.12578	0.18033
H	-0.20359	-8.46439	0.94289
H	1.04347	-7.50169	1.81906
H	-1.39862	-7.50651	-1.07842
H	0.16951	-7.13979	-1.87723
H	-1.05945	-5.84328	-1.66222
C	2.68830	-3.71701	4.61563
H	4.05673	-2.41659	3.59373
H	-0.74305	-3.72027	4.34297

C	1.33521	-4.09176	4.83404
H	1.10409	-4.90725	5.53836
H	3.49661	-4.24469	5.14629
C	1.80950	4.03381	1.84850
C	2.01598	6.40696	3.39879
C	3.17367	5.71170	3.00818
C	3.07337	4.53971	2.24405
C	0.64890	4.73406	2.26714
C	0.75418	5.90769	3.02749
H	2.09544	7.32832	3.99816
H	4.16831	6.08596	3.30206
H	3.98832	4.00432	1.93923
H	-0.34622	4.32882	2.02214
H	-0.16163	6.43331	3.34550
C	0.73902	2.32078	0.30900
H	2.66427	2.17670	1.00732
H	4.10619	-0.99595	2.30722

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	10.62	0.15051	YES	YES
8	a	12.95	0.21276	YES	YES
9	a	14.40	0.15532	YES	YES
10	a	23.97	0.08924	YES	YES
11	a	25.78	0.12696	YES	YES
12	a	26.78	0.39040	YES	YES
13	a	29.84	0.05539	YES	YES
14	a	33.76	0.07702	YES	YES
15	a	36.19	0.18459	YES	YES
16	a	38.54	0.08493	YES	YES
17	a	39.89	0.08542	YES	YES
18	a	43.89	0.23936	YES	YES
19	a	47.76	0.11102	YES	YES
20	a	51.81	0.01456	YES	YES
21	a	54.20	0.15600	YES	YES
22	a	55.50	0.12686	YES	YES
23	a	56.79	0.19308	YES	YES
24	a	62.74	0.58829	YES	YES
25	a	65.17	0.27597	YES	YES
26	a	68.49	1.25021	YES	YES
27	a	71.40	0.08096	YES	YES
28	a	74.38	1.74263	YES	YES
29	a	80.23	0.12535	YES	YES
30	a	83.34	0.22529	YES	YES
31	a	92.35	0.33633	YES	YES
32	a	94.52	0.57134	YES	YES
33	a	100.28	0.77553	YES	YES

34	a	106.36	0.24441	YES	YES
35	a	114.09	0.48884	YES	YES
36	a	118.13	1.19986	YES	YES
37	a	121.76	1.21830	YES	YES
38	a	130.31	2.01170	YES	YES
39	a	153.50	1.13151	YES	YES
40	a	156.02	0.50314	YES	YES
41	a	169.37	1.20691	YES	YES
42	a	180.38	2.62212	YES	YES
43	a	185.63	0.67764	YES	YES
44	a	196.75	0.40996	YES	YES
45	a	203.40	1.30156	YES	YES
46	a	209.99	4.25579	YES	YES
47	a	211.84	1.48055	YES	YES
48	a	216.93	6.30980	YES	YES
49	a	218.16	3.70999	YES	YES
50	a	221.87	2.06221	YES	YES

./16/b

BP86_SV(P) energy (au): -3254.4897516370

PBE0/def2-TZVPP energy (au): -3253.996990878
cosmo_dcm Total energy + OC corr. = -3254.0532018966

Zero point energy (au): 0.8890864
Entropy (kJ mol^-1): 1.42618
Chemical potential (kJ mol^-1): 2069.93

XYZ coordinates:

114

C	-1.68975	4.06806	0.68967
C	-1.58445	4.01251	-0.74675
C	-2.73889	3.19644	1.09623
C	-2.62931	3.13665	-1.22607
C	-3.32410	2.61756	-0.09827
H	-1.06354	4.66876	1.36300
H	-0.89880	4.59319	-1.37671
H	-3.06807	3.03337	2.12921
H	-2.85138	2.93803	-2.28229
H	-4.18325	1.93311	-0.13029
Ru	-1.07858	1.94194	0.04887
C	1.66326	2.54741	1.53071
C	-2.71485	-1.34794	0.62350
P	-1.52479	-0.07318	1.27008
C	-2.18590	0.38232	2.94769
C	-0.06695	-1.15405	1.72856
C	-0.25492	-2.47804	2.10718
N	1.13865	-0.53861	1.76319
C	0.87017	-3.22726	2.56841
C	2.15991	-2.58777	2.59571
C	2.20225	-1.20854	2.16556
O	3.35365	-0.49127	2.16974
C	-0.97647	0.26740	-3.17731
P	0.02178	1.10307	-1.85260
C	0.81037	2.51351	-2.77903
C	1.38929	-0.15604	-1.62539
C	2.75520	0.16544	-1.57739
N	0.93168	-1.41516	-1.51999
C	3.66661	-0.89284	-1.40294
C	3.21118	-2.20971	-1.30133
C	1.81123	-2.42641	-1.38112
N	1.22113	-3.69590	-1.35638
C	1.84002	-4.94773	-1.31810
C	0.88378	-6.15309	-1.53091
O	3.05047	-5.07572	-1.17199
H	-1.24839	-2.95016	2.08101
H	3.11080	1.19783	-1.69025
H	4.74843	-0.68402	-1.36193
H	3.88390	-3.06882	-1.18583

H	0.20110	-3.66133	-1.45090
C	3.29185	-3.32021	3.05274
C	0.76380	-4.57724	3.01839
C	1.98181	4.72749	-4.10780
C	0.99732	3.95776	-4.74749
C	0.41630	2.85671	-4.09223
C	1.78411	3.31227	-2.13374
C	2.37222	4.40113	-2.79697
H	2.43980	5.58567	-4.62608
H	0.67435	4.21057	-5.77075
H	-0.35110	2.26880	-4.61723
H	2.08102	3.09628	-1.09577
H	3.13394	5.00285	-2.27525
C	-2.44833	-0.92153	-5.27945
C	-3.11753	-0.35183	-4.18487
C	-2.38363	0.23551	-3.13815
C	-0.30960	-0.32124	-4.27814
C	-1.04156	-0.90976	-5.32042
H	-3.02148	-1.37988	-6.10205
H	-4.21845	-0.36789	-4.13777
H	-2.91298	0.64711	-2.26581
H	0.79118	-0.31303	-4.32935
H	-0.50875	-1.36005	-6.17407
C	-4.36300	-3.38350	-0.45501
C	-4.61237	-2.87946	0.83148
C	-3.79278	-1.87271	1.37267
C	-2.45500	-1.87959	-0.66009
C	-3.27469	-2.88721	-1.19403
H	-5.01125	-4.16822	-0.87833
H	-5.45068	-3.27428	1.42877
H	-3.99403	-1.51790	2.39413
H	-1.58190	-1.52883	-1.23462
H	-3.06216	-3.28139	-2.20146
C	-3.14251	1.19670	5.48777
C	-4.00990	1.17151	4.38134
C	-3.53451	0.77670	3.11994
C	-1.32223	0.41850	4.06428
C	-1.79847	0.82568	5.32267
H	-3.51538	1.50853	6.47683
H	-5.06676	1.46253	4.49867
H	-4.22958	0.77782	2.26475
H	-0.26382	0.13637	3.95733
H	-1.10841	0.84940	6.18173
C	0.44724	-6.16006	-3.01972
C	-0.35910	-6.06290	-0.61400
C	1.66596	-7.44253	-1.21410
H	-0.97745	-6.97950	-0.73308
H	-1.02171	-5.19982	-0.85271
H	-0.06602	-5.98728	0.45625
H	2.57564	-7.52290	-1.84337
H	1.02397	-8.33106	-1.40030
H	1.99426	-7.46355	-0.15273
H	-0.19779	-7.04383	-3.22152
H	1.32911	-6.22006	-3.69421
H	-0.13236	-5.24994	-3.29286
C	3.15805	-4.63628	3.48001
H	4.29636	-2.86133	3.07917
H	-0.22584	-5.06276	3.01462

C	1.88424	-5.26534	3.46720
H	1.78893	-6.30598	3.81704
H	4.04138	-5.19236	3.83193
C	2.32884	3.85806	1.63296
C	3.69391	6.33648	1.94719
C	4.15057	5.18508	2.61229
C	3.47928	3.96388	2.45730
C	1.88627	5.02796	0.96249
C	2.55932	6.24837	1.12027
H	4.21893	7.29734	2.07138
H	5.04034	5.23859	3.26124
H	3.84418	3.06682	2.98474
H	1.00959	4.97744	0.29855
H	2.19238	7.14328	0.59053
C	0.55355	2.17117	0.88527
H	2.13861	1.71519	2.08336
H	4.10009	-1.05181	2.47746

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	10.34	0.03544	YES	YES
8	a	11.48	0.10432	YES	YES
9	a	15.63	0.22208	YES	YES
10	a	22.71	0.15956	YES	YES
11	a	24.14	0.19162	YES	YES
12	a	29.15	0.12328	YES	YES
13	a	29.69	0.01625	YES	YES
14	a	32.95	0.06444	YES	YES
15	a	34.78	0.22260	YES	YES
16	a	37.20	0.06800	YES	YES
17	a	41.45	0.16495	YES	YES
18	a	43.78	0.03635	YES	YES
19	a	44.21	0.06780	YES	YES
20	a	46.56	0.18466	YES	YES
21	a	49.76	0.15076	YES	YES
22	a	55.69	1.21626	YES	YES
23	a	58.89	0.56523	YES	YES
24	a	62.03	0.48151	YES	YES
25	a	66.63	0.55143	YES	YES
26	a	68.96	0.26062	YES	YES
27	a	70.32	0.19612	YES	YES
28	a	76.70	0.80604	YES	YES
29	a	81.41	1.06988	YES	YES
30	a	84.18	0.37517	YES	YES
31	a	93.97	0.12897	YES	YES
32	a	95.72	0.07480	YES	YES
33	a	106.89	1.16933	YES	YES

34	a	109.55	0.27668	YES	YES
35	a	113.37	0.03549	YES	YES
36	a	120.81	0.64184	YES	YES
37	a	128.26	2.21412	YES	YES
38	a	129.81	1.70763	YES	YES
39	a	153.24	0.69013	YES	YES
40	a	154.93	0.64316	YES	YES
41	a	171.03	0.70715	YES	YES
42	a	180.08	1.07865	YES	YES
43	a	182.42	2.23269	YES	YES
44	a	192.32	0.66646	YES	YES
45	a	202.27	0.20562	YES	YES
46	a	207.49	2.54463	YES	YES
47	a	210.17	0.86091	YES	YES
48	a	216.48	10.25602	YES	YES
49	a	220.54	0.47509	YES	YES
50	a	227.90	0.25247	YES	YES

./17/a

BP86_SV(P) energy (au): -3254.5168127280

PBE0/def2-TZVPP energy (au): -3254.024607585
cosmo_dcm Total energy + OC corr. = -3254.0771101166

Zero point energy (au): 0.8914622
Entropy (kJ mol^-1): 1.37965
Chemical potential (kJ mol^-1): 2085.89

XYZ coordinates:

114

C	-1.40291	3.94393	0.59800
C	-1.45699	3.82603	-0.83427
C	-2.43500	3.12862	1.15230
C	-2.55415	2.94743	-1.15378
C	-3.15970	2.50814	0.06267
H	-0.70555	4.56606	1.17031
H	-0.83904	4.36439	-1.56121
H	-2.66512	3.02835	2.22102
H	-2.88491	2.69084	-2.16929
H	-4.05275	1.87630	0.15752
Ru	-0.98128	1.77297	0.04591
C	1.80289	2.77713	1.26677
C	-2.07788	-1.47540	1.63376
P	-1.08455	0.09535	1.62037
C	-1.38610	0.72820	3.34130
C	0.66795	-0.50701	1.66965
C	1.12649	-1.74796	2.04141
N	1.52628	0.44141	1.11439
C	2.49097	-2.11881	1.81329
C	3.34829	-1.17387	1.15836
C	2.81769	0.11766	0.82265
O	3.60671	0.98957	0.21404
C	-1.75328	-0.27217	-2.86042
P	-0.40949	0.59535	-1.89538
C	0.25345	1.78871	-3.16528
C	0.85678	-0.80404	-1.92059
C	2.09269	-0.75455	-2.58920
N	0.41565	-1.91025	-1.29403
C	2.88089	-1.92257	-2.59630
C	2.43036	-3.08251	-1.96308
C	1.16479	-3.02976	-1.32309
N	0.56649	-4.13373	-0.69620
C	1.06632	-5.43288	-0.56193
C	0.06915	-6.46131	0.03651
O	2.20347	-5.73171	-0.91012
H	0.42485	-2.47187	2.48257
H	2.42665	0.14699	-3.12081
H	3.85075	-1.92842	-3.12072
H	3.00709	-4.01684	-1.95165

H	-0.38621	-3.93388	-0.36719
C	4.70229	-1.50596	0.87753
C	3.02480	-3.38597	2.17256
C	1.26842	3.70057	-4.99917
C	0.03456	3.07449	-5.23771
C	-0.46722	2.12072	-4.33330
C	1.48361	2.44391	-2.92456
C	1.99477	3.37889	-3.83865
H	1.66564	4.43759	-5.71603
H	-0.54718	3.32244	-6.14084
H	-1.43004	1.63224	-4.54971
H	2.05235	2.22073	-2.00748
H	2.96158	3.86890	-3.63680
C	-3.76399	-1.54438	-4.39671
C	-4.11195	-0.78962	-3.26534
C	-3.11128	-0.15942	-2.50232
C	-1.41318	-1.04032	-3.99872
C	-2.41042	-1.66966	-4.75962
H	-4.54598	-2.03791	-4.99663
H	-5.16920	-0.69016	-2.96897
H	-3.38791	0.41319	-1.60415
H	-0.35876	-1.14497	-4.30185
H	-2.12722	-2.26349	-5.64416
C	-3.65664	-3.82111	1.61452
C	-3.14571	-3.32550	2.82678
C	-2.36307	-2.15810	2.83994
C	-2.57749	-1.99046	0.42032
C	-3.36598	-3.15443	0.41140
H	-4.28744	-4.72523	1.60922
H	-3.37412	-3.83783	3.77573
H	-1.98819	-1.77203	3.80086
H	-2.34862	-1.48057	-0.52467
H	-3.76879	-3.53037	-0.54350
C	-1.90510	1.82398	5.89705
C	-2.97187	1.45259	5.05894
C	-2.71601	0.91017	3.78945
C	-0.32291	1.10337	4.18896
C	-0.58286	1.64765	5.45907
H	-2.10633	2.24769	6.89422
H	-4.01300	1.58219	5.39740
H	-3.56363	0.61558	3.14766
H	0.72172	0.97093	3.86460
H	0.25835	1.93092	6.11272
C	-0.37045	-6.02110	1.45381
C	0.78516	-7.82366	0.11643
C	-1.16761	-6.57775	-0.89200
H	0.09577	-8.58927	0.53540
H	1.68748	-7.76979	0.76281
H	1.12047	-8.16164	-0.88726
H	-1.74833	-5.63158	-0.95263
H	-1.85494	-7.36417	-0.50872
H	-0.86848	-6.86363	-1.92411
H	-1.04444	-6.78823	1.89640
H	-0.93311	-5.06125	1.45474
H	0.50613	-5.91902	2.13110
C	5.19346	-2.75632	1.24005
H	5.34759	-0.76399	0.38463
H	2.37185	-4.11750	2.67488

C	4.35160	-3.69848	1.88813
H	4.75287	-4.68595	2.16695
H	6.24222	-3.01713	1.02717
C	1.83963	4.23868	1.07767
C	2.05479	7.06462	0.81478
C	1.72783	6.26795	-0.29834
C	1.62214	4.87548	-0.16893
C	2.19514	5.05609	2.18334
C	2.28998	6.44951	2.05702
H	2.13701	8.15845	0.71018
H	1.56356	6.73764	-1.28249
H	1.38953	4.26128	-1.05044
H	2.39436	4.58389	3.16058
H	2.55572	7.06103	2.93489
C	0.94902	1.79450	0.77085
H	2.51772	2.44369	2.05051
H	3.09834	1.87367	0.19250

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	7.04	0.30754	YES	YES
8	a	14.88	0.16945	YES	YES
9	a	19.34	0.26830	YES	YES
10	a	26.54	0.03014	YES	YES
11	a	28.72	1.23486	YES	YES
12	a	31.66	0.00944	YES	YES
13	a	33.50	0.00865	YES	YES
14	a	35.34	0.24344	YES	YES
15	a	38.27	0.51330	YES	YES
16	a	40.66	0.09014	YES	YES
17	a	45.31	0.06856	YES	YES
18	a	48.16	0.10479	YES	YES
19	a	50.49	0.06656	YES	YES
20	a	55.58	0.01288	YES	YES
21	a	57.78	0.05041	YES	YES
22	a	59.35	0.58788	YES	YES
23	a	63.98	0.29029	YES	YES
24	a	71.47	0.43380	YES	YES
25	a	72.10	0.87088	YES	YES
26	a	74.46	0.25713	YES	YES
27	a	80.73	0.08996	YES	YES
28	a	85.09	0.25430	YES	YES
29	a	90.96	0.33360	YES	YES
30	a	93.42	0.11291	YES	YES
31	a	100.51	0.55673	YES	YES
32	a	107.74	0.13363	YES	YES
33	a	110.74	0.15160	YES	YES

34	a	117.26	1.13357	YES	YES
35	a	124.56	2.19102	YES	YES
36	a	127.56	0.77308	YES	YES
37	a	152.71	0.53144	YES	YES
38	a	165.59	1.02050	YES	YES
39	a	168.52	0.25788	YES	YES
40	a	177.24	3.89381	YES	YES
41	a	184.52	0.69390	YES	YES
42	a	189.37	3.00174	YES	YES
43	a	197.86	0.43837	YES	YES
44	a	199.86	1.35061	YES	YES
45	a	204.50	1.47827	YES	YES
46	a	207.67	1.55349	YES	YES
47	a	212.67	0.55508	YES	YES
48	a	217.45	1.35673	YES	YES
49	a	220.32	0.61008	YES	YES
50	a	223.40	4.48238	YES	YES

./17/b

BP86_SV(P) energy (au): -3254.5216014140

PBE0/def2-TZVPP energy (au): -3254.028475787
cosmo_dcm Total energy + OC corr. = -3254.0809645909

Zero point energy (au): 0.8916519
Entropy (kJ mol^-1): 1.37762
Chemical potential (kJ mol^-1): 2087.13

XYZ coordinates:

114

C	-1.08473	3.93316	1.53409
C	-2.16628	3.75321	0.60062
C	-1.34271	3.11641	2.67811
C	-3.09522	2.82619	1.19544
C	-2.59789	2.43180	2.47871
H	-0.21302	4.58828	1.40619
H	-2.30452	4.26812	-0.35871
H	-0.70862	3.05326	3.57218
H	-4.04409	2.50592	0.74302
H	-3.10311	1.78811	3.21019
Ru	-1.08109	1.76797	0.85152
C	1.00674	3.23487	-0.87293
C	0.09486	-1.31282	2.68119
P	0.38278	0.34540	1.89610
C	1.38624	1.19838	3.20772
C	1.60733	-0.03701	0.54903
C	2.43112	-1.13151	0.45199
N	1.48416	0.86465	-0.51593
C	3.13413	-1.41592	-0.76334
C	2.90452	-0.56114	-1.89137
C	2.04534	0.57534	-1.72852
O	1.81992	1.35044	-2.77118
C	-3.48694	-0.75997	-0.18544
P	-2.10910	0.37794	-0.72067
C	-2.95710	1.42501	-2.01461
C	-1.11889	-0.83525	-1.75770
C	-0.91904	-0.70493	-3.14356
N	-0.66611	-1.88753	-1.05219
C	-0.21501	-1.73351	-3.80028
C	0.24653	-2.84210	-3.08610
C	-0.01976	-2.88154	-1.69263
N	0.33371	-3.95503	-0.86438
C	0.95905	-5.15553	-1.21458
C	1.03684	-6.21079	-0.07767
O	1.40151	-5.35755	-2.34023
H	2.51341	-1.82135	1.30513
H	-1.31545	0.15537	-3.70131
H	-0.04016	-1.67440	-4.88736
H	0.78508	-3.67304	-3.55818

H	-0.00628	-3.83765	0.09747
C	3.54404	-0.82378	-3.13415
C	4.01121	-2.52300	-0.91535
C	-4.16351	3.09795	-3.96085
C	-4.92990	2.14379	-3.27366
C	-4.33269	1.30856	-2.31141
C	-2.19904	2.40505	-2.69807
C	-2.79286	3.22444	-3.67128
H	-4.63285	3.74687	-4.71813
H	-6.00663	2.04115	-3.48666
H	-4.95360	0.56436	-1.78990
H	-1.13074	2.53179	-2.45956
H	-2.18243	3.97352	-4.20235
C	-5.64755	-2.41866	0.58603
C	-5.17823	-1.42107	1.45609
C	-4.10244	-0.60028	1.07217
C	-3.96431	-1.76989	-1.05324
C	-5.03567	-2.59202	-0.66869
H	-6.48987	-3.06393	0.88495
H	-5.64888	-1.28000	2.44293
H	-3.71974	0.16381	1.76516
H	-3.50415	-1.91505	-2.04409
H	-5.39642	-3.37410	-1.35693
C	-0.40976	-3.81864	3.88810
C	0.78430	-3.12996	4.16786
C	1.03574	-1.88228	3.57286
C	-1.09416	-2.01459	2.39826
C	-1.34602	-3.26005	3.00096
H	-0.61308	-4.78904	4.37003
H	1.52166	-3.55988	4.86553
H	1.96388	-1.34371	3.82356
H	-1.83089	-1.58310	1.70627
H	-2.28962	-3.78708	2.78418
C	2.76529	2.65654	5.20176
C	1.62782	1.90153	5.53886
C	0.94097	1.17750	4.55016
C	2.52383	1.96389	2.87796
C	3.21047	2.68589	3.86956
H	3.30442	3.22166	5.97934
H	1.27233	1.87163	6.58197
H	0.05416	0.58591	4.83290
H	2.88508	2.00646	1.83811
H	4.10108	3.27448	3.59538
C	1.86145	-5.65301	1.10827
C	1.72819	-7.46707	-0.64145
C	-0.39489	-6.57299	0.39247
H	1.79893	-8.24589	0.14897
H	2.75282	-7.23701	-1.00172
H	1.16350	-7.88659	-1.50003
H	-0.92411	-5.71208	0.85879
H	-0.34685	-7.38250	1.15419
H	-1.01540	-6.94120	-0.45376
H	1.96164	-6.43173	1.89666
H	1.38829	-4.76551	1.58487
H	2.88798	-5.37103	0.78463
C	4.39720	-1.91660	-3.25107
H	3.36235	-0.15175	-3.98552
H	4.19270	-3.18522	-0.05380

C	4.62974	-2.76804	-2.13904
H	5.30642	-3.63084	-2.24729
H	4.89783	-2.12248	-4.21050
C	2.33128	3.77999	-1.24759
C	4.78862	5.03067	-1.98312
C	4.79002	3.82702	-1.25503
C	3.58430	3.21013	-0.89385
C	2.35571	5.00424	-1.97073
C	3.56128	5.61793	-2.33623
H	5.73903	5.51165	-2.26536
H	5.74554	3.36479	-0.95679
H	3.62605	2.27880	-0.30771
H	1.39955	5.48232	-2.24478
H	3.54233	6.56652	-2.89748
C	0.57662	2.02718	-0.32808
H	0.22211	4.00883	-0.89522
H	1.28201	2.15146	-2.45255

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.88	0.03787	YES	YES
8	a	18.49	0.11906	YES	YES
9	a	21.21	0.68897	YES	YES
10	a	25.27	0.00896	YES	YES
11	a	27.58	0.04176	YES	YES
12	a	29.12	0.03399	YES	YES
13	a	31.23	0.25716	YES	YES
14	a	36.04	0.03772	YES	YES
15	a	37.06	0.60572	YES	YES
16	a	39.14	0.66778	YES	YES
17	a	44.41	0.38154	YES	YES
18	a	47.73	0.07212	YES	YES
19	a	52.19	0.24836	YES	YES
20	a	54.98	0.05465	YES	YES
21	a	56.19	0.01337	YES	YES
22	a	59.39	0.21107	YES	YES
23	a	59.72	0.15688	YES	YES
24	a	63.22	0.22625	YES	YES
25	a	68.29	0.40791	YES	YES
26	a	71.74	0.21478	YES	YES
27	a	75.92	0.11068	YES	YES
28	a	77.86	1.05289	YES	YES
29	a	86.70	0.51033	YES	YES
30	a	88.53	0.01297	YES	YES
31	a	93.96	0.48881	YES	YES
32	a	105.01	0.27568	YES	YES
33	a	108.76	0.65878	YES	YES

34	a	117.77	0.07156	YES	YES
35	a	124.41	1.37829	YES	YES
36	a	135.03	1.02645	YES	YES
37	a	157.14	3.86032	YES	YES
38	a	165.03	0.76701	YES	YES
39	a	170.01	0.90606	YES	YES
40	a	179.17	2.98960	YES	YES
41	a	186.55	1.88276	YES	YES
42	a	189.01	0.55258	YES	YES
43	a	199.51	0.70906	YES	YES
44	a	201.73	1.61766	YES	YES
45	a	208.10	0.59524	YES	YES
46	a	211.88	0.97792	YES	YES
47	a	218.17	3.93790	YES	YES
48	a	218.85	0.35651	YES	YES
49	a	222.77	5.14027	YES	YES
50	a	224.25	2.87326	YES	YES

./18/a

BP86_SV(P) energy (au): -3254.5230801560

PBE0/def2-TZVPP energy (au): -3254.021094273
cosmo_dcm Total energy + OC corr. = -3254.0730530968

Zero point energy (au): 0.8932646
Entropy (kJ mol^-1): 1.33727
Chemical potential (kJ mol^-1): 2101.24

XYZ coordinates:

114

C	3.37025	0.52637	-1.09212
C	2.73441	0.67441	-2.36411
C	3.28417	1.77223	-0.38853
C	2.26219	2.03954	-2.46148
C	2.60156	2.71449	-1.25521
H	3.84657	-0.38893	-0.72019
H	2.69126	-0.08288	-3.15439
H	3.72492	1.99615	0.59082
H	1.76601	2.48634	-3.33259
H	2.42702	3.77530	-1.03915
Ru	1.17704	1.02952	-0.71151
C	1.78156	-1.79296	0.61121
C	-1.33207	2.83149	1.49059
P	0.38138	2.16913	1.13443
C	1.49149	3.52646	1.73832
C	0.38170	0.89363	2.47195
C	0.10641	1.16337	3.78886
N	0.43960	-0.40383	1.96525
C	-0.16475	0.09330	4.70547
C	-0.30278	-1.21935	4.16111
C	-0.11232	-1.46523	2.72283
O	-0.41234	-2.56268	2.20414
C	-2.20220	1.78664	-1.85112
P	-0.71318	0.67351	-1.99801
C	-0.40029	0.79509	-3.85047
C	-1.51556	-1.04524	-2.04071
C	-2.35275	-1.46656	-3.07213
N	-1.17638	-1.94006	-1.05965
C	-2.82821	-2.79520	-3.07452
C	-2.46188	-3.68667	-2.07216
C	-1.60062	-3.25083	-1.02747
N	-1.16198	-4.03298	0.00811
C	-1.31311	-5.45048	0.08366
C	-0.80267	-6.11375	1.37945
O	-1.83540	-6.08026	-0.82340
H	0.03033	2.20837	4.12659
H	-2.61441	-0.77025	-3.88106
H	-3.49773	-3.13722	-3.88071
H	-2.79334	-4.73087	-2.06225

H	-0.71763	-3.52205	0.81255
C	-0.64087	-2.30059	5.01140
C	-0.36804	0.29014	6.09743
C	0.19997	0.98871	-6.61702
C	-0.47999	2.02853	-5.96408
C	-0.78401	1.93220	-4.59347
C	0.27899	-0.24875	-4.52047
C	0.57348	-0.15510	-5.89007
H	0.43261	1.06427	-7.69156
H	-0.78965	2.92589	-6.52444
H	-1.33495	2.75435	-4.11157
H	0.57324	-1.16066	-3.97635
H	1.09761	-0.98447	-6.39270
C	-4.30521	3.67932	-1.77406
C	-2.96931	4.10629	-1.68664
C	-1.92738	3.16596	-1.71237
C	-3.54697	1.36740	-1.92960
C	-4.58991	2.30884	-1.88663
H	-5.12500	4.41534	-1.74611
H	-2.73632	5.17870	-1.58580
H	-0.88008	3.50029	-1.61874
H	-3.80219	0.30013	-2.01307
H	-5.63529	1.96376	-1.94368
C	-3.96477	3.58430	2.20953
C	-2.90306	4.48791	2.36554
C	-1.59217	4.11484	2.01506
C	-2.40847	1.92867	1.33922
C	-3.71173	2.29847	1.69821
H	-4.98880	3.87629	2.49412
H	-3.08692	5.49387	2.77769
H	-0.77419	4.83135	2.18150
H	-2.22315	0.91302	0.95224
H	-4.53610	1.57629	1.58274
C	3.24670	5.60567	2.52923
C	2.30326	5.82780	1.51077
C	1.43753	4.79538	1.11331
C	2.44774	3.31219	2.75468
C	3.31878	4.34538	3.14478
H	3.92696	6.41504	2.83990
H	2.24115	6.81243	1.01883
H	0.71122	4.98674	0.30493
H	2.51842	2.32988	3.24758
H	4.05868	4.15972	3.94041
C	-1.73634	-5.67586	2.53999
C	0.66076	-5.70541	1.67861
C	-0.88693	-7.64118	1.19019
H	1.02297	-6.27333	2.56422
H	0.75741	-4.62536	1.91760
H	1.33260	-5.94521	0.82557
H	-1.92265	-7.96648	0.96047
H	-0.55574	-8.14842	2.12229
H	-0.23672	-7.98281	0.35674
H	-1.41671	-6.18260	3.47751
H	-2.79055	-5.96864	2.33952
H	-1.69304	-4.57961	2.71245
C	-0.82147	-2.08971	6.37894
H	-0.74696	-3.30396	4.57324
H	-0.27387	1.30545	6.51674

C	-0.68719	-0.78847	6.92178
H	-0.83896	-0.62737	8.00172
H	-1.07255	-2.93588	7.03852
C	2.45833	-2.55465	-0.44626
C	3.80773	-4.19611	-2.35479
C	2.78098	-3.32442	-2.76064
C	2.12368	-2.51504	-1.82359
C	3.48433	-3.46027	-0.05654
C	4.15561	-4.25770	-0.99384
H	4.32714	-4.82825	-3.09298
H	2.48835	-3.28046	-3.82328
H	1.32787	-1.83119	-2.15180
H	3.75886	-3.52992	1.01001
H	4.95443	-4.93949	-0.65823
C	1.05129	-0.61780	0.62030
H	1.90935	-2.28900	1.59151
H	-0.44574	-1.61374	-0.36370

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	11.26	0.06336	YES	YES
8	a	18.05	0.07350	YES	YES
9	a	27.11	0.12977	YES	YES
10	a	30.68	0.04628	YES	YES
11	a	33.78	0.02279	YES	YES
12	a	37.48	0.82316	YES	YES
13	a	42.23	0.12123	YES	YES
14	a	46.88	0.16456	YES	YES
15	a	48.18	0.93706	YES	YES
16	a	49.06	0.53102	YES	YES
17	a	52.38	0.42415	YES	YES
18	a	56.10	0.40279	YES	YES
19	a	58.46	0.08057	YES	YES
20	a	61.67	0.15153	YES	YES
21	a	64.84	0.76073	YES	YES
22	a	72.32	0.57317	YES	YES
23	a	73.58	0.05020	YES	YES
24	a	74.74	0.91005	YES	YES
25	a	78.67	2.03828	YES	YES
26	a	85.61	0.24208	YES	YES
27	a	86.90	0.38140	YES	YES
28	a	91.20	0.30264	YES	YES
29	a	96.91	0.61682	YES	YES
30	a	103.97	0.87915	YES	YES
31	a	108.52	0.65481	YES	YES
32	a	117.44	0.40497	YES	YES
33	a	121.45	1.43645	YES	YES

34	a	123.88	1.39687	YES	YES
35	a	139.12	1.55063	YES	YES
36	a	148.66	1.52704	YES	YES
37	a	160.58	0.30719	YES	YES
38	a	164.29	2.04528	YES	YES
39	a	175.51	2.49968	YES	YES
40	a	186.57	0.76861	YES	YES
41	a	192.74	3.32838	YES	YES
42	a	196.13	1.60523	YES	YES
43	a	198.52	4.06224	YES	YES
44	a	201.13	1.53262	YES	YES
45	a	206.98	2.37918	YES	YES
46	a	211.07	0.80785	YES	YES
47	a	214.66	2.38867	YES	YES
48	a	221.84	2.18586	YES	YES
49	a	226.00	1.14284	YES	YES
50	a	228.31	1.23796	YES	YES

./18/b

BP86_SV(P) energy (au): -3254.5157047000

PBE0/def2-TZVPP energy (au): -3254.017884633
cosmo_dcm Total energy + OC corr. = -3254.0763973549

Zero point energy (au): 0.8921631
Entropy (kJ mol^-1): 1.37488
Chemical potential (kJ mol^-1): 2089.78

XYZ coordinates:

114

C	-3.73408	-2.02872	-0.95888
C	-3.78610	-0.99811	-1.96222
C	-2.80284	-3.02712	-1.39454
C	-2.88292	-1.38497	-3.01768
C	-2.28357	-2.64395	-2.68258
H	-4.30645	-2.05830	-0.02297
H	-4.42677	-0.10726	-1.96011
H	-2.55921	-3.94848	-0.84889
H	-2.72032	-0.82210	-3.94745
H	-1.61216	-3.24268	-3.31159
Ru	-1.70440	-1.05696	-1.07757
C	-3.22983	0.40715	1.17196
C	1.55275	-2.55767	-0.10338
P	-0.15196	-1.94724	0.34687
C	-0.78965	-3.34758	1.38240
C	0.18283	-0.57246	1.54816
C	1.28585	-0.42529	2.35512
N	-0.80913	0.39990	1.45665
C	1.45135	0.77451	3.13581
C	0.51477	1.83518	2.94508
C	-0.60669	1.71274	1.98792
O	-1.32715	2.65828	1.66578
C	0.38420	0.54127	-3.57513
P	-0.66016	0.74947	-2.02982
C	-1.88014	2.05473	-2.54662
C	0.59957	1.79923	-1.08912
C	0.47435	3.14942	-0.76613
N	1.76935	1.16559	-0.73804
C	1.53594	3.80552	-0.11266
C	2.71803	3.13616	0.21131
C	2.83436	1.76794	-0.11738
N	3.94289	0.97921	0.11833
C	5.19706	1.41021	0.64106
C	6.27560	0.30757	0.72800
O	5.37816	2.56729	0.97562
H	2.04394	-1.22146	2.40680
H	-0.44609	3.68737	-1.02670
H	1.43807	4.87246	0.14416
H	3.56049	3.62597	0.71149

H	3.86830	-0.01258	-0.13805
C	0.65326	3.04131	3.66914
C	2.51638	0.96103	4.05761
C	-3.89316	3.89521	-3.28796
C	-3.12919	3.25139	-4.27458
C	-2.12244	2.33996	-3.90882
C	-2.66790	2.68876	-1.55507
C	-3.65579	3.61449	-1.93024
H	-4.67647	4.61527	-3.57630
H	-3.31072	3.46064	-5.34153
H	-1.52926	1.85168	-4.69771
H	-2.50947	2.47034	-0.48457
H	-4.24998	4.11521	-1.14821
C	1.89763	0.21376	-5.94472
C	1.15969	-0.86246	-5.42457
C	0.41159	-0.69925	-4.24423
C	1.12765	1.62059	-4.10985
C	1.88060	1.45560	-5.28366
H	2.48477	0.08828	-6.86912
H	1.16238	-1.83670	-5.94048
H	-0.16144	-1.54272	-3.82723
H	1.10905	2.60750	-3.61808
H	2.45171	2.30661	-5.68987
C	4.11132	-3.48757	-0.89335
C	3.60453	-3.80137	0.38182
C	2.33620	-3.34198	0.77622
C	2.06668	-2.25780	-1.38399
C	3.34147	-2.71114	-1.77638
H	5.09865	-3.86606	-1.20423
H	4.19735	-4.42307	1.07286
H	1.94429	-3.62182	1.76745
H	1.43068	-1.71474	-2.10430
H	3.71429	-2.48489	-2.78899
C	-1.94831	-5.46814	2.84815
C	-1.19849	-5.73920	1.68999
C	-0.62341	-4.68641	0.95827
C	-1.55026	-3.08278	2.54175
C	-2.12336	-4.13918	3.27018
H	-2.39719	-6.29495	3.42215
H	-1.05731	-6.77905	1.35224
H	-0.03729	-4.91613	0.05245
H	-1.70531	-2.04652	2.88185
H	-2.71121	-3.91774	4.17567
C	5.79770	-0.81607	1.68225
C	7.56063	0.95078	1.28542
C	6.55043	-0.26410	-0.68654
H	8.36029	0.18262	1.36012
H	7.39229	1.38141	2.29442
H	7.92113	1.77021	0.62900
H	5.67122	-0.79179	-1.11968
H	7.37874	-1.00442	-0.63101
H	6.86023	0.53583	-1.39380
H	6.60483	-1.57274	1.79650
H	4.89871	-1.35376	1.30581
H	5.56648	-0.41363	2.69241
C	1.69971	3.19928	4.58147
H	-0.09161	3.83427	3.50029
H	3.24285	0.14569	4.21342

C	2.63542	2.15523	4.77177
H	3.45980	2.28319	5.49234
H	1.79515	4.13423	5.15714
C	-3.68231	0.93756	2.47082
C	-4.76531	1.91808	4.92151
C	-5.46834	2.09047	3.71668
C	-4.93853	1.59809	2.51591
C	-2.99730	0.76336	3.70168
C	-3.53116	1.24346	4.90567
H	-5.18134	2.29663	5.86945
H	-6.44296	2.60623	3.71378
H	-5.50662	1.72755	1.57849
H	-2.03759	0.22438	3.72559
H	-2.97842	1.08416	5.84647
C	-1.99801	0.06657	0.67193
H	-4.06779	0.25119	0.47248
H	1.84165	0.15628	-0.96219

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	15.12	0.13561	YES	YES
8	a	19.90	0.03495	YES	YES
9	a	21.98	0.13490	YES	YES
10	a	24.88	0.25319	YES	YES
11	a	29.06	0.13317	YES	YES
12	a	33.34	0.17830	YES	YES
13	a	34.56	0.11900	YES	YES
14	a	37.59	0.10537	YES	YES
15	a	41.44	0.75094	YES	YES
16	a	42.85	0.34403	YES	YES
17	a	46.74	0.87729	YES	YES
18	a	50.48	0.02904	YES	YES
19	a	51.94	0.06322	YES	YES
20	a	56.21	0.14264	YES	YES
21	a	56.97	0.32028	YES	YES
22	a	60.49	0.05908	YES	YES
23	a	60.85	1.01985	YES	YES
24	a	65.34	0.02802	YES	YES
25	a	72.33	1.87082	YES	YES
26	a	73.93	2.71298	YES	YES
27	a	76.10	1.49886	YES	YES
28	a	78.23	0.70330	YES	YES
29	a	88.39	0.37528	YES	YES
30	a	92.57	0.32463	YES	YES
31	a	98.27	0.52042	YES	YES
32	a	100.49	2.26968	YES	YES
33	a	108.18	2.45306	YES	YES

34	a	114.37	1.14907	YES	YES
35	a	126.49	0.05418	YES	YES
36	a	132.19	0.99080	YES	YES
37	a	149.42	2.27272	YES	YES
38	a	162.41	0.07305	YES	YES
39	a	163.39	0.49186	YES	YES
40	a	168.38	0.80125	YES	YES
41	a	180.45	1.22351	YES	YES
42	a	188.18	1.12574	YES	YES
43	a	194.93	1.80146	YES	YES
44	a	198.54	3.33182	YES	YES
45	a	206.03	1.01068	YES	YES
46	a	207.71	0.71147	YES	YES
47	a	211.65	1.28322	YES	YES
48	a	214.51	1.31097	YES	YES
49	a	217.13	2.74455	YES	YES
50	a	218.29	1.59003	YES	YES

./TS1617

BP86_SV(P) energy (au): -3254.4859567930

PBE0/def2-TZVPP energy (au): -3253.992067944
cosmo_dcm Total energy + OC corr. = -3254.0484719462

Zero point energy (au): 0.8893094
Entropy (kJ mol^-1): 1.38127
Chemical potential (kJ mol^-1): 2080.78

XYZ coordinates:

114

C	-3.16591	2.72792	-1.07969
C	-2.69712	3.51102	0.04644
C	-2.33833	3.04031	-2.19757
C	-1.59467	4.30209	-0.39306
C	-1.34621	4.00135	-1.77808
H	-4.03309	2.05365	-1.08012
H	-3.13871	3.52963	1.05056
H	-2.44713	2.65273	-3.21873
H	-1.03070	5.01616	0.22033
H	-0.60084	4.47215	-2.42987
Ru	-0.99103	2.09599	-0.56680
C	1.49876	3.23734	1.05250
C	-2.51181	-1.00267	0.90149
P	-1.45731	0.51621	1.08447
C	-2.18670	1.33363	2.58518
C	0.15678	-0.16148	1.73168
C	0.25896	-1.29098	2.52633
N	1.24321	0.55718	1.34661
C	1.54881	-1.72534	2.95965
C	2.70349	-0.99035	2.51600
C	2.46523	0.16485	1.68097
O	3.47360	0.92016	1.19927
C	-0.80361	-0.14875	-3.42202
P	0.16991	0.82902	-2.16526
C	1.18250	1.96439	-3.23351
C	1.37796	-0.52058	-1.66883
C	2.76068	-0.48363	-1.91668
N	0.76542	-1.58186	-1.11608
C	3.51761	-1.61421	-1.55156
C	2.89760	-2.72739	-0.97887
C	1.49104	-2.66978	-0.79248
N	0.73276	-3.73273	-0.28596
C	1.16165	-5.01338	0.07644
C	0.02426	-6.00751	0.43689
O	2.34685	-5.32688	0.08822
H	-0.63720	-1.85362	2.82831
H	3.23614	0.38327	-2.39536
H	4.60528	-1.63090	-1.73417
H	3.44426	-3.63423	-0.69191

H	-0.27251	-3.52472	-0.26198
C	4.00052	-1.41416	2.92302
C	1.73906	-2.85619	3.80691
C	2.71009	3.78757	-4.77143
C	1.62999	3.10403	-5.35257
C	0.87273	2.19433	-4.59248
C	2.25636	2.67763	-2.64846
C	3.02078	3.57087	-3.41695
H	3.30748	4.49337	-5.37139
H	1.37259	3.27256	-6.41119
H	0.03626	1.66197	-5.07091
H	2.49247	2.54375	-1.57991
H	3.85947	4.11061	-2.94745
C	-2.21828	-1.62919	-5.37785
C	-2.91631	-0.86110	-4.43252
C	-2.21182	-0.12729	-3.46003
C	-0.11032	-0.93566	-4.37208
C	-0.81237	-1.66692	-5.34248
H	-2.76841	-2.20234	-6.14201
H	-4.01817	-0.83035	-4.44771
H	-2.76792	0.45260	-2.70832
H	0.99129	-0.97627	-4.35950
H	-0.25584	-2.27174	-6.07713
C	-4.10101	-3.31975	0.55383
C	-4.02143	-2.70110	1.81311
C	-3.23401	-1.54990	1.98885
C	-2.58215	-1.64275	-0.35410
C	-3.37364	-2.79136	-0.52713
H	-4.73208	-4.21281	0.41495
H	-4.58359	-3.11041	2.66848
H	-3.19552	-1.07371	2.98100
H	-2.00310	-1.24853	-1.20045
H	-3.43026	-3.26648	-1.52041
C	-3.29161	2.75030	4.77207
C	-4.13119	2.23315	3.76926
C	-3.58421	1.53311	2.68142
C	-1.35165	1.86129	3.59343
C	-1.90260	2.56383	4.67931
H	-3.72174	3.29846	5.62593
H	-5.22275	2.37309	3.83417
H	-4.25826	1.13335	1.90545
H	-0.25973	1.73167	3.53504
H	-1.23707	2.96679	5.46014
C	-0.86822	-6.23274	-0.81028
C	-0.82566	-5.45499	1.60684
C	0.67319	-7.34080	0.85515
H	-1.59662	-6.20291	1.89687
H	-1.36599	-4.51738	1.34676
H	-0.19438	-5.25796	2.50137
H	1.29764	-7.75834	0.03826
H	-0.11592	-8.08131	1.11082
H	1.33222	-7.20923	1.73918
H	-1.64696	-6.99455	-0.58396
H	-0.27002	-6.60470	-1.67069
H	-1.39363	-5.30581	-1.13147
C	4.15429	-2.52272	3.74779
H	4.90857	-0.87321	2.60149
H	0.85519	-3.41492	4.15458

C	3.01546	-3.24615	4.19268
H	3.15017	-4.12167	4.84795
H	5.16206	-2.84017	4.05900
C	1.68440	4.69689	0.88336
C	2.10816	7.50655	0.69992
C	1.74270	6.76568	-0.43758
C	1.53723	5.37964	-0.34897
C	2.07790	5.45680	2.01603
C	2.28150	6.84148	1.92705
H	2.26990	8.59427	0.62813
H	1.62830	7.27116	-1.41128
H	1.29348	4.80472	-1.25505
H	2.21610	4.94702	2.98442
H	2.57938	7.40705	2.82490
C	0.61903	2.42630	0.41931
H	2.14247	2.80207	1.83220
H	4.33764	0.54924	1.48769

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-92.18	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	12.73	0.12834	YES	YES
9	a	17.88	0.02155	YES	YES
10	a	20.85	0.21809	YES	YES
11	a	24.04	0.62944	YES	YES
12	a	28.73	0.09850	YES	YES
13	a	30.92	0.40806	YES	YES
14	a	33.33	0.15779	YES	YES
15	a	36.25	0.32461	YES	YES
16	a	37.99	0.12684	YES	YES
17	a	40.50	0.27105	YES	YES
18	a	45.18	0.49725	YES	YES
19	a	49.85	0.30288	YES	YES
20	a	52.01	0.01739	YES	YES
21	a	54.67	0.03895	YES	YES
22	a	58.10	0.07679	YES	YES
23	a	61.09	0.67997	YES	YES
24	a	64.06	0.25050	YES	YES
25	a	67.00	1.22445	YES	YES
26	a	68.92	1.16885	YES	YES
27	a	73.96	0.07827	YES	YES
28	a	77.89	0.54705	YES	YES
29	a	81.95	0.29799	YES	YES
30	a	87.93	0.82767	YES	YES
31	a	95.51	0.09481	YES	YES
32	a	97.09	0.87546	YES	YES
33	a	101.79	1.03044	YES	YES

34	a	114.52	0.40540	YES	YES
35	a	116.10	0.59890	YES	YES
36	a	122.74	1.37390	YES	YES
37	a	129.52	3.48535	YES	YES
38	a	139.45	2.46874	YES	YES
39	a	154.17	1.25833	YES	YES
40	a	162.98	2.82347	YES	YES
41	a	171.06	1.01518	YES	YES
42	a	182.79	3.42321	YES	YES
43	a	188.28	0.90400	YES	YES
44	a	199.32	0.62705	YES	YES
45	a	207.30	3.00772	YES	YES
46	a	210.46	0.16947	YES	YES
47	a	211.20	0.55858	YES	YES
48	a	215.68	5.52838	YES	YES
49	a	217.13	2.14724	YES	YES
50	a	221.36	1.97425	YES	YES

./TS1718

BP86_SV(P) energy (au): -3254.4984170890

PBE0/def2-TZVPP energy (au): -3253.997115693
cosmo_dcm Total energy + OC corr. = -3254.0494311333

Zero point energy (au): 0.8906639
Entropy (kJ mol^-1): 1.33566
Chemical potential (kJ mol^-1): 2093.55

XYZ coordinates:

114

C	-1.42477	3.82408	0.92729
C	-2.04630	3.66934	-0.35324
C	-2.22615	3.15382	1.90677
C	-3.27073	2.91893	-0.15771
C	-3.38267	2.60245	1.22428
H	-0.49162	4.36535	1.12410
H	-1.70319	4.10667	-1.29749
H	-2.04163	3.12722	2.98781
H	-4.00218	2.67514	-0.93838
H	-4.22153	2.08108	1.70187
Ru	-1.48467	1.60372	0.44508
C	1.59104	2.32660	0.75318
C	-1.95352	-1.91070	1.78483
P	-1.58112	-0.08922	2.00866
C	-2.43630	0.33864	3.59114
C	0.20170	-0.34548	2.47783
C	0.73898	-1.15214	3.45176
N	1.01038	0.19194	1.48217
C	2.14131	-1.45238	3.44072
C	2.89994	-1.09091	2.27103
C	2.22597	-0.36541	1.22530
O	2.74155	-0.25310	0.01365
C	-2.69609	-0.97714	-1.71334
P	-1.50433	0.47292	-1.61149
C	-2.23478	1.58723	-2.94239
C	-0.03647	-0.20138	-2.65101
C	-0.31081	-0.35017	-4.02400
N	1.15278	-0.61076	-2.11922
C	0.64378	-0.93692	-4.86905
C	1.83469	-1.40624	-4.33016
C	2.05089	-1.24488	-2.93788
N	3.20577	-1.74283	-2.33282
C	4.24682	-2.48586	-2.92123
C	5.36628	-2.90630	-1.93464
O	4.27196	-2.77342	-4.11034
H	0.08535	-1.59609	4.21865
H	-1.27153	-0.01636	-4.43735
H	0.44424	-1.04154	-5.94832
H	2.60850	-1.90088	-4.92925

H	3.28539	-1.56110	-1.32436
C	4.27652	-1.43765	2.18573
C	2.79278	-2.16029	4.48706
C	-3.30535	3.34065	-4.90167
C	-4.11861	2.36792	-4.29972
C	-3.58796	1.49366	-3.33192
C	-1.42399	2.56636	-3.56108
C	-1.95160	3.43248	-4.53197
H	-3.72013	4.01890	-5.66494
H	-5.17793	2.27487	-4.59054
H	-4.24219	0.72556	-2.89070
H	-0.35325	2.63630	-3.31168
H	-1.29634	4.17944	-5.00969
C	-4.69095	-2.99312	-1.80751
C	-4.84337	-1.88737	-0.95423
C	-3.84939	-0.89719	-0.90011
C	-2.55346	-2.09337	-2.56521
C	-3.54034	-3.09435	-2.60599
H	-5.46528	-3.77666	-1.84571
H	-5.73960	-1.79830	-0.31834
H	-3.95785	-0.04428	-0.20936
H	-1.66504	-2.20376	-3.20472
H	-3.40555	-3.96139	-3.27356
C	-2.25823	-4.69840	1.40741
C	-2.89163	-4.05690	2.48349
C	-2.73661	-2.67227	2.67851
C	-1.31629	-2.56646	0.70785
C	-1.46343	-3.94869	0.52216
H	-2.37953	-5.78389	1.25924
H	-3.50955	-4.63734	3.18821
H	-3.22156	-2.19764	3.54471
H	-0.68756	-1.99238	0.00764
H	-0.95760	-4.44355	-0.32280
C	-3.81359	1.13653	5.93191
C	-4.52592	0.61977	4.83563
C	-3.84432	0.22806	3.67140
C	-1.73057	0.86644	4.69449
C	-2.41640	1.26136	5.85643
H	-4.34909	1.44556	6.84408
H	-5.62269	0.52156	4.88467
H	-4.41974	-0.17241	2.81976
H	-0.63572	0.98177	4.64825
H	-1.85030	1.67111	6.70894
C	6.06923	-1.63055	-1.40409
C	6.38102	-3.77301	-2.70401
C	4.76547	-3.73277	-0.77022
H	7.21257	-4.06794	-2.02747
H	6.80678	-3.22333	-3.56872
H	5.90576	-4.69562	-3.09896
H	4.05769	-3.15138	-0.13863
H	5.58082	-4.08744	-0.10177
H	4.22806	-4.62945	-1.14997
H	6.87833	-1.91086	-0.69370
H	5.37119	-0.94464	-0.87525
H	6.53340	-1.05761	-2.23623
C	4.89168	-2.10641	3.24078
H	4.85510	-1.14202	1.29875
H	2.21285	-2.45338	5.37716

C	4.14607	-2.47493	4.39082
H	4.64374	-3.01357	5.21350
H	5.96452	-2.35052	3.18442
C	1.74693	3.63829	0.11608
C	2.19081	6.18652	-1.07089
C	1.40455	5.22196	-1.72804
C	1.18471	3.96850	-1.14057
C	2.56288	4.61392	0.74997
C	2.77162	5.87384	0.17136
H	2.35935	7.17384	-1.53074
H	0.96543	5.45092	-2.71347
H	0.57998	3.20818	-1.65394
H	3.03107	4.37557	1.72050
H	3.39774	6.61754	0.69118
C	0.54656	1.42144	0.76152
H	2.48218	2.05857	1.35726
H	1.97271	-0.16039	-0.73752

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-45.01	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	11.26	1.06556	YES	YES
9	a	12.42	0.05279	YES	YES
10	a	18.98	1.39504	YES	YES
11	a	27.50	0.15740	YES	YES
12	a	35.78	0.73753	YES	YES
13	a	37.00	0.27016	YES	YES
14	a	40.20	0.28194	YES	YES
15	a	42.69	0.72575	YES	YES
16	a	47.37	0.53466	YES	YES
17	a	47.97	0.39370	YES	YES
18	a	53.33	2.04213	YES	YES
19	a	56.70	1.01575	YES	YES
20	a	57.85	0.25750	YES	YES
21	a	64.27	0.96143	YES	YES
22	a	66.62	0.35573	YES	YES
23	a	67.54	0.53459	YES	YES
24	a	73.55	0.22925	YES	YES
25	a	75.07	0.79721	YES	YES
26	a	77.01	0.29759	YES	YES
27	a	80.40	1.49929	YES	YES
28	a	88.08	0.04655	YES	YES
29	a	94.80	0.30210	YES	YES
30	a	98.48	0.06158	YES	YES
31	a	98.60	0.37843	YES	YES
32	a	108.37	0.20371	YES	YES
33	a	120.27	2.05959	YES	YES

34	a	121.65	0.19435	YES	YES
35	a	132.41	3.05197	YES	YES
36	a	145.24	1.14761	YES	YES
37	a	147.97	10.91648	YES	YES
38	a	164.91	3.25587	YES	YES
39	a	171.03	1.19923	YES	YES
40	a	182.01	1.03063	YES	YES
41	a	187.95	3.35773	YES	YES
42	a	191.28	0.80293	YES	YES
43	a	195.99	1.66042	YES	YES
44	a	204.86	1.87792	YES	YES
45	a	209.23	1.51218	YES	YES
46	a	210.72	1.54966	YES	YES
47	a	217.69	1.09026	YES	YES
48	a	219.44	3.02722	YES	YES
49	a	224.00	2.17868	YES	YES
50	a	226.05	2.29493	YES	YES

./TS1815

BP86_SV(P) energy (au): -3254.5126766050

PBE0/def2-TZVPP energy (au): -3254.004646051
cosmo_dcm Total energy + OC corr. = -3254.0568191662

Zero point energy (au): 0.8878974
Entropy (kJ mol^-1): 1.34141
Chemical potential (kJ mol^-1): 2085.40

XYZ coordinates:

114

C	3.41064	0.77647	-1.18262
C	2.78331	0.90318	-2.46601
C	3.31468	2.02261	-0.48942
C	2.29558	2.25749	-2.57261
C	2.60971	2.94468	-1.35695
H	3.89522	-0.13055	-0.80227
H	2.75101	0.13694	-3.24900
H	3.74249	2.25512	0.49347
H	1.80342	2.69544	-3.45092
H	2.42126	4.00506	-1.15042
Ru	1.19619	1.28258	-0.86386
C	1.95557	-1.48015	0.53109
C	-1.37973	3.00950	1.32282
P	0.34956	2.38800	0.98047
C	1.42649	3.77371	1.58252
C	0.37981	1.12294	2.32584
C	0.10652	1.42658	3.63747
N	0.49797	-0.18617	1.86703
C	-0.07610	0.38619	4.60651
C	-0.08716	-0.95951	4.13271
C	0.12413	-1.26185	2.70902
O	0.00006	-2.42091	2.26360
C	-2.11287	2.22317	-2.04259
P	-0.69490	1.02484	-2.15688
C	-0.37535	1.05820	-4.00547
C	-1.49479	-0.67366	-2.05257
C	-2.40314	-1.09987	-3.02629
N	-1.05834	-1.50640	-1.07094
C	-2.89973	-2.41460	-2.94867
C	-2.44653	-3.26961	-1.95192
C	-1.48371	-2.80865	-1.00649
N	-0.96140	-3.62854	-0.02484
C	-1.02734	-5.04881	-0.04713
C	-0.52249	-5.78892	1.21376
O	-1.48282	-5.65076	-1.01068
H	-0.02121	2.47902	3.93384
H	-2.70110	-0.42610	-3.84233
H	-3.63905	-2.77497	-3.68258
H	-2.78440	-4.30923	-1.89014

H	-0.48495	-3.15453	0.78214
C	-0.31074	-2.02395	5.03985
C	-0.29402	0.63584	5.98801
C	0.22948	1.10513	-6.77564
C	-0.42360	2.19230	-6.17442
C	-0.72935	2.16930	-4.80109
C	0.27736	-0.03376	-4.62292
C	0.57439	-0.01236	-5.99487
H	0.46319	1.12292	-7.85241
H	-0.71056	3.06902	-6.77783
H	-1.25881	3.02692	-4.35815
H	0.54534	-0.92531	-4.03328
H	1.07586	-0.87792	-6.45812
C	-4.12289	4.21473	-2.02209
C	-2.76873	4.57933	-1.93026
C	-1.77237	3.59009	-1.93197
C	-3.47516	1.86699	-2.12694
C	-4.47184	2.85754	-2.11337
H	-4.90683	4.98927	-2.01475
H	-2.48654	5.64153	-1.84835
H	-0.71088	3.87739	-1.84128
H	-3.77815	0.81092	-2.18606
H	-5.53194	2.56161	-2.17362
C	-4.02566	3.68972	2.06100
C	-2.98220	4.60974	2.24331
C	-1.66473	4.27259	1.88331
C	-2.43712	2.08960	1.14454
C	-3.74760	2.42463	1.51297
H	-5.05534	3.95311	2.35290
H	-3.18619	5.60024	2.68240
H	-0.86092	5.00050	2.06842
H	-2.23220	1.08747	0.73173
H	-4.55792	1.69028	1.37593
C	3.13663	5.89729	2.35427
C	2.18212	6.09253	1.34053
C	1.33838	5.03831	0.95277
C	2.39322	3.58667	2.59408
C	3.24180	4.64186	2.97488
H	3.79930	6.72388	2.65767
H	2.09325	7.07349	0.84552
H	0.60129	5.20924	0.15011
H	2.48866	2.60937	3.09268
H	3.98977	4.47725	3.76756
C	-1.42498	-5.39868	2.41326
C	0.95712	-5.44073	1.50752
C	-0.64644	-7.30284	0.94880
H	1.31214	-6.05222	2.36690
H	1.09256	-4.37396	1.77952
H	1.60586	-5.67489	0.63532
H	-1.69423	-7.59311	0.72620
H	-0.30811	-7.86419	1.84700
H	-0.02399	-7.61690	0.08448
H	-1.11245	-5.97681	3.31133
H	-2.49073	-5.64495	2.20952
H	-1.34481	-4.31917	2.65759
C	-0.51195	-1.75952	6.39522
H	-0.31552	-3.05402	4.65375
H	-0.29611	1.67590	6.35360

C	-0.50573	-0.42446	6.86861
H	-0.67136	-0.22290	7.93967
H	-0.67884	-2.59015	7.09966
C	2.55086	-2.31495	-0.50645
C	3.77251	-4.08071	-2.37817
C	2.71745	-3.23674	-2.77710
C	2.12564	-2.35981	-1.86123
C	3.60724	-3.18864	-0.12231
C	4.21730	-4.04862	-1.04517
H	4.24214	-4.76321	-3.10489
H	2.35722	-3.26611	-3.81868
H	1.31570	-1.69134	-2.18597
H	3.94748	-3.18850	0.92710
H	5.03894	-4.70744	-0.72002
C	0.99907	-0.46464	0.48239
H	2.31021	-1.77140	1.53791
H	-0.06335	-0.96185	-0.34220

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-1144.65	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	6.78	0.01628	YES	YES
9	a	14.72	0.09105	YES	YES
10	a	26.14	0.20701	YES	YES
11	a	30.44	0.34554	YES	YES
12	a	33.54	0.84164	YES	YES
13	a	34.27	0.39943	YES	YES
14	a	39.35	0.08502	YES	YES
15	a	44.77	0.67463	YES	YES
16	a	47.68	0.09544	YES	YES
17	a	48.24	0.25591	YES	YES
18	a	53.63	0.64612	YES	YES
19	a	55.09	0.23299	YES	YES
20	a	57.02	0.14725	YES	YES
21	a	58.94	0.29520	YES	YES
22	a	62.08	0.38446	YES	YES
23	a	68.16	0.15759	YES	YES
24	a	72.47	0.10009	YES	YES
25	a	75.35	0.46610	YES	YES
26	a	82.69	0.81220	YES	YES
27	a	84.24	1.51308	YES	YES
28	a	86.28	0.30637	YES	YES
29	a	90.56	0.27424	YES	YES
30	a	100.36	0.81920	YES	YES
31	a	107.07	1.80316	YES	YES
32	a	111.41	0.36433	YES	YES
33	a	121.04	0.40409	YES	YES

34	a	124.45	1.02790	YES	YES
35	a	131.16	0.23820	YES	YES
36	a	146.45	1.82398	YES	YES
37	a	152.99	1.84538	YES	YES
38	a	163.72	4.23607	YES	YES
39	a	166.11	0.27952	YES	YES
40	a	178.11	1.75778	YES	YES
41	a	185.36	1.27844	YES	YES
42	a	191.97	3.15812	YES	YES
43	a	194.02	0.34761	YES	YES
44	a	201.33	2.58139	YES	YES
45	a	204.04	0.17809	YES	YES
46	a	206.90	1.28058	YES	YES
47	a	210.74	0.28157	YES	YES
48	a	217.83	1.21860	YES	YES
49	a	220.68	0.99721	YES	YES
50	a	227.43	1.13106	YES	YES

References

1. F. Chevallier and B. Breit, *Angewandte Chemie International Edition*, 2006, 45, 1599-1602.
2. A. Ali, M. Hussain, I. Malik, A. Villinger, C. Fischer and P. Langer, *Helvetica Chimica Acta*, 2010, 93, 1764-1772.
3. R. C. Clark and J. S. Reid, *Acta Crystallographica Section A*, 1995, 51, 887-897.
4. J. J. P. Stewart, L. P. Davis and L. W. Burggraf, *J. Comput. Chem.*, 1987, 8, 1117-1123.
5. S. A. Maluendes and M. Dupuis, *J. Chem. Phys.*, 1990, 93, 5902-5911.
6. P. Csaszar and P. Pulay, *Journal of Molecular Structure*, 1984, 114, 31-34.
7. R. Ahlrichs, M. Bar, M. Haser, H. Horn and C. Kolmel, *Chemical Physics Letters*, 1989, 162, 165-169.
8. K. Eichkorn, O. Treutler, H. Ohm, M. Haser and R. Ahlrichs, *Chemical Physics Letters*, 1995, 240, 283-289.
9. O. Treutler and R. Ahlrichs, *Journal of Chemical Physics*, 1995, 102, 346-354.
10. K. Eichkorn, F. Weigend, O. Treutler and R. Ahlrichs, *Theoretical Chemistry Accounts*, 1997, 97, 119-124.
11. M. v. Arnim and R. Ahlrichs, *The Journal of Chemical Physics*, 1999, 111, 9183-9190.
12. P. Deglmann and F. Furche, *Journal of Chemical Physics*, 2002, 117, 9535-9538.
13. P. Deglmann, F. Furche and R. Ahlrichs, *Chemical Physics Letters*, 2002, 362, 511-518.
14. P. Deglmann, K. May, F. Furche and R. Ahlrichs, *Chemical Physics Letters*, 2004, 384, 103-107.
15. W. M. Haynes, *CRC Handbook of Chemistry and Physics ISBN 1439820775* 2010.