Supplementary Information

DLPNO-CCSD(T) and DFT study of the acetate-assisted C-H activation of benzaldimine at [$RuCl_2$(*p*-cymene)]$_2$: relevance of the ligand exchange processes at ruthenium(II) complexes in polar protic media

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Rationale for the selection of methods

DFT methods. It would be desirable to have a benchmark of the performance of DFT methods for reproducing the geometry of ruthenium(II) complexes in methanol solution. However, the lack of the experimental data required as reference make such assessment unfeasible. Guided by previous benchmarks for ruthenium complexes,[1] we have assessed in vaccum the performance of 12 DFT methods for reproducing selected distances of the coordination center for a small set of ruthenium(II) complexes (whose structures have been determined by X-ray diffraction analysis) by using an affordable double-ζ basis set with a pseudopotential for ruthenium. The evaluation set included 3 cycloruthenated complexes derived from Schiff bases (with Cambridge Structural Database (CSD) deposit codes MEJYOR, MEJYUX and ZUGVUU) and the intermediate chloro-acetate(*p*-cymene)ruthenium complex **B[1]** (with CSD deposit code OMATUR), as depicted in Figure S1. Among the selected DFT methods, we considered 5 standard functionals not including dispersion (BP86,[2] RevTPSS,[3] B3LYP,[4] PBE0 [5] and ωB97X,[6] 2 functionals designed to include dispersion effects at an electronic level (M06 [7] and MN15 [8]) and 7 DFT methods adding dispersion energy corrections in the protocol (BP86-D3(BJ), B3LYP-D3(BJ), PBE0-D3(BJ), TPSS-D3(BJ) and ωB97X-D3 [9]). With this purpose, the coordinates from the crystal structures were subjected to DFT geometry optimization in the gas phase using the cc-pVDZ-PP[Ru] basis set (see Computational methods for a description) and the computed distances for 12 ruthenium-ligand bonds (Ru-C, Ru-N, Ru-O and Ru-Cl) were compared to the corresponding bond distances determined by X-ray diffraction analysis (see Table S1). The best performances were observed for ωB97X-D3 and M06 functionals, which showed the smallest mean unsigned errors (MUE) for the selected interatomic distances (MUEs close to 0.008 Å).[10] BP86, B3LYP, and RevTPSS optimized bond distances also agreed satisfactorily with the reference values (with MUEs lower than 0.01 Å). The largest deviation from experiment were associated to MN15 and PBE0 functionals (MUEs close to of 0.02 Å). Inclusion of the Grimme´s model for dispersion correction with the original D3 [11] or the Becke-Johnson damping function (D3(BJ)) [12] to M06 or B3LYP had small effects on the calculated distances but, going from BP86, PBE0 or RevTPSS to BP86-D3(BJ), PBE0-D3(BJ) and TPSS-D3(BJ), respectively, the agreement between the calculated and the experimental distances was clearly reduced.[13] For ωB97X-D3, the best performing functional, the change of the basis set and ruthenium pseudopotential from cc-pVDZ-PP[Ru] to def2-SVP reduced the agreement of the computed distances with the experimental ones (MUE increased from 0.0079 to 0.0113 Å). Thus, among the best performers, we considered the

M06 as the functional of choice, due to its broad success for the estimation stabilities of conformers, binding energies and barrier heights in transition metal chemistry,[14] particularly in the area of ruthenium-based catalysts.[15] Also selected ωB97X-D3 as a suitable functional for comparison purposes, due to its accuracy for the evaluation of non-covalent interactions and its performance for the thermodynamic and kinetic estimations according to MOR41 [16] and MOBH35 [17] benchmark databases.

Solvation models. Looking for a compromise between computational cost and accuracy, we have selected the conductor-like polarizable continuum (CPCM) solvation model for performing the geometry optimizations. CPCM model is integrated in all parts of ORCA program, including analytical calculation of hessians and frequencies. Conversely, analytical hessians and frequencies are not yet implemented for the solvation model based on density (SMD) and its necessary to switch to the numerical calculation. It is well known that calculations of numerical frequencies are inherently less accurate and quite more expensive than the analytical ones. This can become a very important limitation for studies challenging many reaction manifolds, where a considerable number of intermediates have to be characterized in multiple conformations. This issue may also become critical for the location of transition state structures, usually requiring several evaluations of the hessian in the protocol. In addition, we expected small changes in our benchmark energies when switching between SMD and CPCM models for geometry optimization, as structural changes resulting from the use of different DFT methods (and/or basis sets) in geometry optimization has been reported to produce a small impact in the DLPNO-CCSD(T) energies, usually lower than 1 kcal/mol (see reference 40c in the main article). Trying to maintain simplicity and consistency in our computational scheme, we also selected the CPCM solvation model for the final single point energy calculations. Nevertheless, as the SMD solvation model provides a more realistic description of the non-electrostatic solute-solvent interactions and is recommended for the estimation of the solvation energies of charged species, we also performed benchmark energy evaluations with the SMD model and compared them with the results using the CPCM model.

Refined DFT energy evaluations. We considered three double-hybrid functionals, B2K-PLYP,[18] B2GP-PLYP [19] and PWPB95 [20] (alone and including D3(BJ) or D4 dispersion energy corrections) which were shown to outperform to most of the tested DFT methods in the MOR41 and the MOBH35 databases and were reported as especially suitable for transition metal thermochemistry. We also selected one hybrid GGA and two hybrid meta-GGA DFT methods of lower computational cost with

different schemes for the treatment of the dispersion corrections. Thus, we considered PBE0-D3BJ (with atom-pairwise Grimme´s dispersion corrections with a Becke-Johnson damping scheme), *w*B97M-V [21] (range-separated hybrid with VV10 non-local correlation), and highly parameterized M06-2X [22] (constructed to account for dispersion). The two last were recommended for systems where non-covalent interactions, hydrogen bonds or interactions between ions and aromatic rings may be of relevance,[23] while the two first functionals are among the best hybrid DFT methods according to the MOR41 or MOBH35 benchmark databases.

Computational methods

Full geometry optimizations for all the molecular structures were performed in the self-consistent reaction field [24] of implicit methanol with two different hybrid functionals, M06 [7] and ωB97X-D3 [8], using the cc-pVDZ-PP[Ru] basis set (see below for a description). Calculations with the M06 method were performed with GAUSSIAN 16 [25] program using the integral equation formalism variant for the polarizable continuum model (IEF-PCM) [26] while those made with the ωB97X-D3 method were performed with the ORCA program (version 5.0.3) [27] and the conductor like polarizable continuum model (CPCM).[28] For all the located stationary points different orientations of the *p*-cymene ring were assessed and the lowest energy structures and energies are reported. Vibrational frequencies were calculated analytically at the same level to ensure that each minimum was a true local minimum (only positive frequencies) and that each transition structure had only a single imaginary frequency (negative eigenvalue in the Hessian matrix, associated with the normal mode connecting reactant to product). These calculations were also used to extract thermodynamic corrections. Intrinsic Reaction Coordinates (IRC) [29] were employed to verify the connection of relevant transition structures to the respective minima.

The difference between the Gibbs and electronic energies (G-E) were determined at two different conditions. Since entropic contribution calculated within the ideal gas approximation at 1 atm is likely exaggerating the expected values in the condensed phase, the thermochemical analysis was first performed including a correction for the change in standard state from gas phase at 1 atm to 1 M. To further model the reduction of the translational degrees of freedom at the concentration of liquid solvent, a second thermochemical analysis was performed following the proposal by Martin, Hay and Pratt.[30] With this purpose, the necessary pressure parameter was derived from P = (*d*/M)*RT (where M and *d* are the molar mass and the density of the solvent, respectively, and T is the temperature) by using M = 32.04 g/mol and *d* = 787 g/L for liquid methanol. Thus, a second set of entropy corrections was obtained at condensed phase with a pressure parameter of 601 atm to achieve a methanol concentration of 24.56 M. In all calculations a quasi-harmonic-oscillator approximation (qh) was used in which the treatment of the vibrational entropies switches from the standard rigid-rotor-harmonic-oscillator model to a free rotor description for frequencies below 100 cm^{-1}, as first proposed by Grimme.[31]All these thermodynamic corrections were calculated at T = 298.15 K, by using ORCA or applying the GoodVibes program [32] to the output files generated by GAUSSIAN 16.

Refined energies were obtained from single-point energy calculations with ORCA (version 5.0.3) at the DLPNO-CCSD(T) [33] level of theory, using the accurate iterative (T_1) algorithm for the perturbative triples correction [34] and the NormalPNO threshold settings,[35] with the energies extrapolated to the complete basis set limit (CBS). SCF energies were extrapolated with the method of Petersson *et al* [36] by using the cc-pVTZ-PP[Ru] and cc-pVQZ-PP[Ru] basis sets, while the correlation energies were extrapolated with the method of Helgaker *et al* [37] by using the cc-pVDZ-PP[Ru] and cc-pVTZ-PP[Ru] basis sets. The optimum values for the parameters required in the CBS extrapolations (α(3/4) = 5.46 and β(2/3) = 2.46) were taken from the literature.[38] Additional single-point energy evaluations were performed with ORCA (version 4.2.1) [39] using the PWPB95,[20] B2GP-PLYP,[19] B2K-PLYP,[18] *w*B97M-V,[21] M06-2X [22] and PBE0 [5] functionals with the aug-cc-pVTZ-PP[Ru] basis set. The atom-pairwise Grimme´s dispersion corrections with either the Becke-Johnson damping scheme (D3BJ) [12] or the 4th generation charge dependent scheme (D4) [40] were calculated for the PBE0 and PWP95 functionals using the DFT-D3 (version 3.1) and DFT-D4 (version 2.5) programs, respectively. All the single point energy evaluations were performed with implicit solvation in methanol (by using CPCM or SMD solvation models).[28] Thus, all energies given in text are quasi-harmonic Gibbs energies of solutes in the solution phase, which were calculated by adding the qh-G corrections to the refined single point energies calculated in solution.

With cc-pVDZ-PP[Ru], cc-pVTZ-PP[Ru], cc-pVQZ-PP[Ru] and aug-cc-pVTZ-PP[Ru] basis sets, C, H, Cl, N and O atoms were described with the Dunning´s correlation-consistent polarized double-, triple-, quadruple- or augmented triple-ζ basis sets [41] (cc-pVDZ, cc-pVTZ, cc-pVQZ or aug-cc-pVTZ keywords, respectively), while the inner electrons of Ru were described by the Stuttgart/Cologne fully relativistic effective core potential (ECP28MDF, replacing 28 core electrons) and the outer electrons of Ru were described by the associated double-, triple-, quadruple- or augmented triple-ζ basis set (ECP28MDF_VDZ, ECP28MDF_VTZ, ECP28MDF_VQZ or ECP28MDF_AVTZ, using the cc-pVDZ-PP, cc-pVTZ-PP, cc-pVQZ-PP or aug-cc-pVTZ-PP keywords).[42,43]

Calculations in ORCA were performed with “TightSCF” convergence criteria and the default frozen-core approximation for the MP2 part. To speed up the SCF calculations, resolution-of-identity (RI) method [44] was used with def2/J,[45] cc-pVnZ/C and cc-pVnZ-PP/C (where n = D, T or Q) or aug-cc-pVTZ/C and aug-cc-pVTZ-PP/C auxiliary basis sets [46] in conjunction with the RIJCOSX [47] approximation. DFT integration grids with 99 radial and 590 angular points were used in GAUSSIAN 16 (“ultrafine” integration grid) and the equivalent “Grid6” and “GridX6” were used with ORCA 4.2.1.

References

1 (a) J. P. Cerón-Carrasco, J. Ruiz, C. Vicente, C. de Haro, D. Bautista, J. Zúñiga and A. Requena *J. Chem. Theory Comput.* **2017**, *13*, 3898−3910. (b) A. Poater, E. Pump, S. V. C. Vummaleti, and L. Cavallo *J. Chem. Theory Comput.* **2014**, *10*, 4442−4448. (c) Y. Minenkov, A. Singstad, G. Occhipinti, and V. R. Jensen, *Dalton Trans.* **2012**, *41*, 5526−5541. (d) A. D. Kulkarni and D. G. Truhlar *J. Chem. Theory Comput.* **2011**, *7*, 2325–2332.

2 (a) A. D. Becke *Phys. Rev. A*, **1988**, 38, 3098-3100. (b) J. P. Perdew *Phys. Rev. B*, **1986**, 33, 8822-8824.

3 (a) J. P. Perdew, A. Ruzsinsky, G. I. Csonka, L. A. Constantin, and J. Sun, *Phys. Rev. Lett.* **2009**, *103*, 026403. (b) J. P. Perdew, A. Ruzsinsky, G. I. Csonka, L. A. Constantin, and J. Sun, *Phys. Rev. Lett.* **2011**, *106*, 179902.

4 P. J. Stephens, F. J. Devlin, C. F. Chabalowski, and M. J. Frisch, *J. Phys. Chem.* **1994**, *98*, 11623-11627.

5 C. Adamo and V. Barone *J. Chem. Phys.*, **1999**, *110*, 6158-6170.

6 J.-D. Chai and M. Head-Gordon *J. Chem. Phys.* **2008**, *128*, 084106.

7 Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, **2008**, *120*, 215-241.

8 H. S. Yu, X. He, S. L. Li, and D. G. Truhlar *Chemical Science* **2016**, *7*, 5032-5051.

9 S. Dohm, A. Hansen, M. Steinmetz, S. Grimme, and M. P. Checinski. *J. Chem. Theory Comput.* **2018**, *14*, 2596–2608.

10 The performance of M06 and wB97BX-D for predicting structural parameters of ruthenium complexes have been previously reported superior to BP86, B3LYP or PBE0 and comparable to that achieved with MP2, see refs. 1(a), 1(b) and 1(d).

11 S. Grimme, J. Antony, S. Ehrlich, and H. Krieg *J. Chem. Phys*. **2010**, *132*, 154104S.

12 S. Grimme, S. Ehrlich and L. Goerigk *J. Comp. Chem*. **2011**, *32*, 1456-1465.

13 The inclusion of dispersion corrections (D3) on the geometry optimizations of ruthenium complexes with either BP86 or B3LYP functionals has been previously reported to give less reproducibility with respect to the experimental data, see ref. 1(b).

14 (a) M. S. G. Ahlquist, and P.-O. Norrby *Angew. Chem. Int. Ed.* **2011**, *50*, 11794-11797. (b) B. B. Averkiev, Y. Zhao, and D. G. Truhlar *J. Mol Catal. A* **2010**, *324*, 80-88. (c) Y. Minenkov, G. Occhipinti, and V. R. Jensen *J. Phys. Chem. A* **2009,** *113,* 11833–11844.

15 (a) P. Sliwa, and J. Handzlik *Chem. Phys. Lett.* **2010**, 493, 273-278. (b) I. C. Stewart, D. Benitez, D. J. O'Leary, E. Tkatchouk, M. W. Day, W. A. Goddard III, and R. H. Grubbs *J. Am. Chem. Soc.* **2009**, *131*, 1931-1938. (c)

D. Benitez, E. Tkatchouk, and W. A. Goddard III *Organometallics*, **2009**, *28*, 2643-2645. (d) Y. Zhao, and D. G. Truhlar *Acc. Chem. Res.* **2008**, *41*, 157-167.

16 S. Dohm, A. Hansen, M. Steinmetz, S. Grimme, and M. P. Checinski. *J. Chem. Theory Comput.* **2018**, *14*, 2596–2608.

17 M. A. Iron, and T. Janes, J. Phys. Chem. A **2019**, *123*, 3761-3781.

18 A. Tarnopolsky, A. Karton, R. Sertchook, D. Vuzman, and J. M. L. Martin *J. Phys. Chem.* A **2008**, *112*, 3−8.

19 A. Karton, A. Tarnopolsky, J.-F. Lamére, G. C. Schatz, and J. M. L. Martin *J. Phys. Chem.* A **2008**, *112*, 12868-12886.

20 L. Goerigk, and S. *J.* Grimme, *Chem. Theory Comput.* **2011**, *7*, 291-309.

21 (a) N. Mardirossian, and M. Head-Gordon *J. Chem. Phys.* **2016**, *144*, 214110. In ORCA dispersion is included into *ω*B97M-V functional by using the VV10 nonlocal correlation as a non-self-consistent correction to the final SCF energy. See: (b) A. Najibi, and L. Goerigk *J. Chem. Theory Comput.* **2018**, *14*, 5725−5738; (c) O. A. Vydrov, and T. Van Voorhis *J. Chem. Phys.* **2010**, *133*, 244103.

22 Y. Zhao, and D. G. Truhlar *Theor. Chem. Acc.* **2008**, *120*, 215-241.

23 (a) N. Mardirossian and M. Head-Gordon *Molecular Physics* **2017**, *115*, 2315-2372. (b) A. D. Boese *Chem. Phys. Chem* **2015**, *16*, 978-985. (c) D. Papp, P. Rovó, I. Jákli, A. G. Császár and A. Perczel *J. Comput. Chem.* **2017**, *38*, 1762-1773.

24 (a) V. Dillet, D. Rinaldi, and J. L. Rivail *J. Phys. Chem.* **1994**, *98*, 5034-5039. (b) V. Dillet, D. Rinaldi, J. Bertran, and J. L. Rivail, *J. Chem. Phys.* **1996**, *104*, 9437-9444. (c) For a review on quantum mechanical continuum solvation models, see: J. Tomasi, B. Mennucci, and R. Cammi *Chem. Rev*. **2005**, *105*, 2999-3093.

25 Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2019.

26 The IEF-PCM parameters were selected for pure methanol as solvent (dielectric constant of 32.613) and atomic radii from universal force field were used for the solute atomic radii. See: E. Cancès, B. Mennucci, and J. Tomasi, *J. Chem. Phys.* **1997**, *107,* 3032-3041.

27 F. Neese *WIREs Comput. Mol. Sci.* **2022**, *12*:e1606 (DOI: 10.1002/wcms.1606).

28 (a) V. Barone and M. Cossi *J. Phys. Chem. A*, **1998**, 102, 1995-2001. (b) A. V. Marenich, C. J. Cramer, and D. G. Truhlar *J. Phys. Chem. B* 2009, **113**, 6378–6396.

29 K. Fukui *Acc. Chem. Res.*, 1981, **14**, 363-68.

30 R. L. Martin, P. J. Hay, L. R Pratt. *J. Phys. Chem. A* 1998, **102**, 3565–3573.

31 S. Grimme *Chem. Eur. J*. **2012**, *18*, 9955–9964.

32 G. Luchini, J. V. Alegre-Requena, I. Funes-Ardoiz, R. S. Paton *F1000Research*, **2020**, *9*, 291.

33 (a) C. Riplinger and F. Neese, *J. Chem. Phys.*, **2013**, *138*, 034106. (b) C. Riplinger, P. Pinski, U. Becker, E. F. Valeev and F. Neese *J. Chem. Phys*., **2016**, *144*, 024109.

34 (a) Y. Guo, C. Riplinger, U. Becker, D. G. Liakos, Y. Minenkov, L. Cavallo, and F. Neese *J. Chem. Phys.* **2018**, *148*, 011101. (b) Y. Guo, C. Riplinger, D. G. Liakos, U. Becker, M. Saitow, and F. Neese *J. Chem. Phys.* **2020**, *152*, 024116.

35 D. G. Liakos, M. Sparta, M. K. Kesharwani, J. M. L. Martin, and F. Neese, *J. Chem. Theory Comput.* **2015**, *11*, 1525–1539.

36 S. J. Zhong, E. C. Barnes, and G. A. Petersson *J. Chem. Phys.* **2008**, *129*, 184116.

37 T. Helgaker, W. Klopper, H. Koch, and J. Noga *J. Chem. Phys.* **1997**, *106*, 9639-9646.

38 F. Neese, A. Hansen, and D. G. Liakos *J. Chem. Phys.* **2009**, *131*, 064103.

39 (a) F. Neese *Computational Molecular Science*, **2012**, *2*, 73-78; (b) Neese, F. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2017**, *8*, e1327.

40 E. Caldeweyher, S. Ehlert, A. Hansen, H. Neugebauer, S. Spicher, C. Bannwarth, and S. Grimme *J. Chem. Phys.* **2019**, *150*, 154122 (and *ChemRxiv* 2019, DOI: 10.26434/chemrxiv.7430216.v2).

41 (a) T. H. Jr. Dunning *J. Chem. Phys.*, **1989**, *90*, 1007-1023; (b) R. A. Kendall, T. H. Jr. Dunning, and R. J. Harrison *J. Chem. Phys.*, **1992**, *96*, 6796-6806; (c) D. E. Woon and T. H. Jr. Dunning *J. Chem. Phys.*, **1993**, *98*, 1358-1371.

42 K. A. Peterson, D. Figgen, M. Dolg, and H. Stoll *J. Chem. Phys.* **2007**, 126, 124101.

43 Stuttgart/Cologne effective core potentials for Ru and the associated basis set were obtained from the web of the group (http://www.tc.uni-koeln.de/PP/index.en.html) and used in the GAUSSIAN calculations via the GENECP keyword.

44 (a) K. Eichkorn, O. Treutler, H. Öhm, M. Häser, and R. Ahlrichs, *Chem. Phys. Lett.* **1995**, *240*, 283−290. (b) F. Weigend, and M. Häser *Theor. Chem. Acc.* **1997**, *97*, 331-340.

45 F. Weigend *Phys. Chem. Chem. Phys.* **2006**, *8*, 1057−1065.

46 F. Weigend, A. Kohn, and C. Hattig *J. Chem. Phys.* **2002**, *116*, 3175-3183.

47 (a) F. Neese, F. Wennmohs, A. Hansen, and U. Becker *Chem. Phys.* **2009**, *356*, 98-109. (b) R. Izsak, and F. Neese *J. Chem. Phys.* **2011**, *135*, 144105.

Figure S1. Structures derived from X-ray diffraction analysis and CSD deposit codes for the evaluation set.

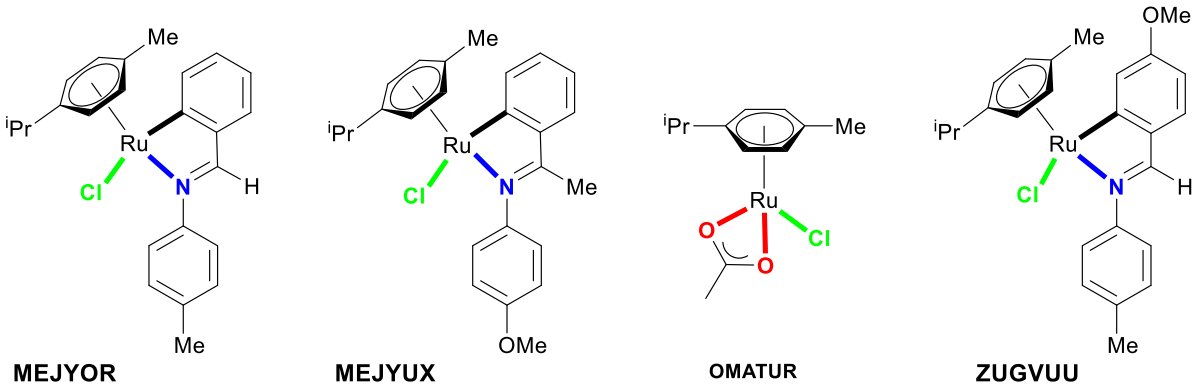
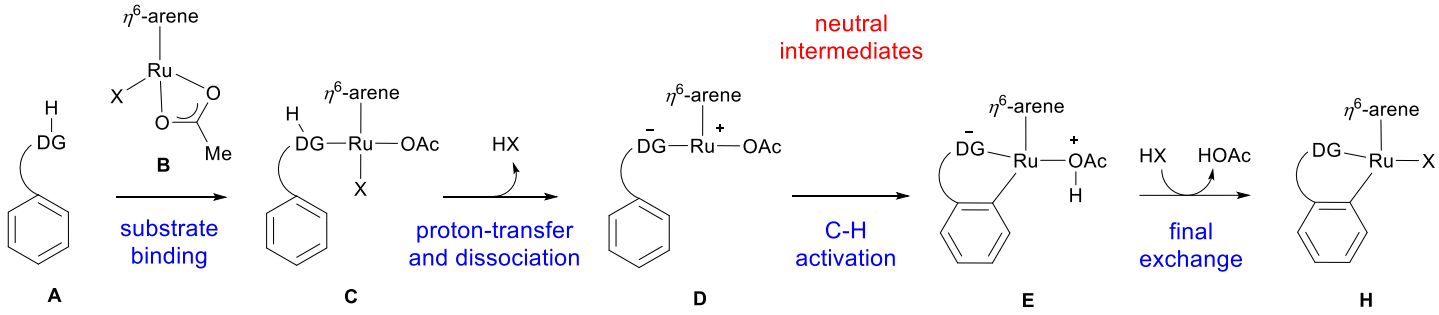


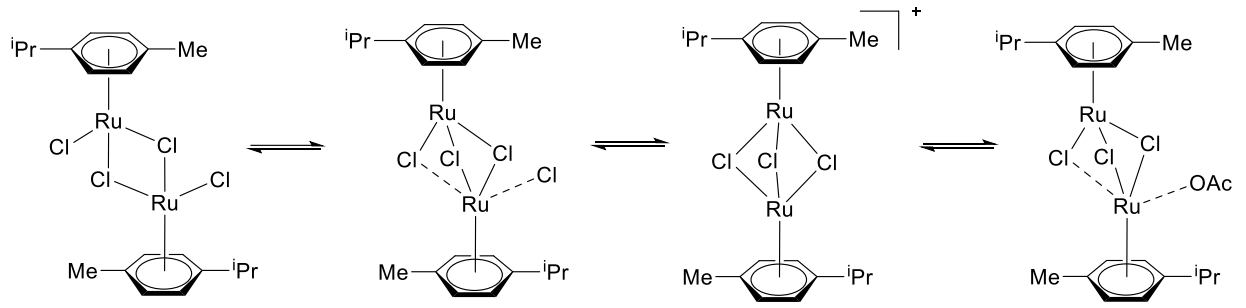
Table S1. Computed bond distances at DFT/cc-PVDZ-PP[Ru] levels and mean unsigned errors (MUEs).

METHOD	Distances (Å)												MUE (Å)
	MEJYOR			MEJYUX			OMATUR			ZUGVUU			
	Ru-C	Ru-N	Ru-Cl	Ru-C	Ru-N	Ru-Cl	Ru-O1	Ru-O2	Ru-Cl	Ru-C	Ru-N	Ru-Cl	
X-Ray	**2.0463**	**2.1115**	**2.4161**	**2.0460**	**2.1160**	**2.4150**	**2.1660**	**2.1510**	**2.3890**	**2.0480**	**2.0966**	**2.4183**	
ωB97X-D3	2.0527	2.1033	2.4146	2.0474	2.1033	2.4235	2.1512	2.1463	2.3677	2.0530	2.1043	2.4156	0.0079
M06	2.0543	2.1045	2.4242	2.0498	2.1022	2.4313	2.1620	2.1563	2.3763	2.0565	2.1092	2.4251	0.0084
M06-D3	2.0540	2.1013	2.4244	2.0481	2.1037	2.4307	2.1623	2.1565	2.3762	2.0556	2.1054	2.4255	0.0085
BP86	2.0420	2.0931	2.4177	2.0370	2.0892	2.4253	2.1560	2.1558	2.3739	2.0384	2.0811	2.4146	0.0088
B3LYP	2.0509	2.1169	2.4286	2.0443	2.1114	2.4365	2.1513	2.1528	2.3881	2.0466	2.1082	2.4257	0.0090
RevTPSS	2.0454	2.0784	2.4114	2.0459	2.0916	2.4194	2.1451	2.1418	2.3692	2.0512	2.0992	2.4143	0.0092
ωB97X	2.0598	2.1227	2.4202	2.0529	2.1197	2.4304	2.1569	2.1513	2.3733	2.0598	2.1247	2.4222	0.0103
B3LYP-D3BJ	2.0394	2.0869	2.4169	2.0364	2.0829	2.4251	2.1557	2.1469	2.3779	2.0339	2.0797	2.4135	0.0111
TPSS-D3BJ	2.0454	2.0784	2.4114	2.0432	2.0759	2.4182	2.1478	2.1418	2.3703	2.0470	2.0822	2.4125	0.0155
PBE0	2.0353	2.0893	2.3993	2.0300	2.0861	2.4063	2.1345	2.1309	2.3585	2.0369	2.0926	2.4001	0.0183
BP86-D3BJ	2.0305	2.0631	2.4065	2.0287	2.0615	2.4147	2.1579	2.1531	2.3640	2.0324	2.0684	2.4081	0.0196
MN15	2.0419	2.0799	2.3945	2.0388	2.0814	2.4000	2.1143	2.1182	2.3583	2.0432	2.0825	2.3951	0.0227
PBE0-D3BJ	2.0299	2.0732	2.3946	2.0261	2.0715	2.4015	2.1557	2.1469	2.3779	2.0309	2.0763	2.3954	0.0251

Scheme S1. Routes for C-H activation at Ru(II) arene complexes featuring a protic directing-group. (DG stands for directing-group, X stands for chloro or acetate).



Scheme S2. Initial steps for the reaction of ruthenium dimeric precursor (**B^0**) with acetate to form the monomer derivatives **B^1** and **B^2**. Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(CPCM) level (298 K, 1 M) using the geometries optimized at M06/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in blue color. The corresponding values calculated at the same level by using the geometries optimized at ωB97X-D3/cc-pVDZ-PP[Ru](CPCM) level are shown in red color and between brackets.



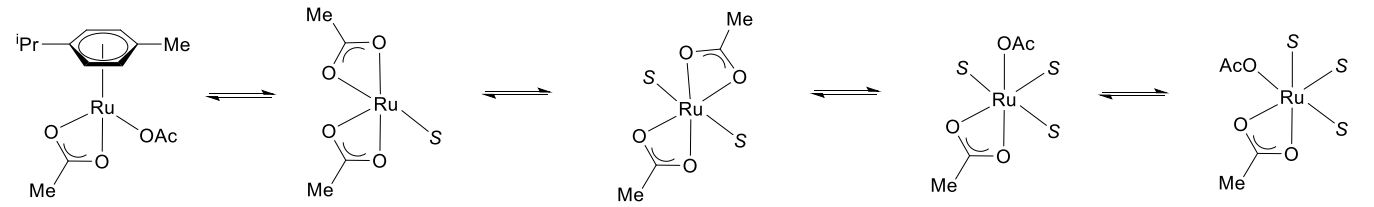
B^0
+2AcO$^-$ **0.0** [**0.0**]

TS(B^0-B^{0+})
+2AcO$^-$ **20.2** [**18.9**]

B^{0+}
+Cl$^-$+2AcO$^-$ **2.7** [**0.9**]

TS(B^0-B^{0*})
+Cl$^-$+AcO$^-$ **23.0** [**22.0**]

Scheme S3. Solvent-assisted dissociation of *p*-cymene from **B^2** to form free *p*-cymene and mono-, di- or three-solvated $Ru(OAc)_2$ complexes. Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(CPCM) level (298 K, 1 M) on the geometries optimized at M06/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in blue color. The corresponding values calculated at the same level at condensed phase (298 K, 24.6 M) are shown in green color. *S* stands for solvent (MeOH) and *p*-cym for the *p*-cymene ligand.



B^2
+3*S*+2Cl$^-$ **-12.2**
+3*S*+2*S*•Cl$^-$ **-13.5**

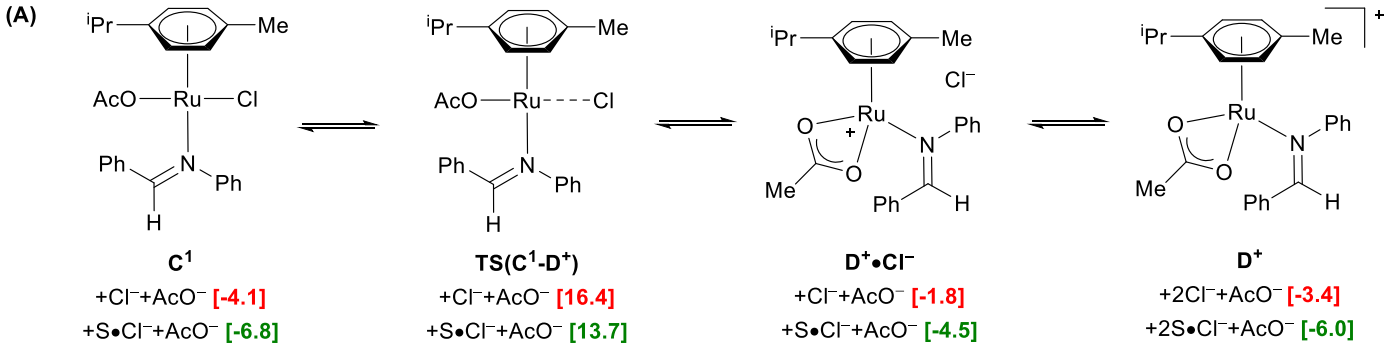
Ru(OAc)$_2$•S
+2Cl$^-$+2S+*p*-cym **29.3**
+2S•Cl$^-$+2S+*p*-cym **28.9**

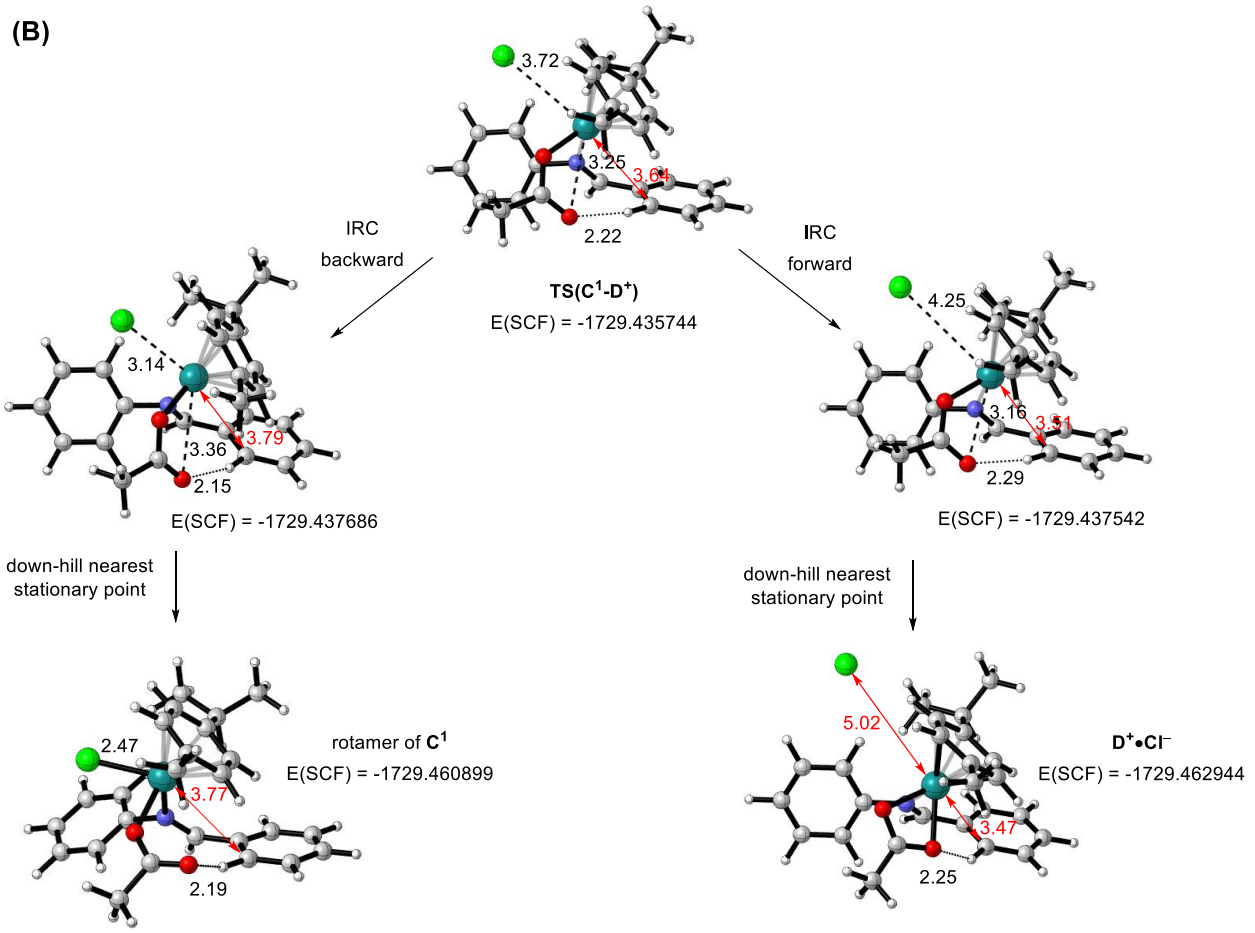
Ru(OAc)$_2$•2S
+2Cl$^-$+S+*p*-cym **13.7**
+2S•Cl$^-$+S+*p*-cym **11.3**

Ru(OAc)$_2$•3S^{fac}
+2Cl$^-$+*p*-cym **14.7**
+2S•Cl$^-$+*p*-cym **10.4**

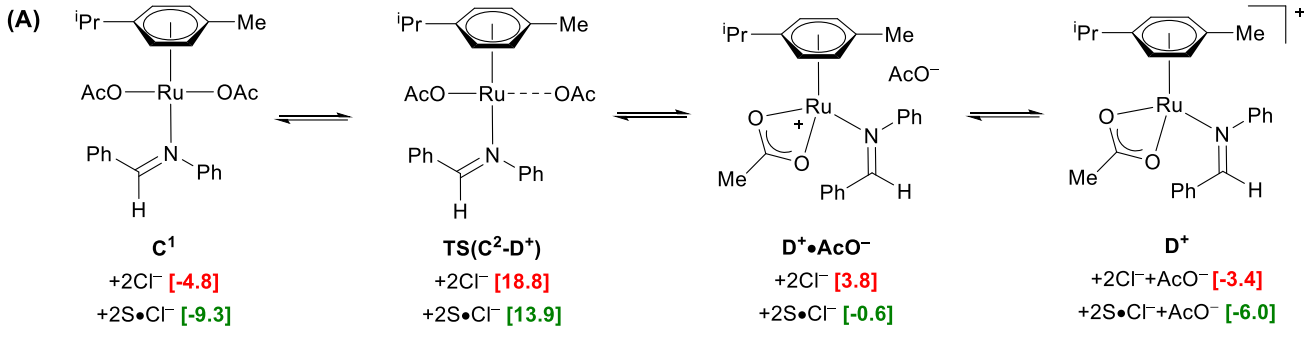
Ru(OAc)$_2$•3S^{mer}
+2Cl$^-$+*p*-cym **12.4**
+2S•Cl$^-$+*p*-cym **8.1**

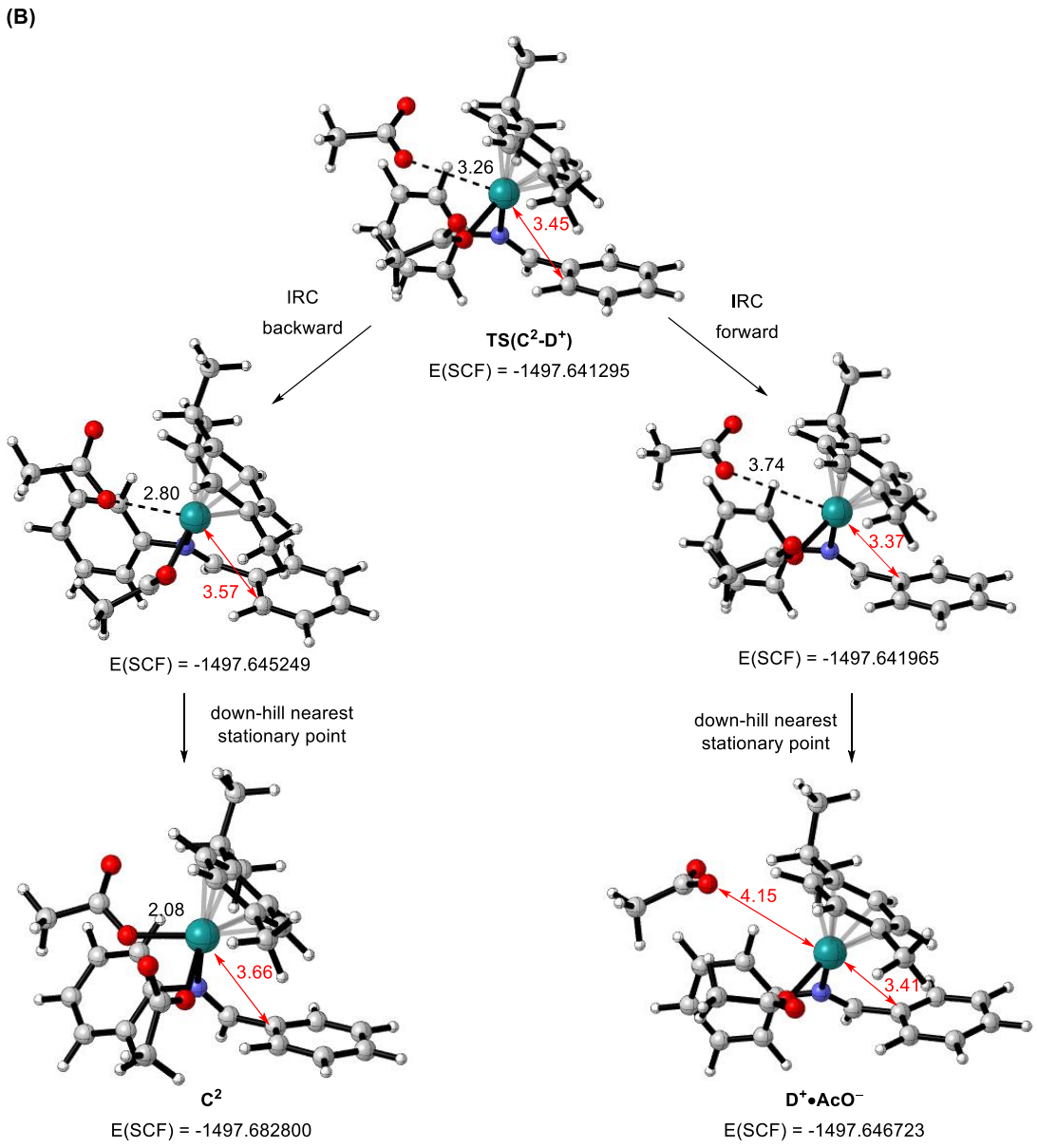
Scheme S4a. Formation of key cationic ruthenium intermediate **D⁺** *via* transition state structure **TS(C¹-D⁺)**. (A) Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(CPCM) level (298 K, 1 M) on the geometries optimized at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in red color. The corresponding values calculated at the same level at condensed phase (298 K, 24.6 M) are shown in green color. *S* stands for solvent (MeOH). (B) 3D CYLview representations for the IRC path calculated at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol from **TS(C¹-D⁺)**, showing relevant distances in Ångstroms.





Scheme S4b. Formation of key cationic ruthenium intermediate **D⁺** *via* transition state structure **TS(C²-D⁺)**.
(A) Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(CPCM) level (298 K, 1 M) on the geometries optimized at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in red color. The corresponding values calculated at the same level at condensed phase (298 K, 24.6 M) are shown in green color. *S* stands for solvent (MeOH). (B) 3D CYLview representations for the IRC path from **TS(C²-D⁺)** calculated at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol, showing relevant distances in Ångstroms.





Scheme S4c. Reaction pathways towards $\mathbf{D^+}$ involving coordination of the ligand (**A**) to the unsolvated or the solvated cationic precursor ($\mathbf{B^+}$ and $\mathbf{B^{+S}}$, respectively). Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(CPCM) level (298 K, 1 M) using the geometries optimized at M06/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in blue color. The corresponding values calculated at the same level in condensed phase (298 K, 24.6 M) are shown in green color. *S* stands for solvent (MeOH).

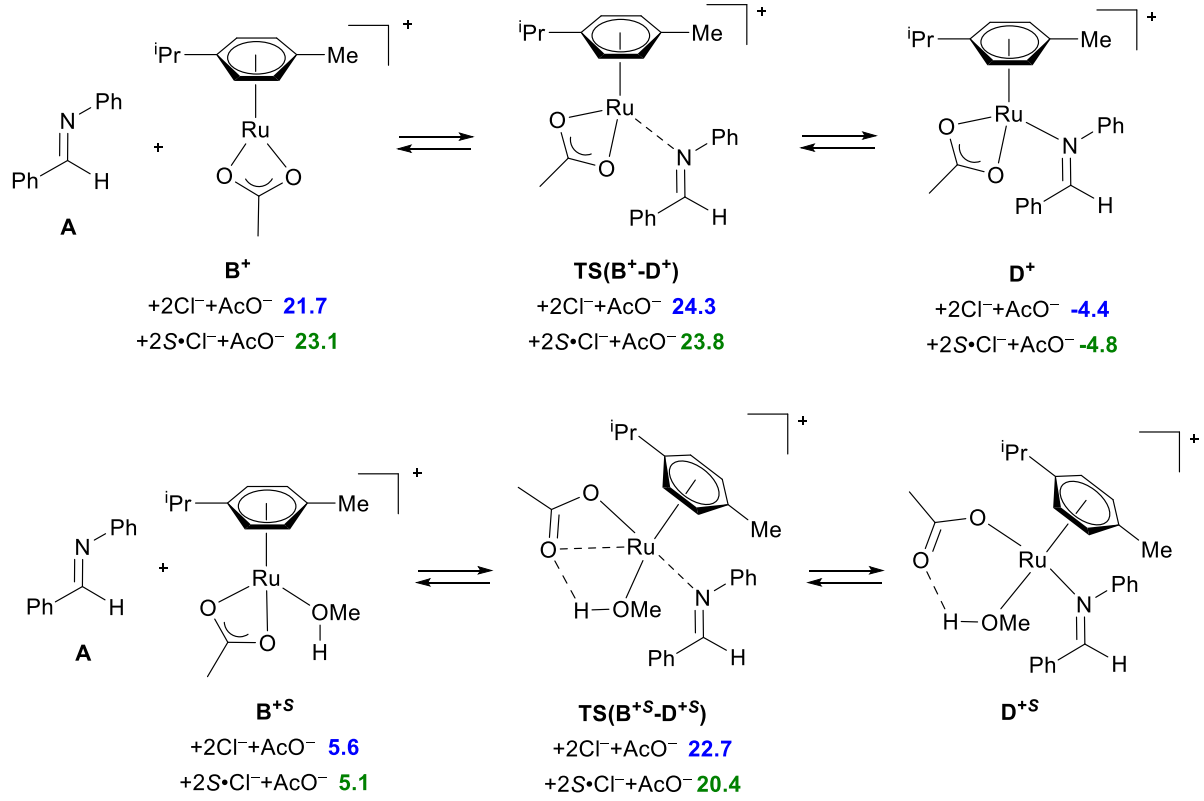
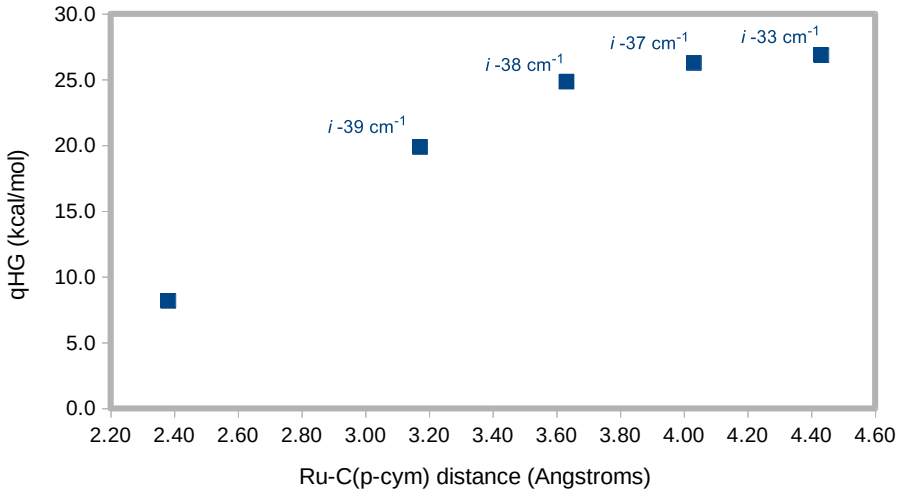
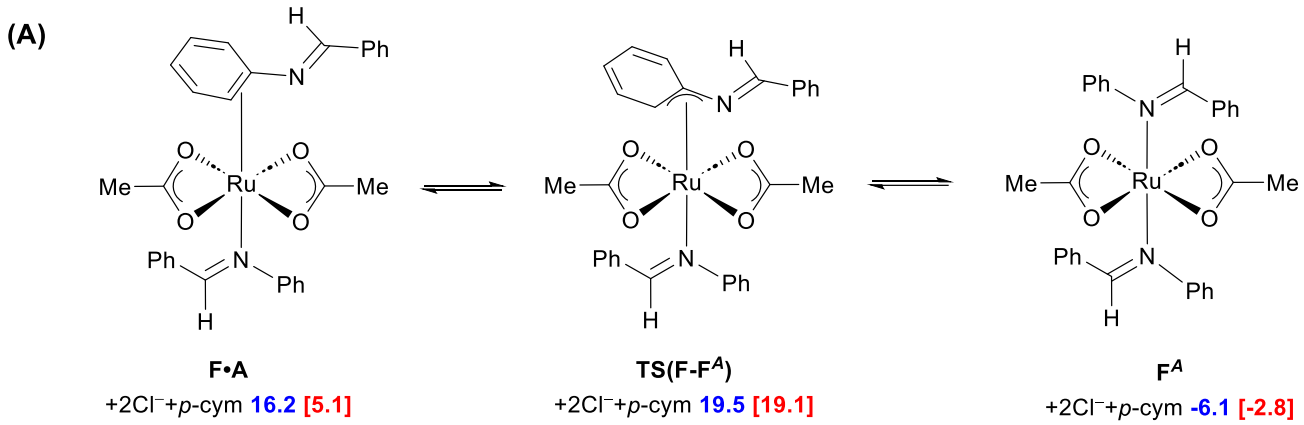
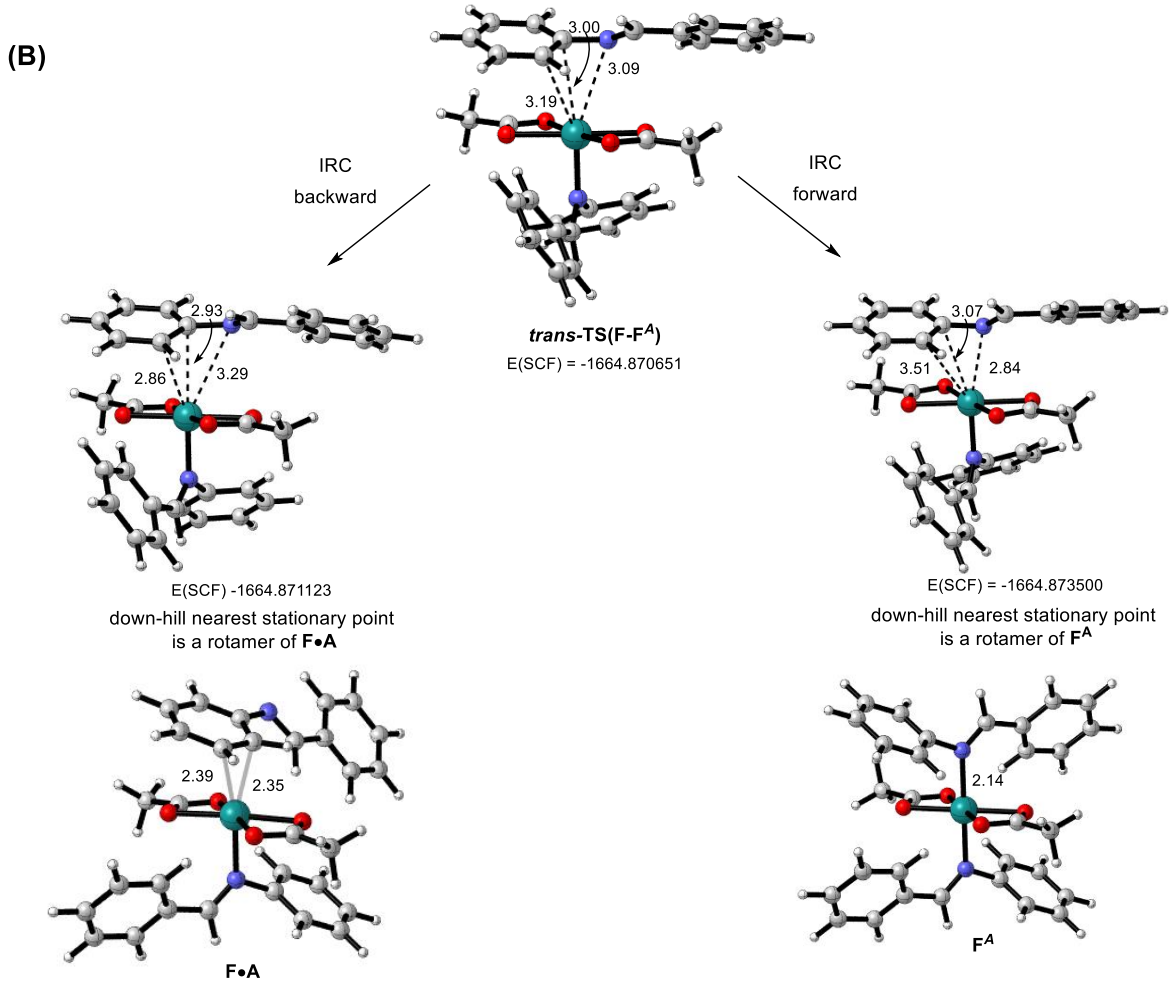


Chart S1. Constrained energy profile for *p*-cymene dissociation from $\mathbf{F^c}$ leading to **F**. Relative quasi-harmonic free energies (in kcal/mol) calculated for **TS($\mathbf{F^c}$-F)** at DLPNO-CCSD(T)/CBS(CPCM) level (298 K, 1 M) on the geometries optimized at ωB97X-D3/cc-pVDZ-PP[Ru](CPCM) level in methanol.

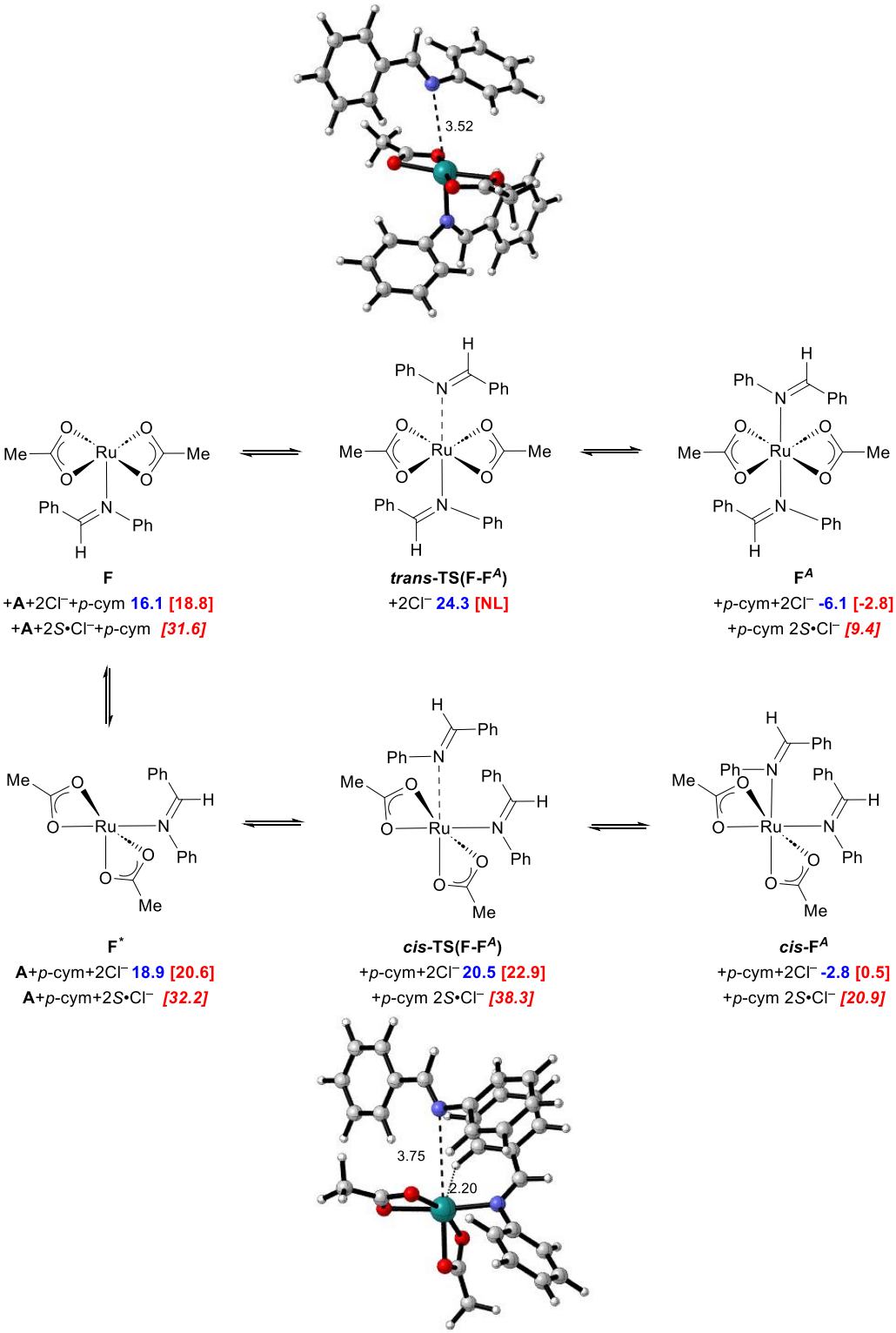


Scheme S5a. Transition state structures **TS(F-F^A)** towards bis-imine intermediate **F^A**. (A) Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(CPCM) level (298 K, 1 M) using the geometries optimized at M06/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in blue color. The corresponding values calculated at the same level by using the geometries optimized at ωB97X-D3/cc-pVDZ-PP[Ru](CPCM) level are shown in red color and between brackets. (B) 3D CYLview representations for the IRC paths from **TS(F-F^A)** calculated at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol, showing relevant distances in Ångstroms.

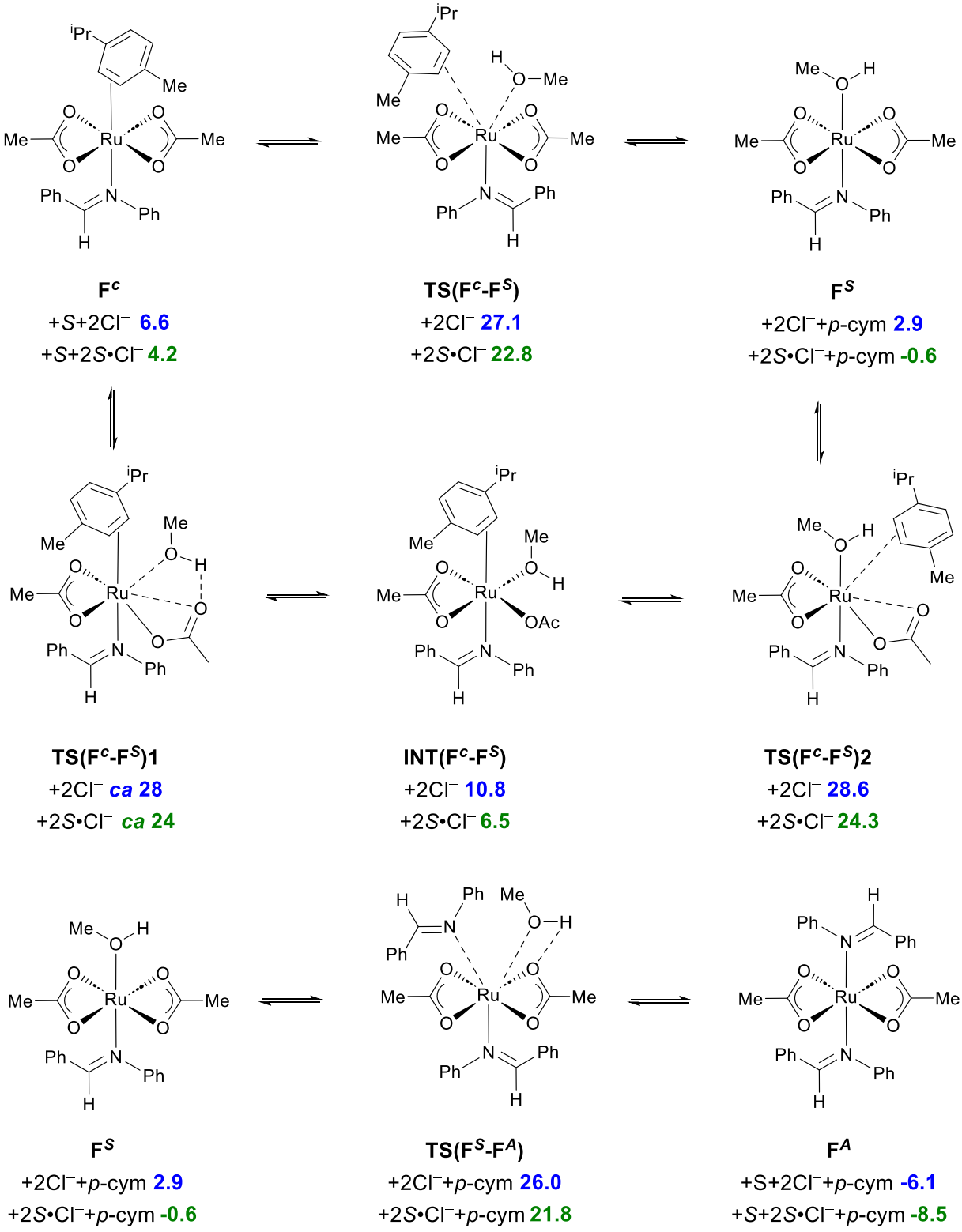




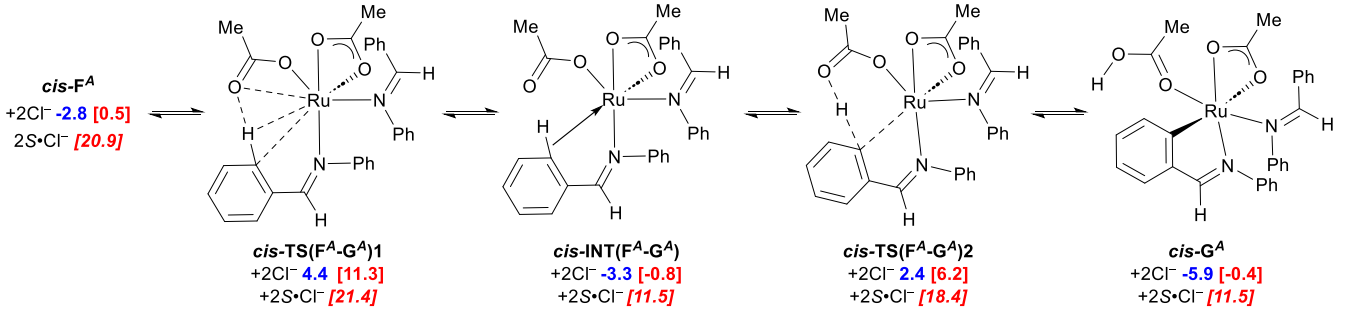
Scheme S5b. Alternative transition state structures **TS(F-F^A)** in the dissociative pathways towards bis-imine intermediates **F^A** and ***cis*-F^A**. Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(CPCM) level (298 K, 1 M) using the geometries optimized at M06/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in blue color. The corresponding values calculated at the same level by using the geometries optimized at ωB97X-D3/cc-pVDZ-PP[Ru](CPCM) level are shown in red color and between brackets.



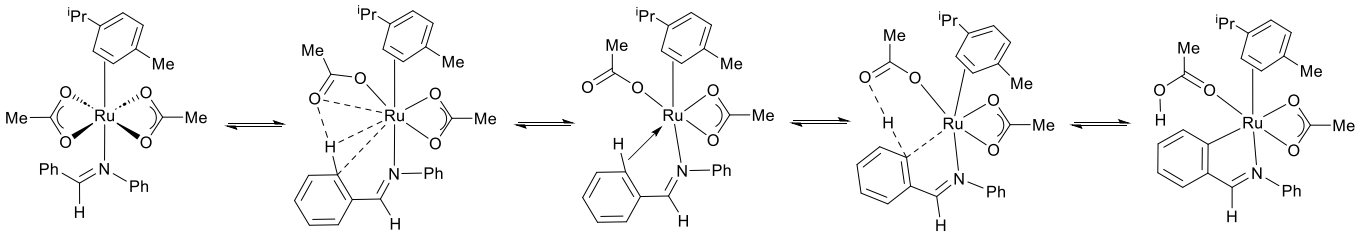
Scheme S5c. Solvent-assisted interchange pathways from $\mathbf{F^c}$ to $\mathbf{F^S}$ or $\mathbf{F^A}$. Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(CPCM) level (298 K, 1 M) on the geometries optimized at M06/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in blue color. The corresponding values calculated at the same level in condensed phase (298 K, 24.6 M) are shown in green color. *S* stands for solvent (MeOH) and *p*-cym for *p*-cymene.



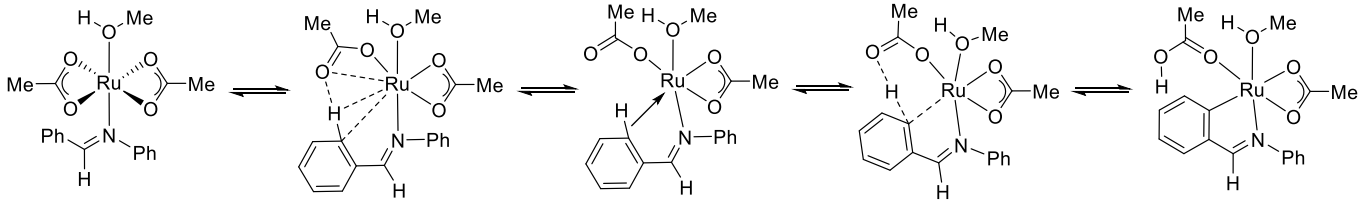
Scheme S6. Reaction pathway for the carboxylate-assisted C-H activation of neutral bis-imine diacetate ruthenium intermediates ***cis*-F^A**, involving the formation of the agostic intermediate ***cis*-INT(F^A-G^A)** and subsequent intramolecular proton abstraction leading to acetate-ruthenacycle ***cis*-G^A**. Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(CPCM) level (298 K, 1 M) using the geometries optimized at M06/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in blue color while those values calculated by using the geometries optimized at ωB97X-D3/cc-pVDZ-PP[Ru](CPCM) level in methanol are shown in red color and brackets. The corresponding values calculated at ωB97X-D3/cc-pVDZ-PP[Ru](SMD) level in methanol are shown in brackets and italics. *S* stands for solvent (MeOH).



Scheme S7. Reaction pathway for the carboxylate-assisted C-H activation of neutral diacetate ruthenium intermediates (**F^c**), involving the formation of the agostic intermediate (**INT(F^c-G^c)**) and subsequent intramolecular proton abstraction leading to acetate-ruthenacycle (**G^c**). Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(CPCM) level (298 K, 1 M) using the geometries optimized at M06/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in blue color while those values calculated by using the geometries optimized at ωB97X-D3/cc-pVDZ-PP[Ru](CPCM) level in methanol are shown in red color and brackets. The corresponding values calculated at the ωB97X-D3/cc-pVDZ-PP[Ru](SMD) level in methanol are shown in italics and brackets. *S* stands for solvent (MeOH).



Scheme S8. Reaction pathway for carboxylate-assisted C-H activation of neutral monosolvated diacetate ruthenium intermediates (**F^{S}**), involving the formation of the agostic intermediate (**INT(F^{S}-G^{S})**) and subsequent intramolecular proton abstraction leading to acetate-ruthenacycle (**G^{S}**). Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(CPCM) level (298 K, 1 M) using the geometries optimized at M06/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in blue color while those values calculated by using the geometries optimized at ωB97X-D3/cc-pVDZ-PP[Ru](CPCM) level in methanol are shown in red color and brackets. The corresponding values calculated at the same levels in condensed phase (298 K, c24 M) are shown in green color. *S* stands for solvent (MeOH).



F^{S}
+2Cl^{-} 2.9 [5.8]
+2*S*•Cl^{-} -0.6 [1.3]

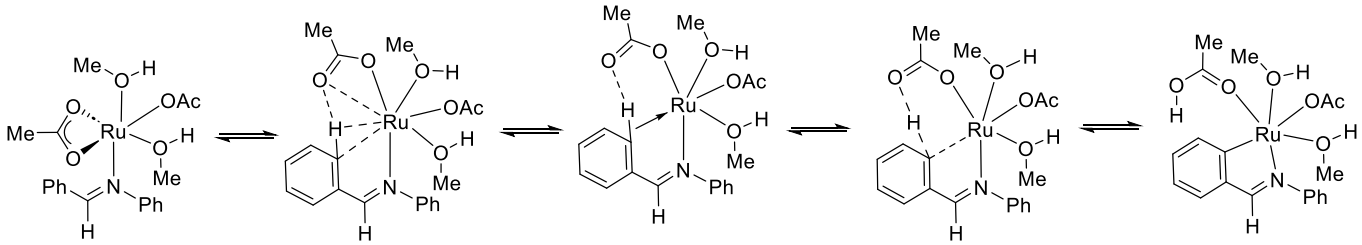
TS(F^{S}-G^{S})1
+2Cl^{-} 14.9 [18.2]
+2*S*•Cl^{-} 12.6 [13.7]

INT(F^{S}-G^{S})
+2Cl^{-} 3.2 [7.4]
+2*S*•Cl^{-} 0.8 [1.0]

TS(F^{S}-G^{S})2
+2Cl^{-} 8.5 [11.1]
+2*S*•Cl^{-} 6.2 [7.6]

G^{S}
+2Cl^{-} 5.7 [8.3]
+2*S*•Cl^{-} 3.3 [3.8]

Scheme S9. Reaction pathway for carboxylate-assisted C-H activation from neutral disolvated diacetate ruthenium intermediates (**F^{2S}**), involving the formation of the agostic intermediate (**INT(F^{2S}-G^{2S})**) and subsequent intramolecular proton abstraction leading to acetate-ruthenacycle (**G^{2S}**). Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(CPCM) level (298 K, 1 M) using the geometries optimized at M06/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in blue color. The corresponding values calculated at the same levels in condensed phase (298 K, c 24 M) are shown in green color. *S* stands for solvent (MeOH).



F^{2S}
+2Cl^{-} 5.4
+2*S*•Cl^{-} 1.1

TS(F^{2S}-G^{2S})1
+2Cl^{-}15.8
+2*S*•Cl^{-} 11.6

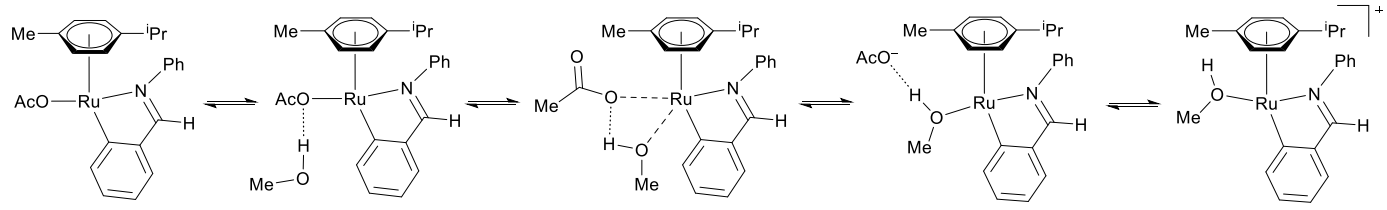
INT(F^{2S}-G^{2S})
+2Cl^{-} 4.6
+2*S*•Cl^{-} 0.3

TS(F^{2S}-G^{2S})2
+2Cl^{-} 7.9
+2*S*•Cl^{-} 3.7

G^{2S}
+2Cl^{-} 6.0
+2*S*•Cl^{-} 1.7

Scheme S10a. Formation of cationic ruthenacycle intermediate **INT(E-H)$^+$•*S*** *via* transition state structure **TS(E-H)1•*S***. (A) Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(CPMC) level (298 K, 1 M) on the geometries optimized at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in red color. The corresponding values calculated at the same level at condensed phase (298 K, 24.6 M) are shown in green color. *S* stands for solvent (MeOH). (B) 3D CYLview representations for the IRC pathways calculated at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol from **TS(E-H)1•*S***, showing relevant distances in Ångstroms.

(A)



E
S+Cl⁻+AcOH•Cl⁻ [-17.8]
2S+Cl⁻+AcOH•Cl⁻ [-20.5]

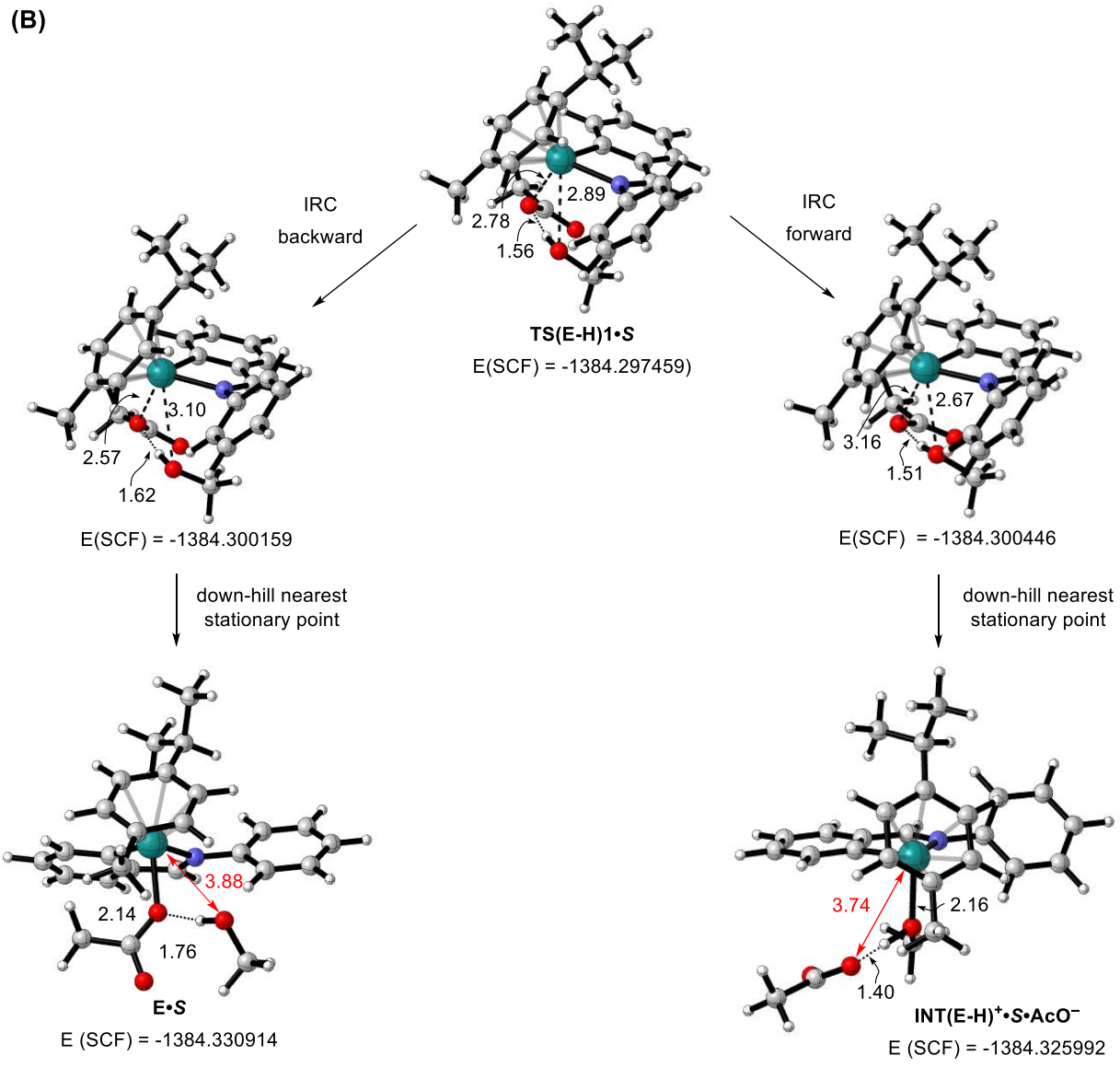
E•*S*
+Cl⁻+AcOH•Cl⁻ [10.1]
+*S*•Cl⁻+AcOH•Cl⁻ [-14.7]

TS(E-H)1•*S*
+Cl⁻+AcOH•Cl⁻ [10.7]
+*S*•Cl⁻+AcOH•Cl⁻ [6.1]

INT(E-H)$^+$•*S*•AcO⁻
+Cl⁻+AcOH•Cl⁻ [-9.3]
S•Cl⁻+AcOH•Cl⁻ [-14.0]

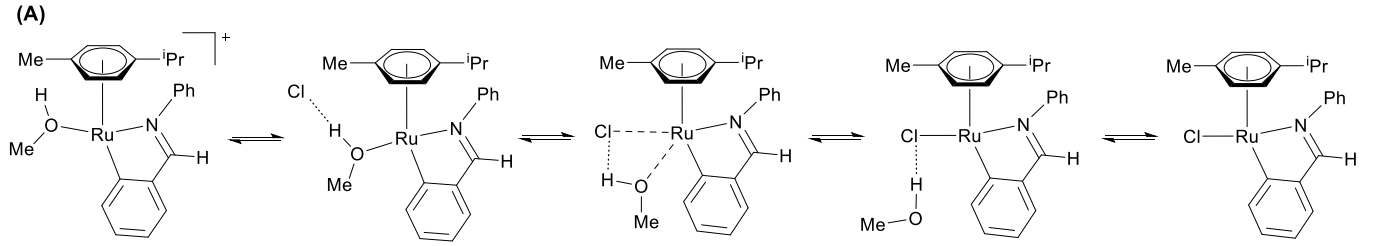
INT(E-H)$^+$•*S*
+2Cl⁻+AcO⁻•HOAc [-4.7]
S•Cl⁻+AcO⁻•HOAc [-9.1]

(B)



Scheme S10b. Formation of chloro ruthenacycle **H•*S*** *via* transition state structure **TS(E-H)2•*S***. (A) Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(CPCM) level (298 K, 1 M) on the geometries optimized at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in red color. The corresponding values calculated at the same level at condensed phase (298 K, 24.6 M) are shown in green color. *S* stands for solvent (MeOH). (B) 3D CYLview representations for the IRC pathways calculated at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol from **TS(E-H)2•*S***, showing relevant distances in Ångstroms.

(A)



INT(E-H)$^+$•*S*
+2Cl$^-$+AcO$^-$•HOAc **[-4.7]**
+*S*•Cl$^-$+AcO$^-$•HOAc **[-9.1]**

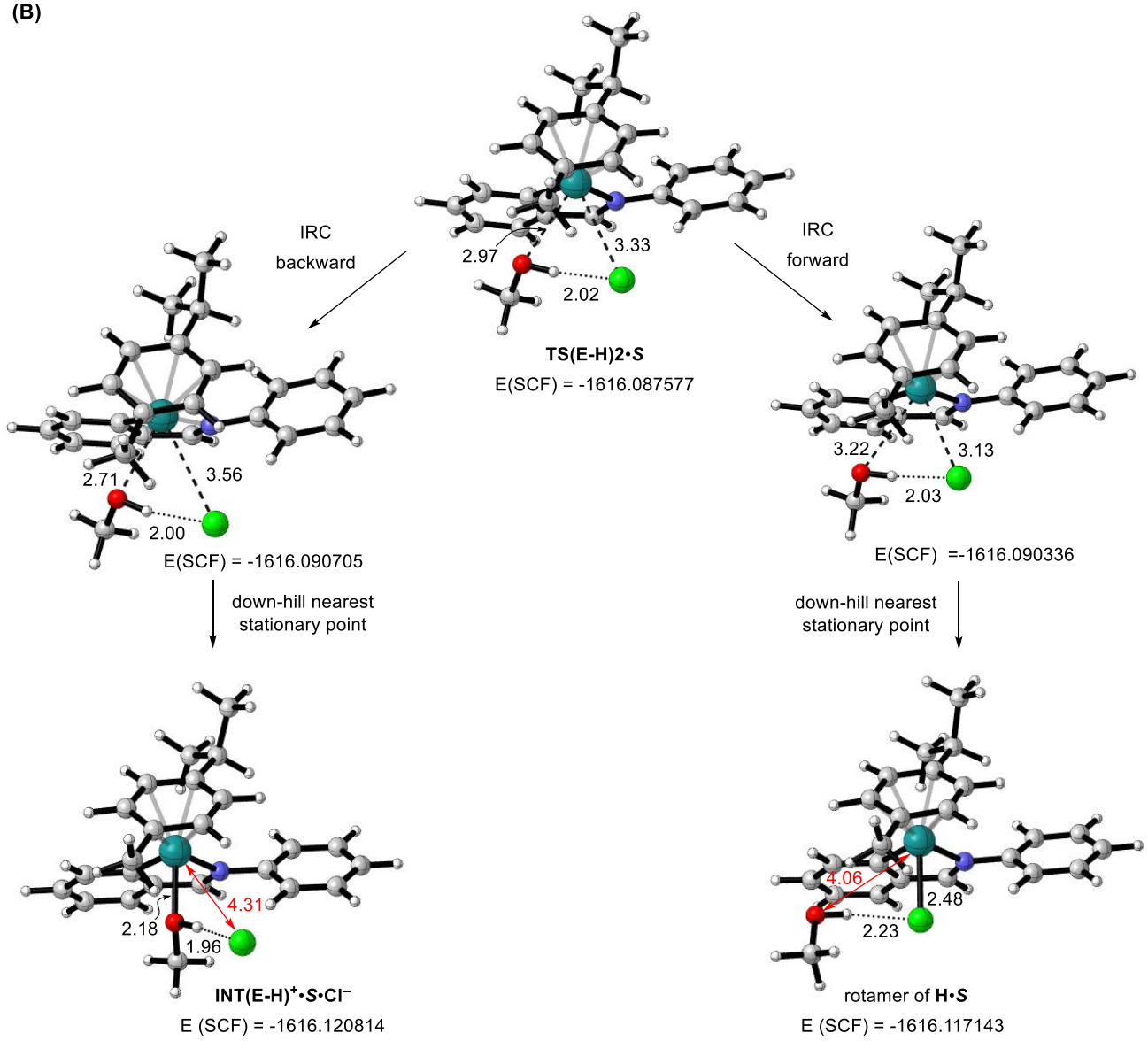
INT(E-H)$^+$•*S*•Cl$^-$
+Cl$^-$+AcO$^-$•HOAc **[-10.4]**
+*S*•Cl$^-$+AcO$^-$•HOAc **[-15.0]**

TS(E-H)2•*S*
+Cl$^-$+AcO$^-$•HOAc **[9.5]**
+*S*•Cl$^-$+AcO$^-$•HOAc **[6.7]**

H•*S*
+Cl$^-$+AcO$^-$•HOAc **[-11.3]**
+*S*•Cl$^-$+AcO$^-$•HOAc **[-15.9]**

H
S+Cl$^-$+AcO$^-$•HOAc **[-18.3]**
+*S*•Cl$^-$+AcO$^-$•HOAc **[-21.0]**

(B)



Scheme S10c. Direct associative route and dissociative route for acetate/chloride exchange on cycloruthenates. Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(CPCM) level (298 K, 1 M) on the geometries optimized at M06/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in blue color. The corresponding values calculated at the same level in condensed phase (298 K, c 24 M) are shown in green color. *S* stands for solvent (MeOH).

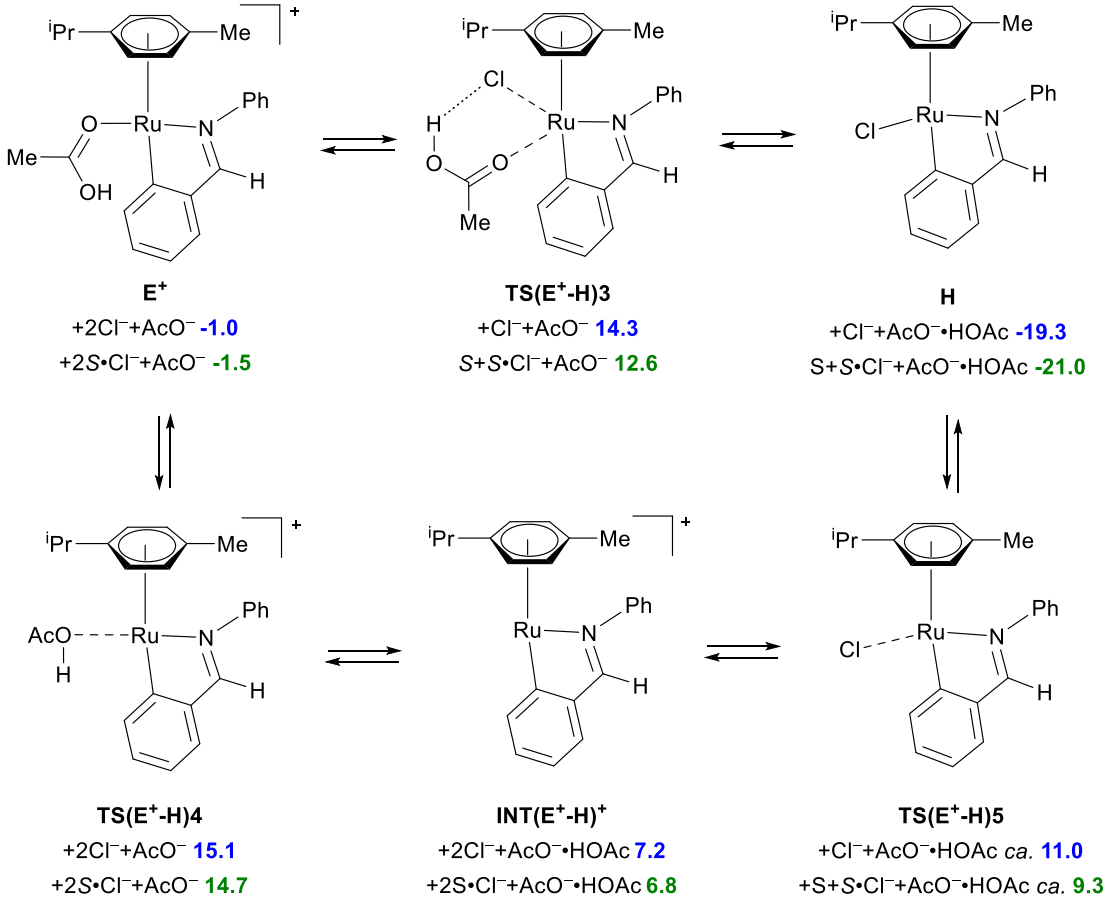
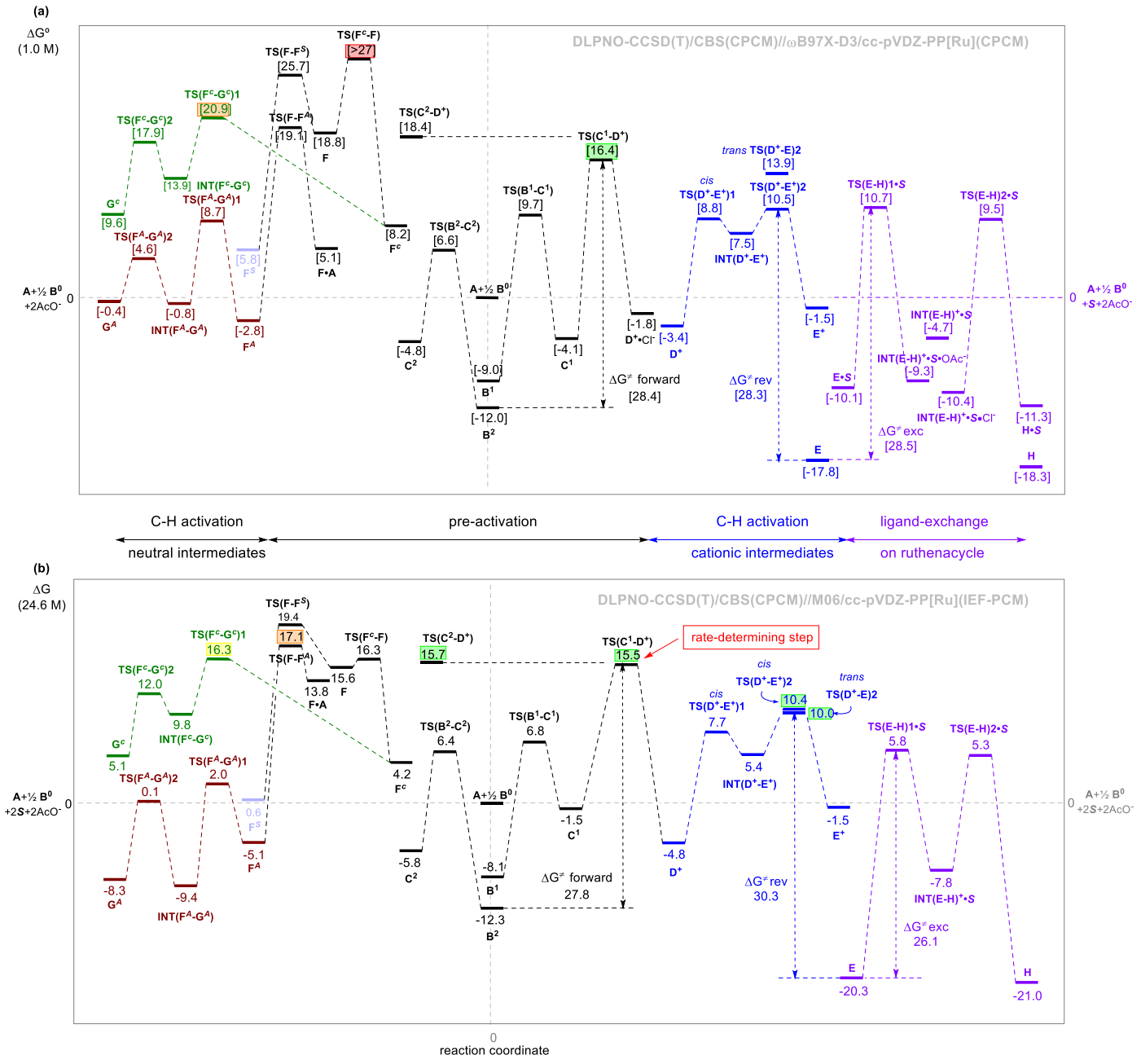
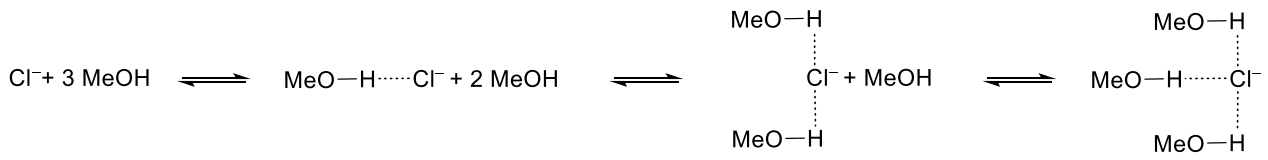


Figure S2. Relative quasi-harmonic Gibbs energy plots calculated at DLPNO-CCSD(T)/CBS(CPCM) level in methanol (in kcal/mol). (a) At 298 K and 1 M after geometry optimizations at ωB97X-D3/cc-pVDZ-PP[Ru](CPCM) level. (b) At 298 K and c 24 M after geometry optimizations at M06/cc-pVDZ-PP[Ru](IEF-PCM) level, including one or two explicit MeOH molecules to monosolvate the chloride anions. Pre-activation by anion dissociation and ligand exchange processes at ruthenium are shown in black color, C-H activations involving cationic intermediates are shown towards the right in blue color and the corresponding processes involving neutral intermediates are shown towards the left in brown and green colors. The final ligand exchange processes at ruthenacycles are shown towards the right in purple color.



Scheme S11. Selected equilibria between solvent, chloride anion, acetate anion and acetic acid in methanol solution. Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(CPCM) level (298 K, 1 M) using the geometries optimized at M06/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in blue color while those calculated by using the geometries optimized at ωB97X-D3/cc-pVDZ-PP[Ru](CPCM) level are shown between brackets in red color. The corresponding values calculated at the same levels in condensed phase (298 K, c 24 M) are shown below in green color. Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(SMD) level are shown in italics. *S* stands for solvent (MeOH). Hydrogen bonds are represented by dotted lines.

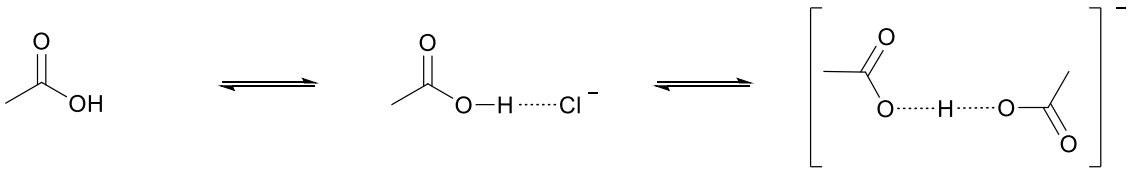


0.0 [0.0] *[0.0]*
0.0 [0.0] *[0.0]*

1.2 [0.1] *[-1.0]*
-0.7 [-1.8] *[-2.9]*

[5.9] *[4.1]*
[2.1] *[0.4]*

[11.8] *[10.1]*
[6.2] *[4.4]*



+Cl⁻+AcO⁻ **0.0** [0.0] *[0.0]*
+*S*•Cl⁻+AcO⁻ -0.7 [-1.8] *[-2.9]*

+AcO⁻ **-0.8** [-0.1] *[-2.1]*
+*S*+AcO⁻ -2.7 [-2.0] *[-4.0]*

+Cl⁻ **-2.1** [-1.0] *[2.0]*
+*S*•Cl⁻ -4.0 [-2.9] *[0.1]*

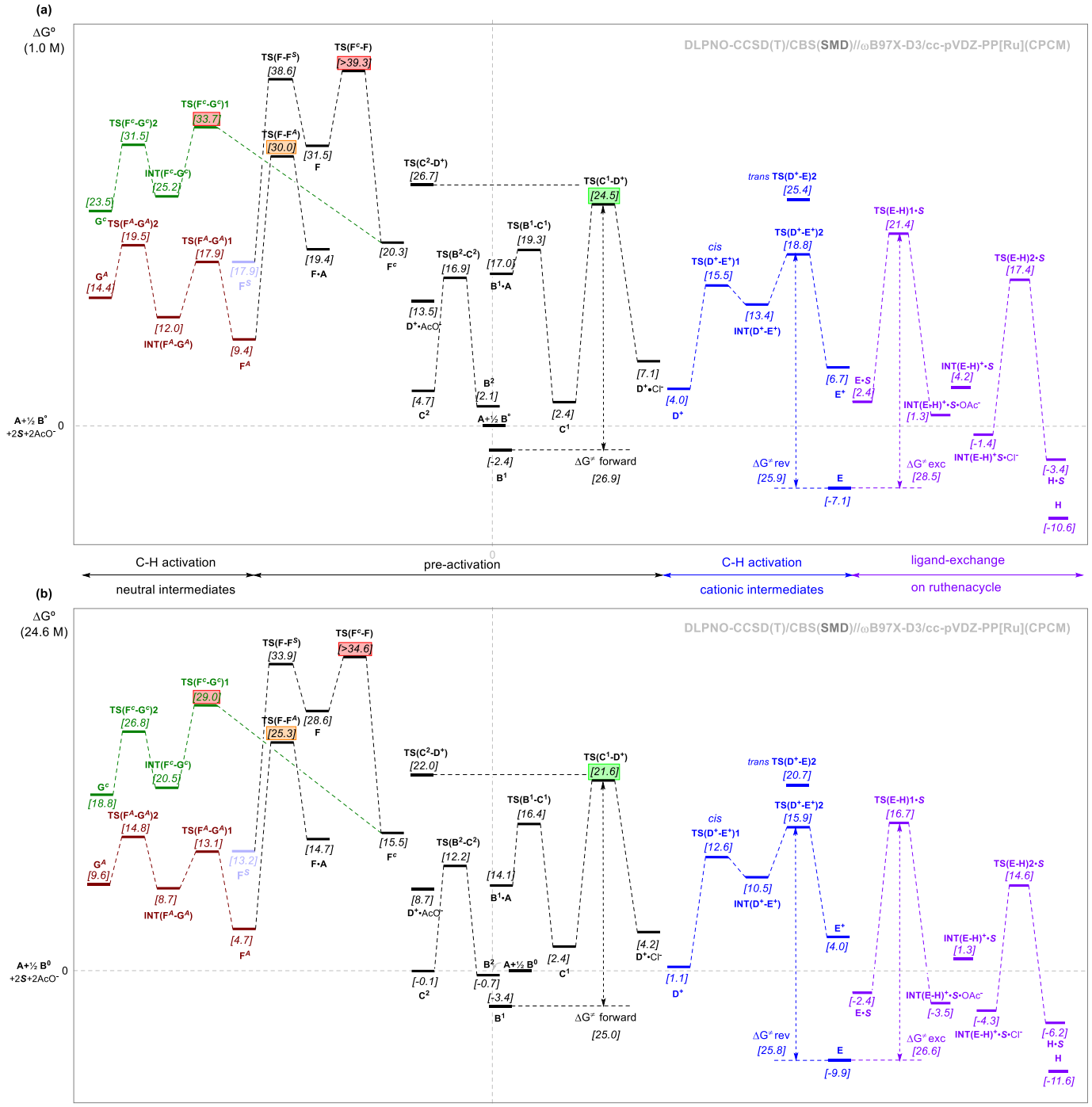
Table S2. Relative quasi-harmonic Gibbs energies (ΔG) and barriers heights (ΔG≠) calculated with DFT/aug-cc-pVTZ-PP[Ru](CPCM) levels for significative intermediates and TS structures as well as mean unsigned errors (MUEs) of the DFT methods relative to the benchmark energies calculated at DLPNO-CCSD(T)/CBS(CPCM) level (at 298 K and c = 1 M). Values calculated on the geometries optimized with the M06 functional are reported first, followed by the corresponding values calculated by using the ωB97X-D3 geometries, which are shown in brackets. All values are in kcal/mol.

entry	structure	benchmark	DFT method							
			PBE0-D3(BJ)	M06-2X	ωB97M-V	B2G-PLYP	B2K-PLYP	PWPB95	PWPB95+D3(BJ)	PWPB95+D4
1	**B¹**	-8.1 [-9.0]	-7.4 [-8.2]	-8.4 [-8.2]	-8.2 [-8.4]	-9.9 [-9.2]	-9.5 [-8.6]	-9.6 [-9.7]	-6.7 [-6.8]	-8.5 [-8.5]
2	**B²**	-12.3 [-12.0]	-9.7 [-9.8]	1.9 [-10.8]	1.3 [-11.2]	0.0 [-10.7]	0.5 [-10.3]	0.0 [-10.9]	3.0 [-8.6]	1.0 [-10.6]
3	**E**	-18.6 [-17.8]	-15.1 [-14.9]	-2.8 [-6.9]	-9.3 [-13.0]	-8.2 [-13.0]	-9.4 [-14.2]	-5.7 [-9.7]	-9.0 [-13.0]	-10.0 [-13.9]
4	**H**	-19.3 [-18.3]	-17.5 [-15.8]	-6.9 [-7.4]	-11.2 [-12.5]	-12.7 [-13.5]	-13.2 [-14.7]	-9.2 [-9.9]	-12.2 [-13.0]	-13.0 [-13.7]
5	ΔG MUE	0.0 [0.0]	2.2 [2.2]	10.7 [6.0]	7.8 [3.0]	7.8 [2.8]	7.4 [2.3]	9.3 [4.6]	8.4 [3.9]	7.2 [2.6]
6	**TS(C¹-D⁺)**	29.0[b] [28.4][b]	30.3[b] [30.2][b]	31.7[a] [29.3] [b]	30.5[a] [29.6][b]	38.5[a] [33.7][b]	38.8[a] [32.4][b]	38.1[a] [35.4][b]	31.1[a] [28.8][b]	32.4[a] [30.4][b]
7	**TS(F[c]-F)**	30.6[b] [32.9][b]	27.4[b] [35.0][b]	25.5[a] [27.4][b]	26.1[a] [31.3][b]	48.0[a] [43.8][b]	50.4[a] [44.8][b]	43.2[a] [43.1][b]	37.0[a] [40.1][b]	36.1[a] [39.1][b]
8	**TS(F-F[S])**	33.6[b] [37.7][b]	30.2[b] [33.7][b]	23.8[a] [21.2][b]	30.2[a] [29.0][b]	42.0[a] [42.0][b]	43.1[a] [43.0][b]	41.7[a] [40.9][b]	39.6[a] [37.9][b]	37.5[a] [37.4][b]
9	**TS(F-F[A])**	32.4[b] [34.9][b]	29.9[b] [32.8][b]	34.3[a] [25.2][b]	34.5[a] [28.2][b]	57.2[a] [44.2][b]	59.3[a] [44.4][b]	51.5[a] [43.3][b]	44.1[a] [36.6][b]	43.5[a] [36.1][b]
10	**TS(D⁺-E⁺)1**	20.1[b] [20.8][b]	20.9[b] [21.5][b]	26.1[a] [24.5][b]	21.3[a] [22.3][b]	28.3[a] [24.1][b]	28.4[a] [23.3][b]	28.0[a] [25.7][b]	22.1[a] [20.6][b]	23.8[a] [22.4][b]
11	**TS(D⁺-E⁺)2**	22.8[b] [22.5][b]	20.5[b] [19.7][b]	32.2[a] [32.5][b]	24.1[a] [24.8][b]	26.6[a] [24.3][b]	26.0[a] [23.4][b]	28.7[a] [27.7][b]	22.2[a] [22.3][b]	24.2[a] [24.1][b]
12	**TS(F[c]-G[c])1**	30.6[b] [32.9][b]	29.1[b] [30.2][b]	20.7[a] [24.4][b]	27.4[a] [26.4][b]	49.9[a] [41.5][b]	45.1[a] [41.2][b]	37.4[b] [41.2][b]	37.4[a] [33.4][b]	36.5[a] [33.1][b]
13	**TS(F[c]-G[c])2**	26.2[b] [29.9][b]	22.7[b] [25.9][b]	33.4[a] [26.5][b]	27.3[a] [27.8][b]	43.9[a] [39.0][b]	45.4[a] [38.6][b]	41.4[a] [39.4][b]	32.0[a] [30.9][b]	32.0[a] [30.3][b]
14	**TS(F[A]-G[A])1**	16.3[b] [20.7][b]	15.2[b] [17.6][b]	27.4[a] [13.6][b]	22.0[a] [15.7][b]	46.8[a] [31.2][b]	49.6[a] [30.8][b]	42.1[a] [32.7][b]	32.6[a] [22.4][b]	31.9[a] [23.6][b]
15	**TS(F[A]-G[A])2**	14.3[b] [16.6][b]	10.3[b] [14.6][b]	15.1[a] [17.9][b]	17.2[a] [16.3][b]	23.1[a] [27.6][b]	21.6[a] [27.2][b]	28.1[a] [30.1][b]	18.6[a] [21.0][b]	18.4[a] [21.1][b]
16	**TS(F[S]-G[S])1**	26.8[b] [30.2][b]	24.1[b] [25.6][b]	16.2[a] [14.5][b]	23.1[a] [22.4][b]	34.5[a] [33.7][b]	35.2[a] [34.5][b]	36.2[a] [34.2][b]	33.0[a] [31.0][b]	31.2[a] [30.6][b]
17	**TS(F[S]-G[S])2**	20.4[b] [23.1][b]	16.1[b] [18.5][b]	19.2[a] [17.6][b]	23.1[a] [21.2][b]	27.6[a] [26.8][b]	28.3[a] [27.6][b]	30.5[a] [28.9][b]	27.2[a] [26.2][b]	25.7[a] [25.1][b]
18	**TS(E-H)1**	27.9[c] [28.5][c]	28.2[c] [28.3][c]	31.4[a] [28.9][b]	29.2[c] [28.2][c]	34.0[a] [32.0][c]	32.7[a] [31.8][c]	36.5[a] [32.7][b]	29.6[c] [29.2][c]	29.4[a] [29.0][c]
19	**TS(E-H)2**	27.4[c] [27.3][c]	25.7[c] [26.5][c]	26.7[a] [26.0][b]	26.3[c] [27.3][c]	31.7[a] [30.0][c]	30.8[a] [30.1][c]	30.8[a] [9.6][b]	26.3[a] [27.3][b]	26.3[a] [27.5][c]
20	ΔG≠ MUE	0.0 [0.0]	2.3 [2.7]	5.7 [6.8]	2.6 [3.7]	12.4 [5.8]	12.6 [5.8]	11.1 [6.6]	5.6 [1.2]	5.2 [1.3]
21	$\Delta G^{\neq}$ $MUE_{cationic}$[d]	0.0 [0.0]	1.5 [1.3]	4.6 [3.3]	1.3 [1.1]	6.4 [3.3]	5.9 [2.7]	6.5 [4.7]	1.5 [0.3]	2.2 [1.2]

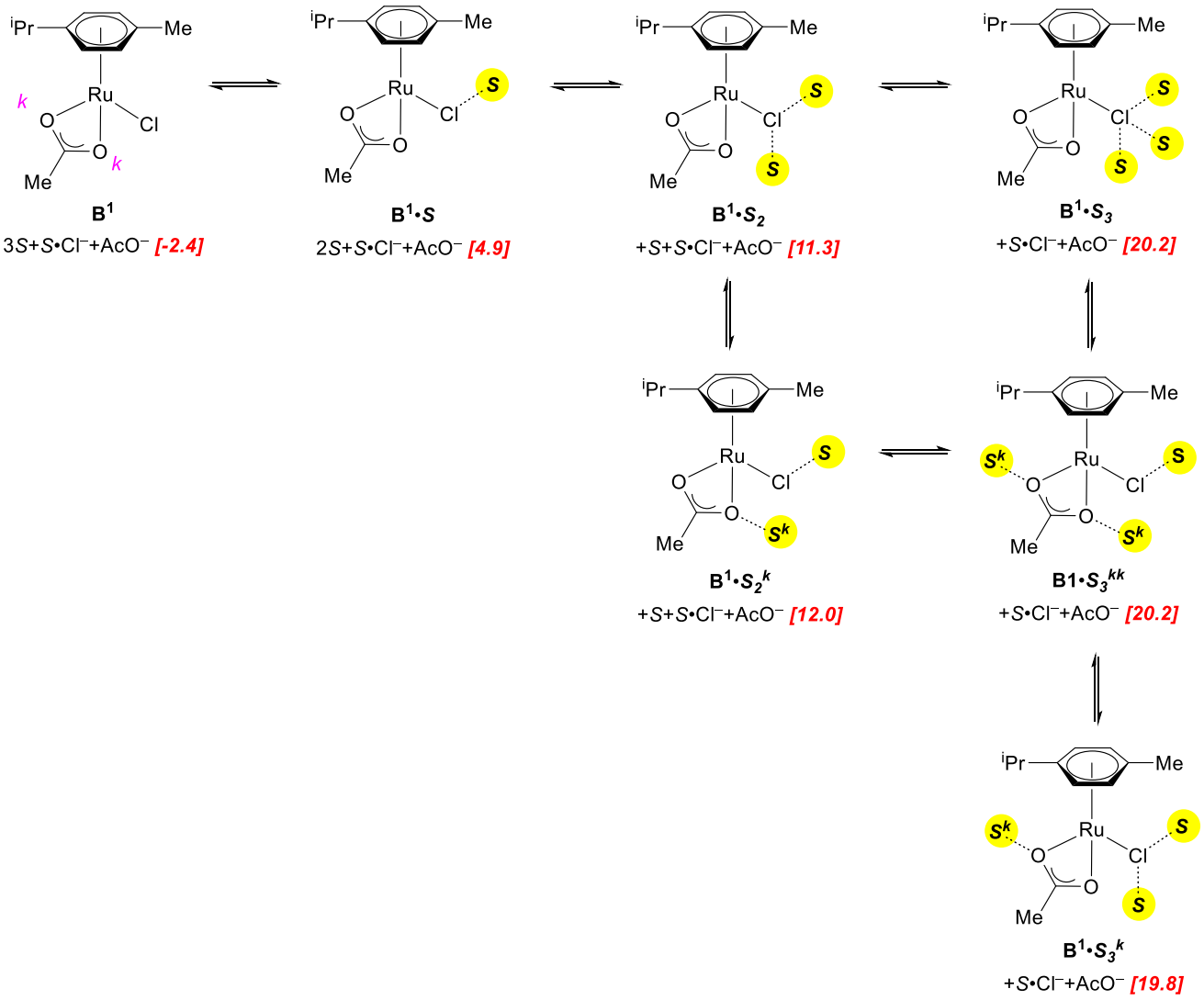
[a] relative to **B¹**. [b] relative to **B²**. [c] relative to **E**. [d] Considering barrier heights to **TS(C¹-D⁺)**, **TS(D⁺-E⁺)1**, **TS(D⁺-E⁺)2**, **TS(E-H)⁺ˢ1** and **TS(E-H)⁺ˢ2**.

Performance of hybrid DFT methods. Single point energy evaluations with the selected DFT methods using an augmented polarized triple-ζ basis set did not allow to reproduce the DLPNO-CCSD(T)/CBS(CPCM) energy results. Calculations with either PBE0-D3(BJ),[5] M06-2X [22] or ωB97M-V [21] functionals indicate that reaction pathways involving neutral diacetate intermediates should be kinetically favoured over [or competitive with] those involving the cationic ones. In particular, according to the energy evaluations with the M06-2X functional, the lowest energy barriers for the C-H activation event were located in the pathway involving neutral and solvated intermediates (see entries 16 and 17), the final ligand exchange at ruthenacycle would be the RDS (see entry 18) and the transformation of the monomeric ruthenium precursors to the cycloruthenates should be endergonic (see entries 1-4). Energy evaluations with either ωB97M-V or PBE0-D3(BJ) functionals indicate that the pathway involving neutral diacetate intermediates with the *p*-cymene moiety acting as an η^2-ligand should be kinetically favoured or competitive with the pathway involving the cationic intermediates (compare entry 6 with entries 12 and 13). Calculations with ωB97M-V functional incorrectly predict the final ligand exchange process at ruthenacycles as the RDS (se entry 18) but provide the best agreement with the benchmark results among the hybrid DFT methods for the activation barriers involving cationic intermediates ($\Delta G^{\neq}$ $MUE_{cationic}$ of *ca.* 1 kcal/mol, see entry 21). Conversely, energy evaluations with PBE0-D3(BJ) correctly indicate that the ligand exchange processes on the ruthenacycles are faster than the C-H activation events on the neutral intermediates (compare entries 12 and 18). Thus, calculations with the PBE0-D3(BJ) functional does not afford the correct energy gap between the pathways involving cationic and neutral intermediates but show the lowest MUEs among the tested hybrid DFT methods for the thermodynamics of the global process (ΔG MUEs of *ca.* 2 kcal/mol, see entry 5) as well as for the whole set of activation barriers ($\Delta G^{\neq}$ MUEs below 3 kcal/mol, see entry 20).

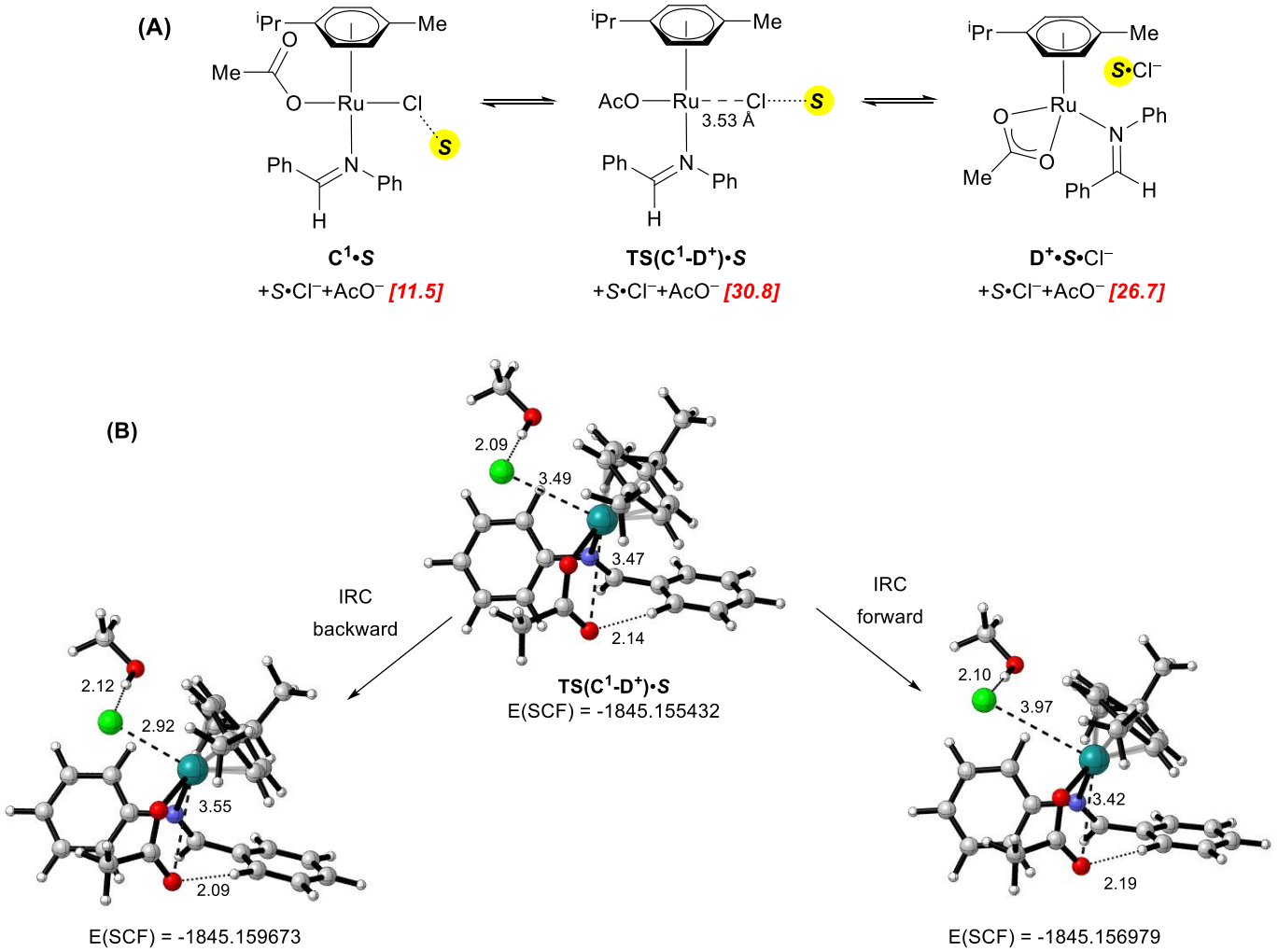
Figure S3. Relative quasi-harmonic Gibbs energy plots calculated at DLPNO-CCSD(T)/CBS(SMD) level in methanol after geometry optimizations at ωB97X-D3/cc-pVDZ-PP[Ru](CPCM) level (in kcal/mol). (a) At 298 K and 1 M. (b) At 298 K and 24 M, including one or two explicit MeOH molecules to monosolvate the chloride anions. Pre-activation by anion dissociation and ligand exchange processes at ruthenium are shown in black color, C-H activations involving cationic intermediates are shown towards the right in blue color and the corresponding processes involving neutral intermediates are shown towards the left in brown and green colors.



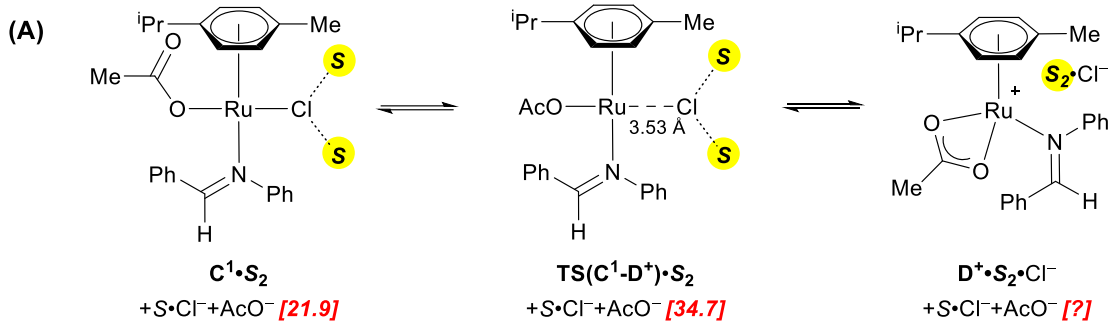
Scheme S12. Equilibria between **B^1•*S*$_n$** precursors in methanol solution. Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(SMD) level (298 K, 1 M) using the geometries optimized at wB97X-D3/cc-pVDZ-PP[Ru](CPCM) level in methanol are shown in brackets, italics and red colour. *S* stands for solvent (MeOH). Hydrogen bonds are represented by dotted lines.

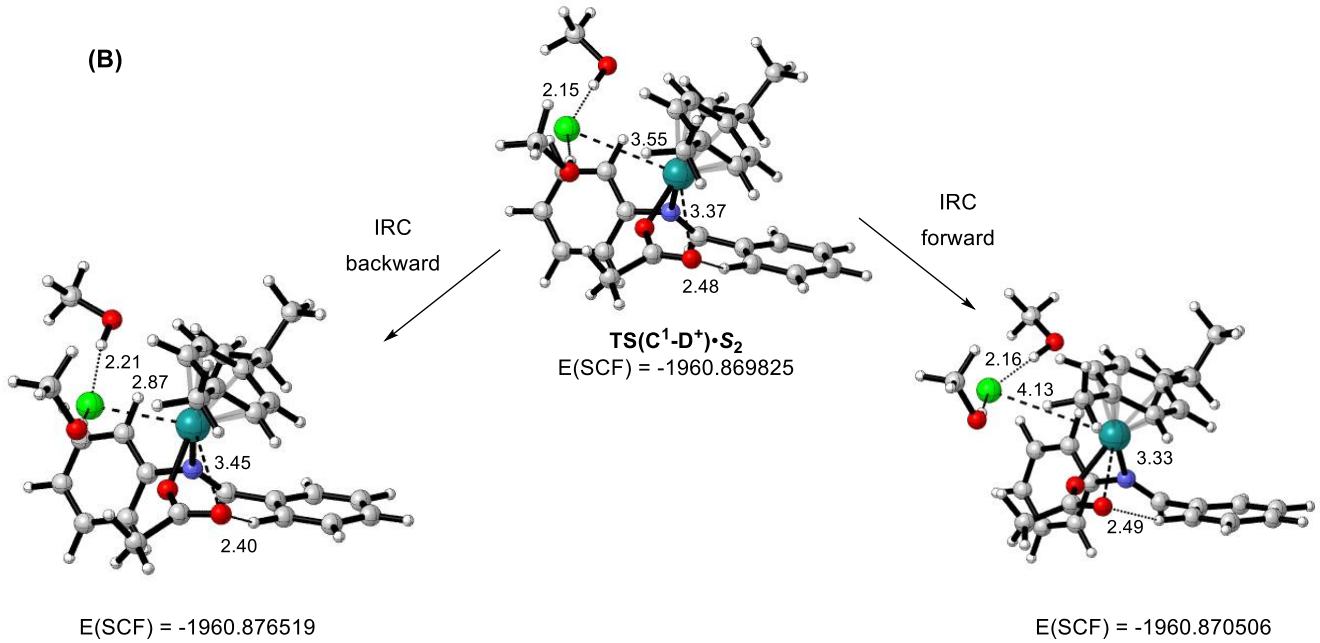


Scheme S13a. Formation of key cationic ruthenium intermediate **D**$^{+}$ *via* transition state structure **TS(C^{1}-D^{+})•*S***. (A) Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(SMD) level (298 K, 1 M) on the geometries optimized at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in red color. *S* stands for solvent (MeOH). (B) 3D CYLview representations for the IRC path calculated at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol from **TS(C^{1}-D^{+})•*S*$_1$**, showing relevant distances in Ångstroms.

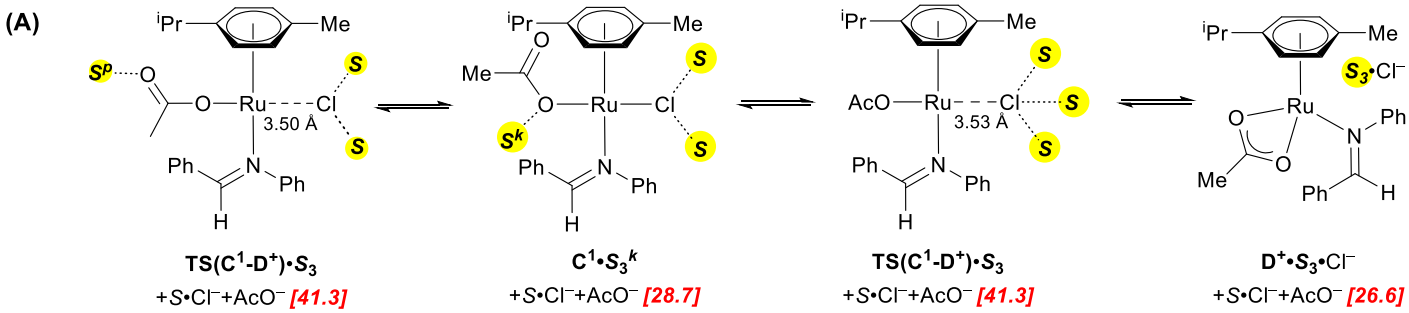


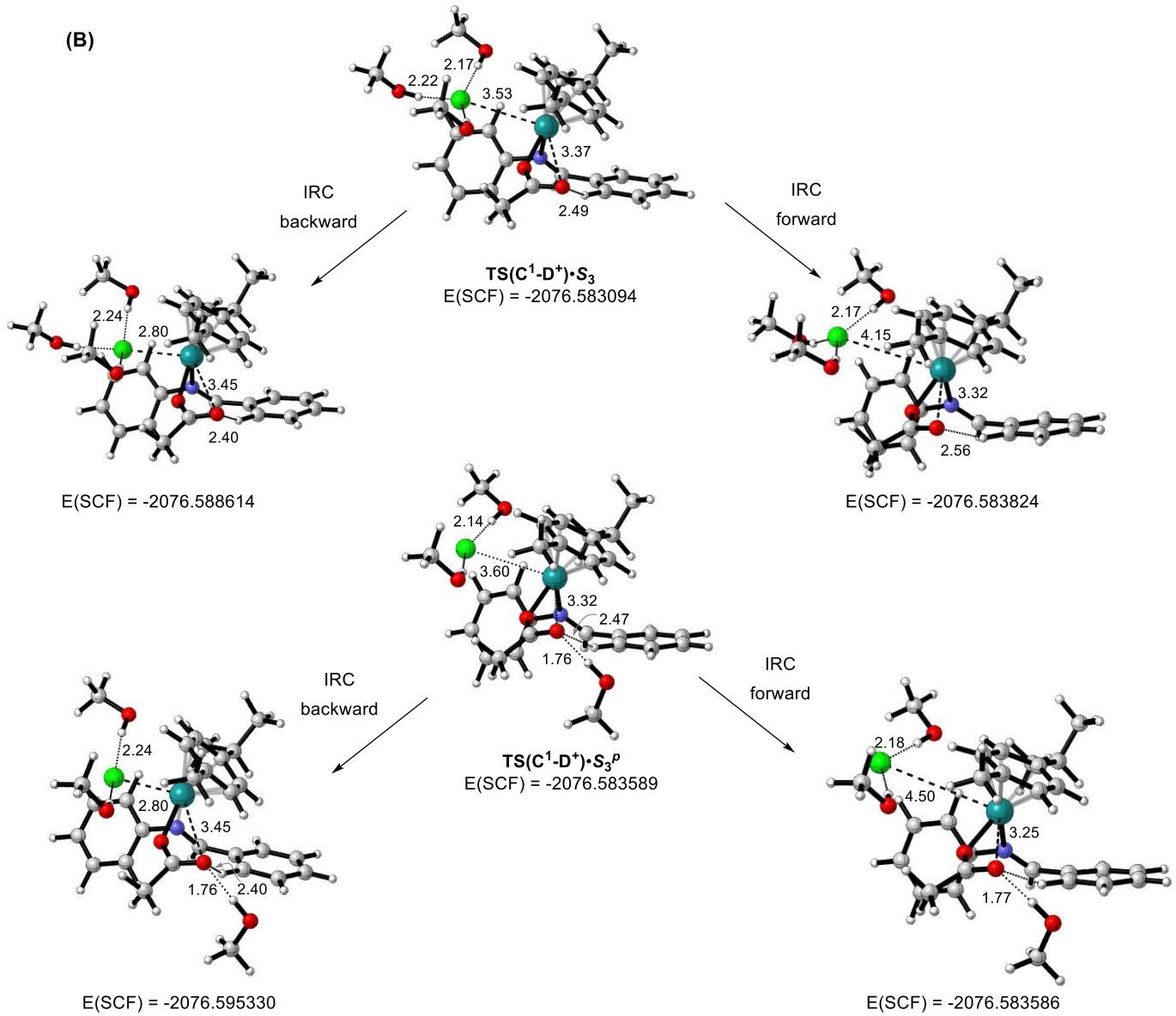
Scheme S13b. Formation of key cationic ruthenium intermediate **D**$^{+}$ *via* transition state structure **TS(C^{1}-D^{+})•*S*$_2$**. (A) Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(SMD) level (298 K, 1 M) on the geometries optimized at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in red color. *S* stands for solvent (MeOH). (B) 3D CYLview representations for the IRC path calculated at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol from **TS(C^{1}-D^{+})•*S*$_2$**, showing relevant distances in Ångstroms.



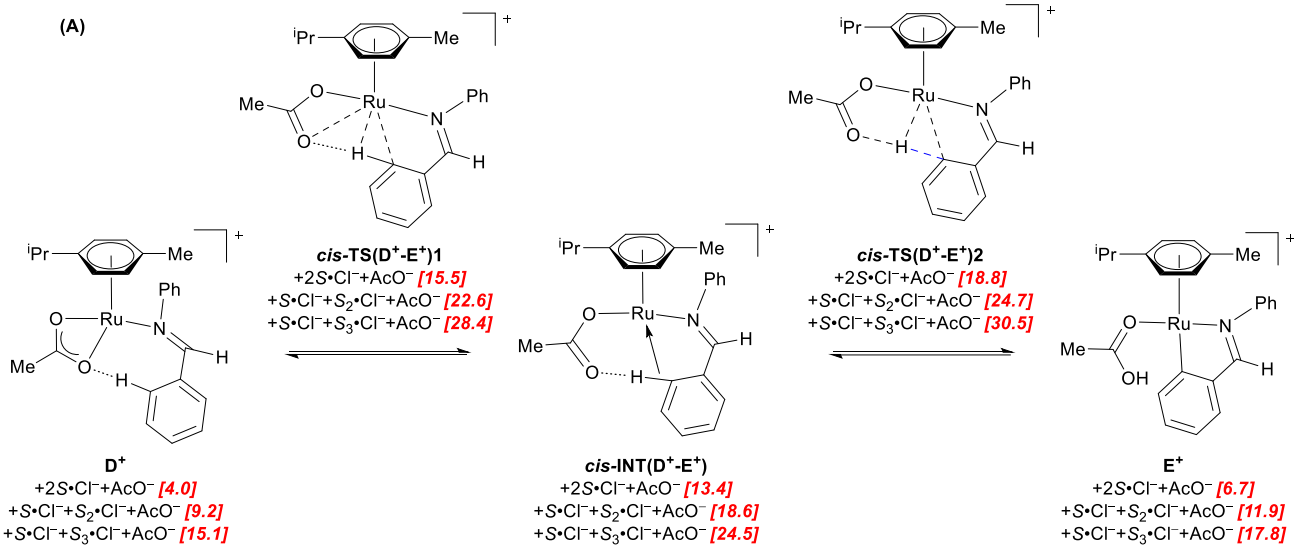


Scheme S13c. Formation of key cationic ruthenium intermediate **D**$^{+}$ *via* transition state structure **TS(C^{1}-D^{+})•*S*$_{3}$**. (A) Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(SMD) level (298 K, 1 M) on the geometries optimized at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in red color. *S* stands for solvent (MeOH). (B) 3D CYLview representations for the IRC paths calculated at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol from **TS(C^{1}-D^{+})•*S*$_{3}$** and **TS(C^{1}-D^{+})•*S*$_{3}^{p}$**, showing relevant distances in Ångstroms.





Scheme S14. Lowest energy non-solvated TS structures located for the C-H bond activation process from **D⁺** *to* **E⁺** in the S_1-, S_2- and S_3-reaction channels. (A) Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(SMD) level (298 K, 1 M) on the geometries optimized at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in brackets and italics, in red color. *S* stands for solvent (MeOH). (B) 3D CYLview representations for the IRC paths calculated at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol from ***cis*-TS(D⁺-E⁺)1** and ***cis*-TS(D⁺-E⁺)2**, showing relevant distances in Ångstroms.



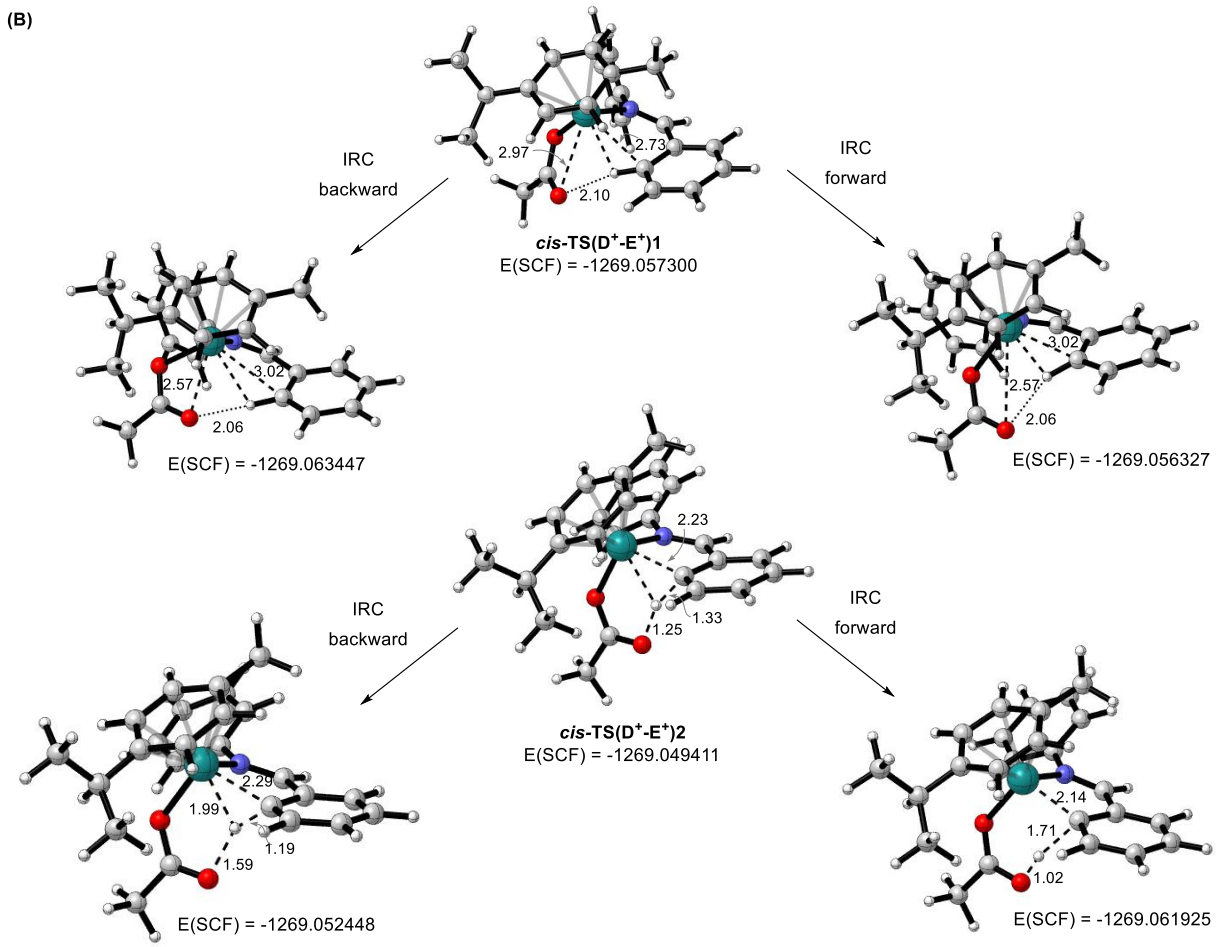


Figure S4. Energy plot for chloride dissociation from **C**[1] and subsequent C-H bond activation leading to cycloruthenate **E** in the S_1-reaction channel, calculated at DLPNO-CCSD(T)/CBS(SMD) level in methanol (298 K, 1 M), after geometry optimizations at ωB97X-D3/cc-pVDZ-PP[Ru](CPCM) level. Quasi-harmonic Gibbs energies are shown between brackets, in italics and red colour, relative to separated reagents (**A**+½**B**^{0}+2AcO$^-$) plus two explicit MeOH molecules: one active MeOH molecule (close to the reaction center in any intermediate or transition state, shadowed in yellow) and one stoichiometric MeOH molecule required to monosolvate the chloride anion freed in the formation of the **B**^{1}•***S*** precursor (bluish, omitted). Characteristic activation energies in the S_1-reaction channel are shown in magenta color. The hydrogen bonds are represented by dotted lines.

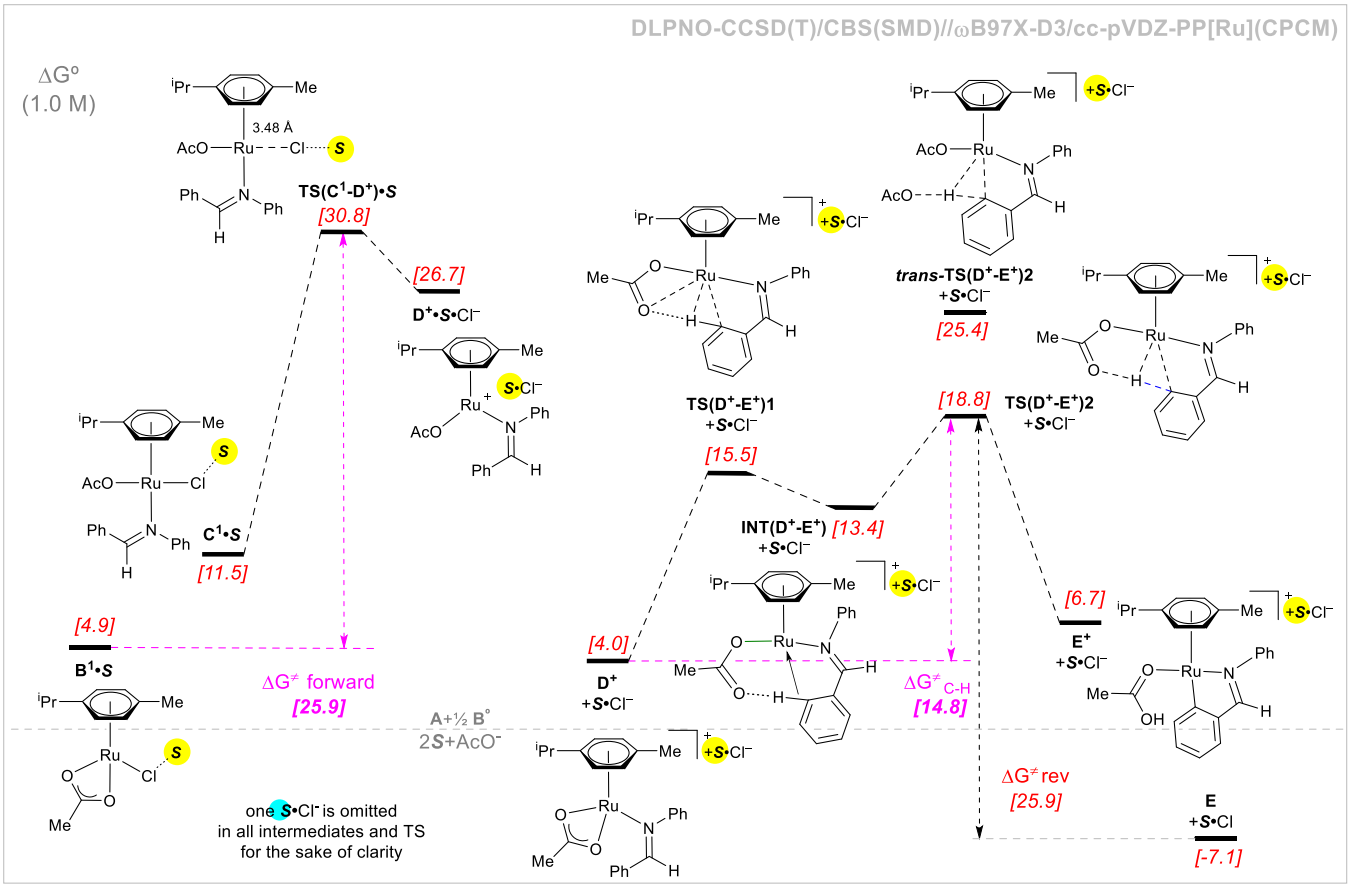


Figure S5. Energy plot for for chloride dissociation from **C**[1] and subsequent C-H bond activation leading to cycloruthenate **E** in the S_2-reaction channel, calculated at DLPNO-CCSD(T)/CBS(SMD) level in methanol (298 K, 1 M), after geometry optimizations at ωB97X-D3/cc-pVDZ-PP[Ru](CPCM) level. Quasi-harmonic Gibbs energies are shown between brackets, in italics and red colour, relative to separated reagents (**A**+½**B**[0]+2AcO$^-$) plus three explicit MeOH molecules: two active MeOH molecule (close to the reaction center in any intermediate or transition state, shadowed in yellow) and one stoichiometric MeOH molecule required to monosolvate the chloride anion freed in the formation of the **B**[1]•***S*** precursor (bluish, omitted). Characteristic activation energies in the S_2-reaction channel are shown in green color. The hydrogen bonds are represented by dotted lines.

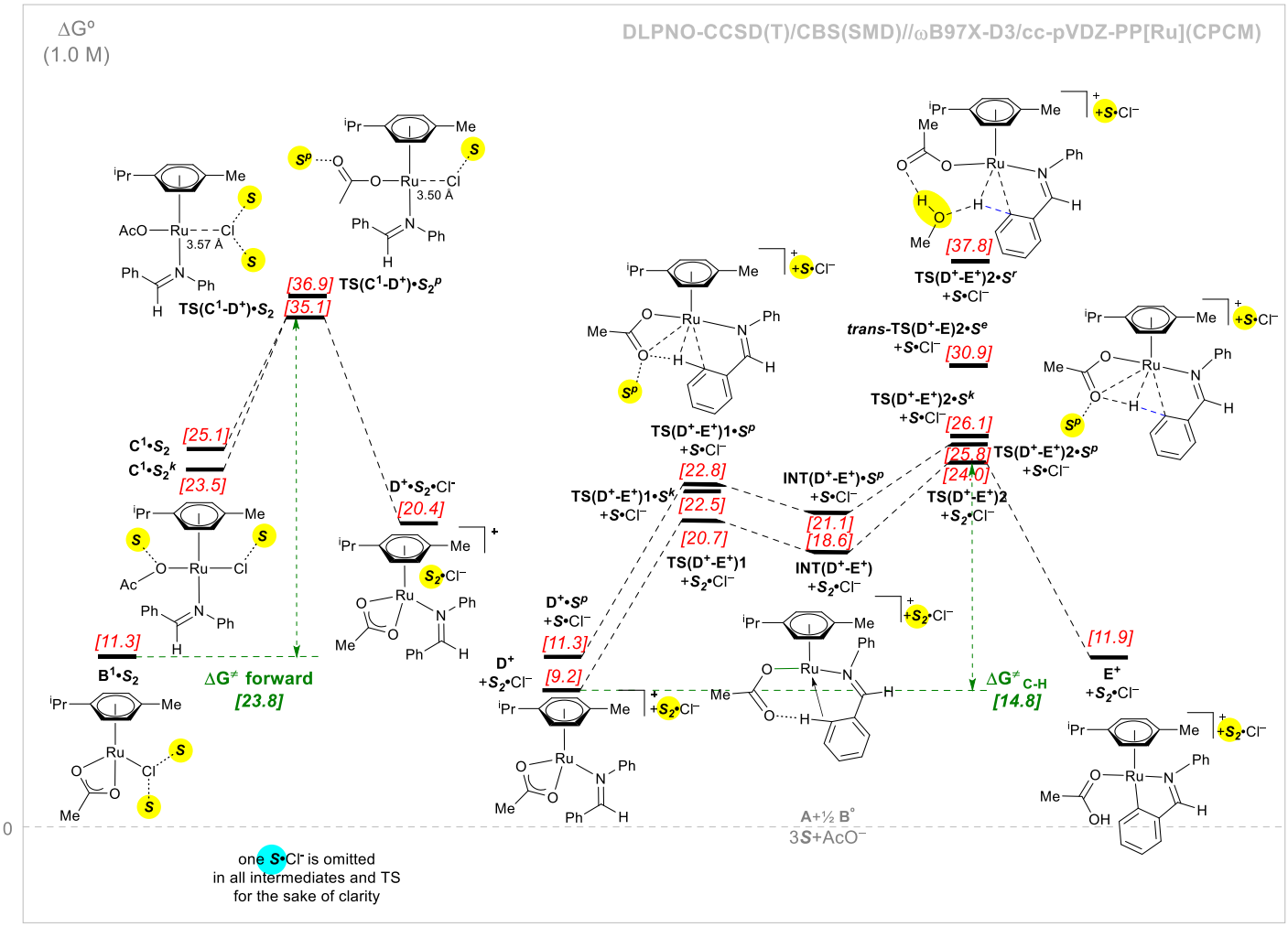
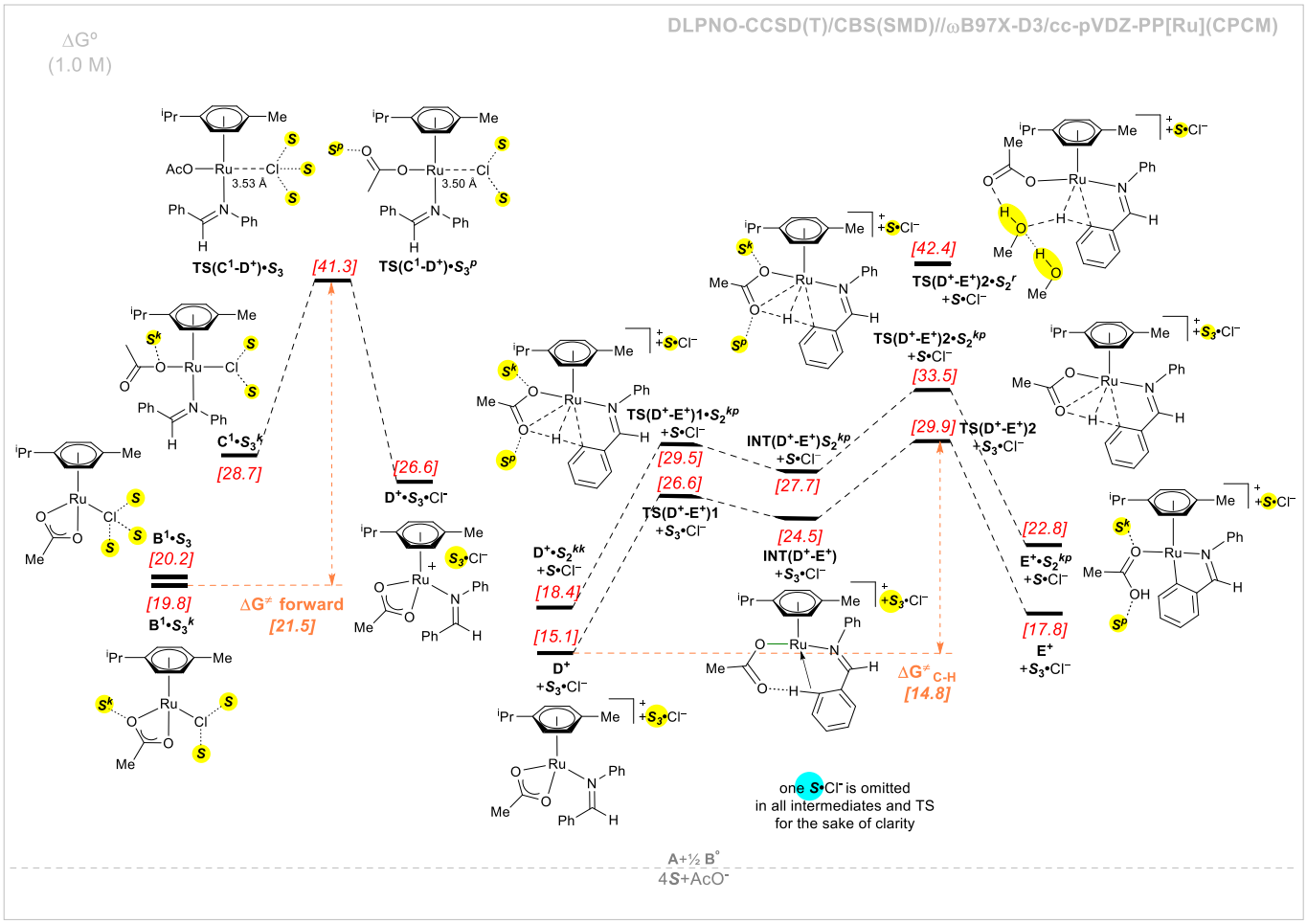
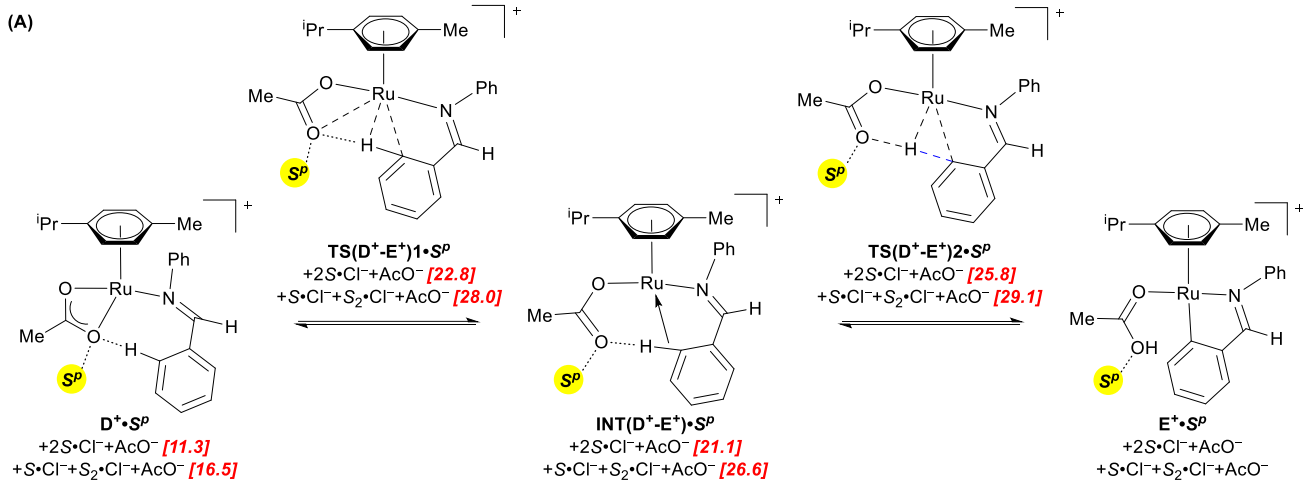
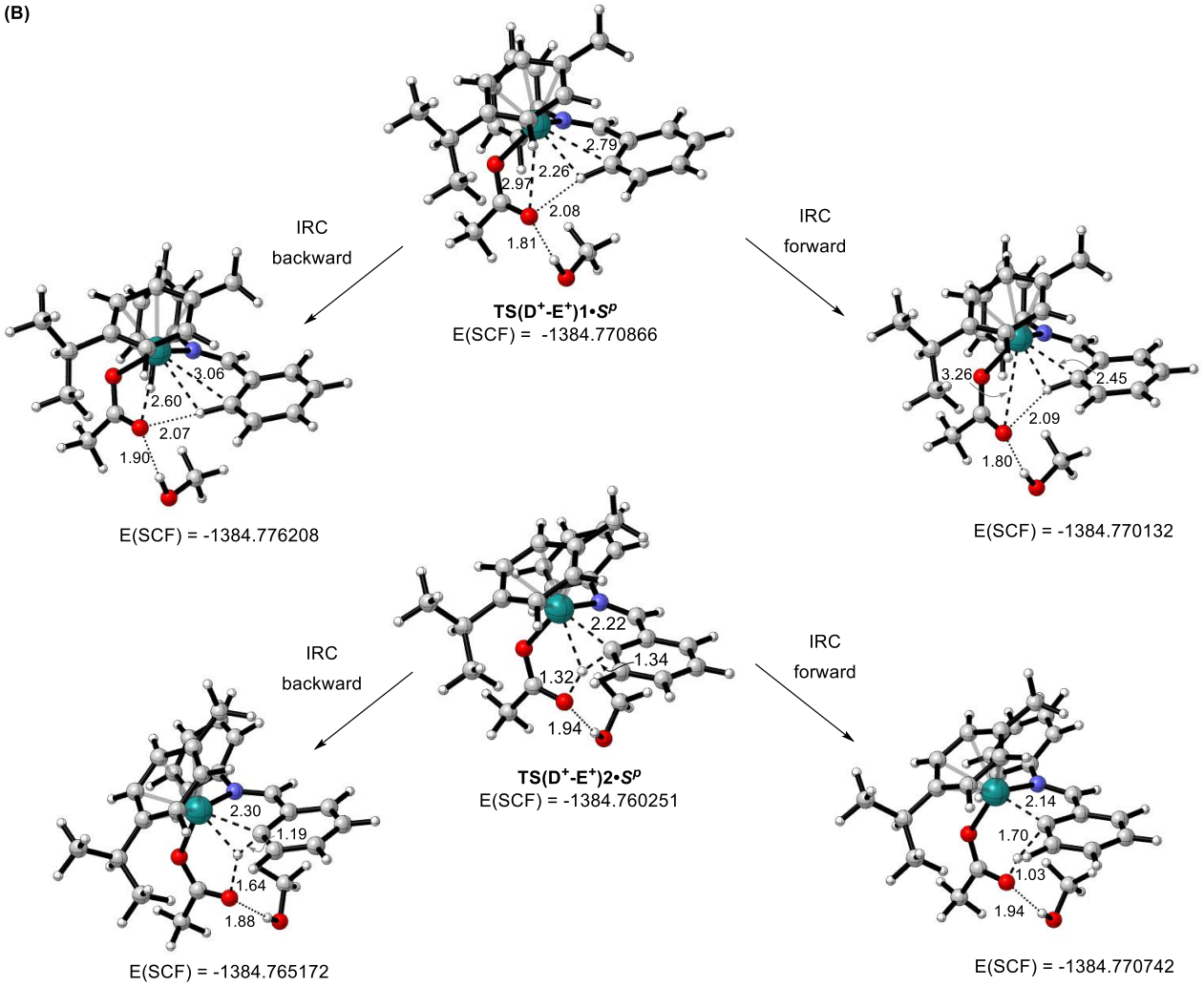


Figure S6. Energy plot for chloride dissociation from **C**[1] and subsequent C-H bond activation leading to cycloruthenate **E** in the S_3-reaction channel calculated at DLPNO-CCSD(T)/CBS(SMD) level in methanol (298 K, 1 M) after geometry optimizations at ωB97X-D3/cc-pVDZ-PP[Ru](CPCM) level. Quasi-harmonic Gibbs energies are shown between brackets, in italics and red colour, relative to separated reagents (**A**+½**B**[0]+2AcO$^-$) plus four explicit MeOH molecules: three active MeOH molecule (close to the reaction center in any intermediate or transition state, shadowed in yellow) and one stoichiometric MeOH molecule required to monosolvate the chloride anion freed in the formation of the **B**[1]•***S*** precursor (bluish, omitted). Characteristic activation energies in the S_3-reaction channel are shown in orange color.
The hydrogen bonds are represented by dotted lines.

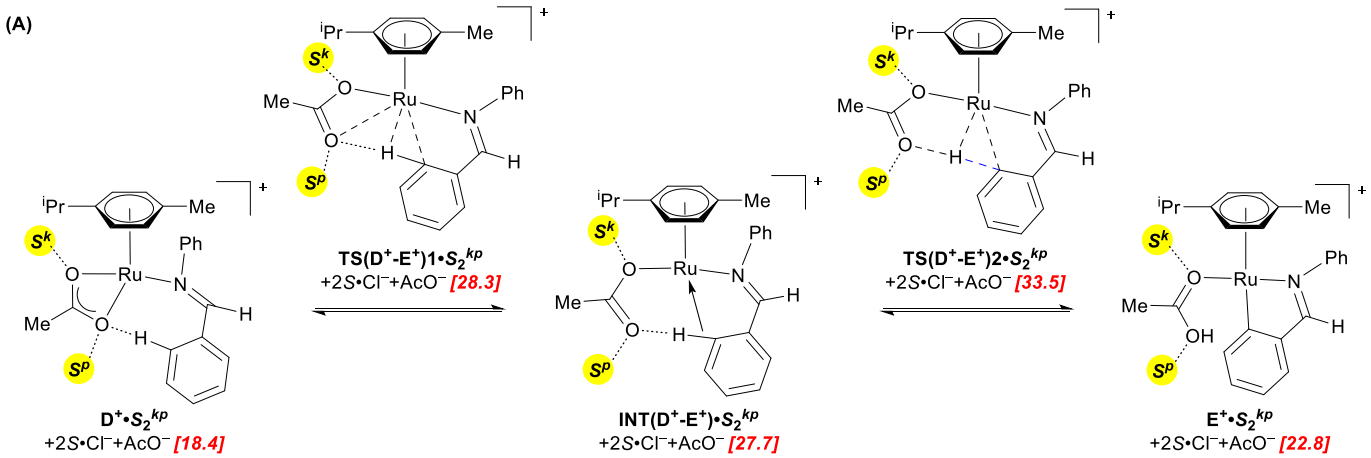


Scheme S15a. Lowest energy solvated TS structures located for the C-H bond activation process from $\mathbf{D^+}$ *to* $\mathbf{E^+}$ in the S_2-reaction channel. (A) Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(SMD) level (298 K, 1 M) on the geometries optimized at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in brackets and italics, in red color. *S* stands for solvent (MeOH). (B) 3D CYLview representations for the IRC paths calculated at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol from $\mathbf{TS(D^+\text{-}E^+)1\bullet}S^p$ and $\mathbf{TS(D^+\text{-}E^+)2\bullet}S^p$, showing relevant distances in Ångstroms.





Scheme S15b. Lowest energy solvated TS structures located for the C-H bond activation process from **D⁺** *to* **E⁺** in the S_3-reaction channel. (A) Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(SMD) level (298 K, 1 M) on the geometries optimized at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in brackets and italics, in red color. *S* stands for solvent (MeOH). (B) 3D CYLview representations for the IRC paths calculated at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol from **TS(D⁺-E⁺)1•** S_2^{kp} and **TS(D⁺-E⁺)2•**S_2^{kp}, showing relevant distances in Ångstroms.



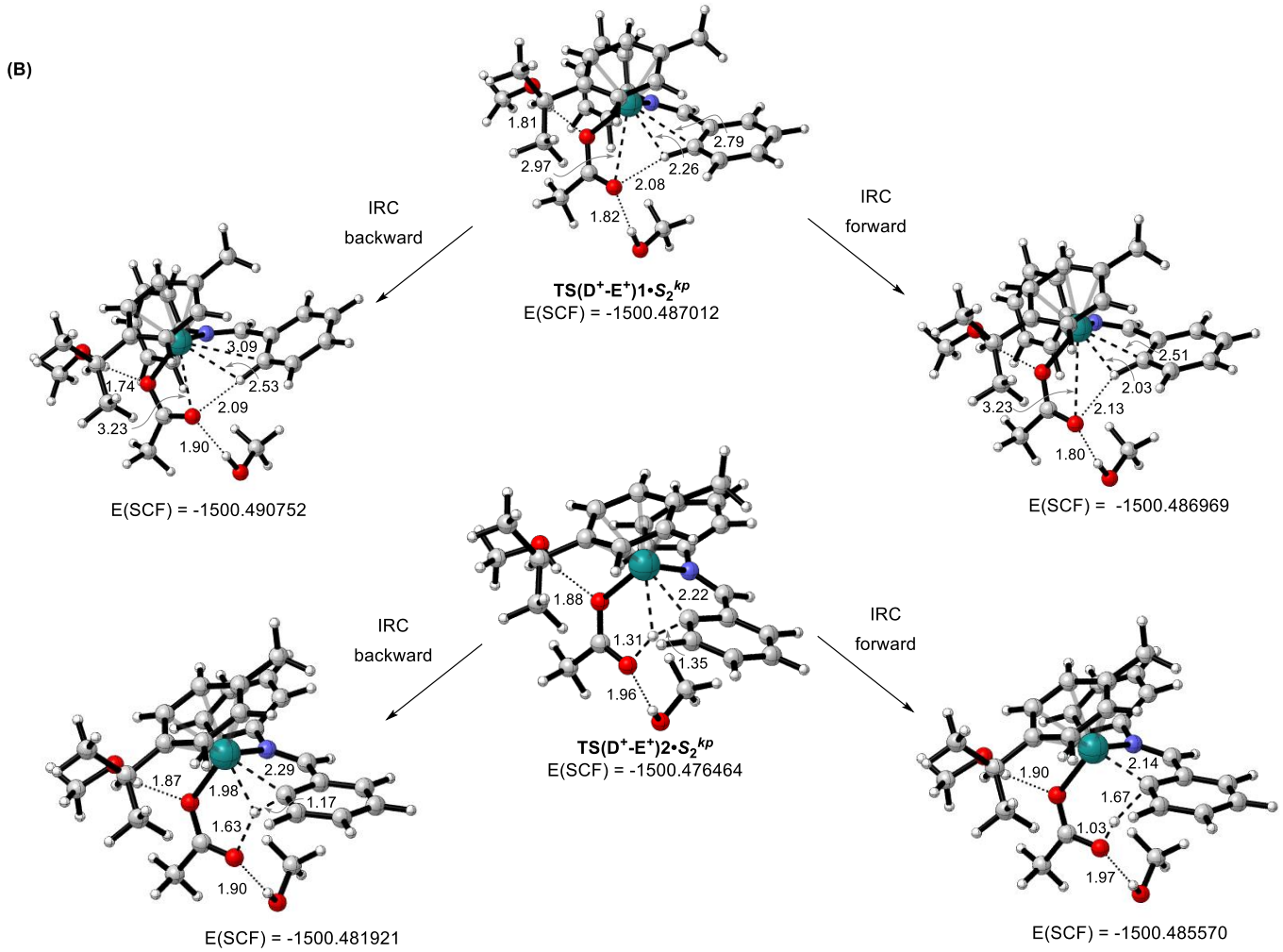


Figure S7. Alternative TS structures of higher energy located for the C-H bond activation process from **D⁺** *to* **E⁺** in the S_2- or S_3-reaction channel. Relative quasi-harmonic free energies (in kcal/mol) calculated at DLPNO-CCSD(T)/CBS(SMD) level (298 K, 1 M) on the geometries optimized at ωB97X-D3/cc-pVDZ-PP[Ru](IEF-PCM) level in methanol are shown in brackets and italics, in red color. Activation barriers with respect to the corresponding lowest energy precursor **D⁺** in the S_2- and S_3-reaction channels are shown in green and orange colour, respectively. *S* stands for solvent (MeOH). 3D CYLview representations show relevant distances in Ångstroms.

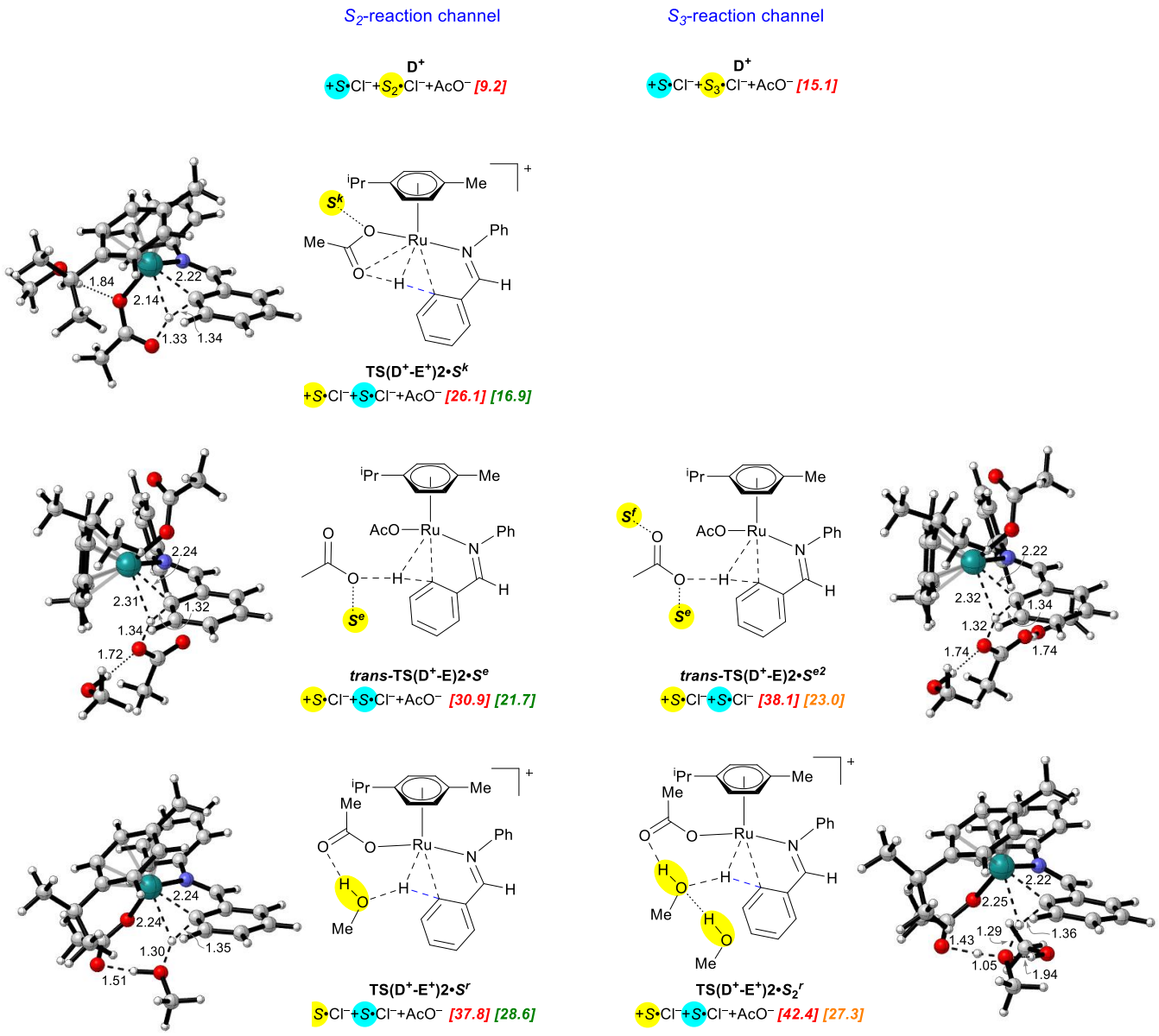


Figure S8a. Energy plot for the acetate/chloride exchange on cycloruthenates E and H in the S_1-reaction channel calculated at DLPNO-CCSD(T)/CBS(SMD) level in methanol (298 K, 1 M) after geometry optimizations at ωB97X-D3/cc-pVDZ-PP[Ru](CPCM) level. Quasi-harmonic Gibbs energies are shown between brackets, in italics and red colour, relative to separated reagents (**A**+½**B**^{0}+2AcO$^-$) plus three explicit MeOH molecules: two active MeOH molecule (close to the reaction center and shadowed in yellow) and one stoichiometric MeOH molecule required to monosolvate one chloride anion (bluish, omitted). Characteristic activation energies in the S_2-reaction channel are shown in magenta color. The hydrogen bonds are represented by dotted lines.

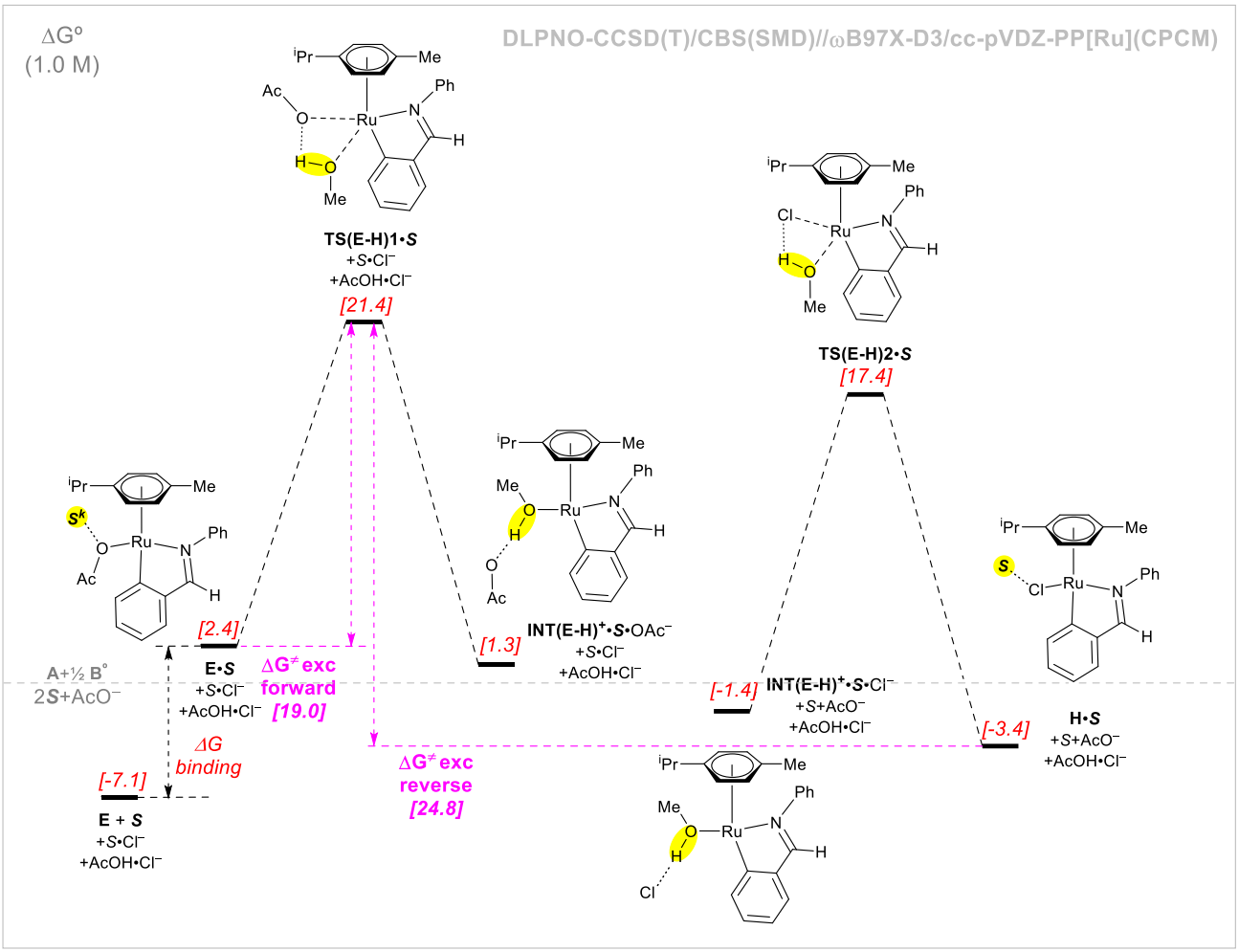
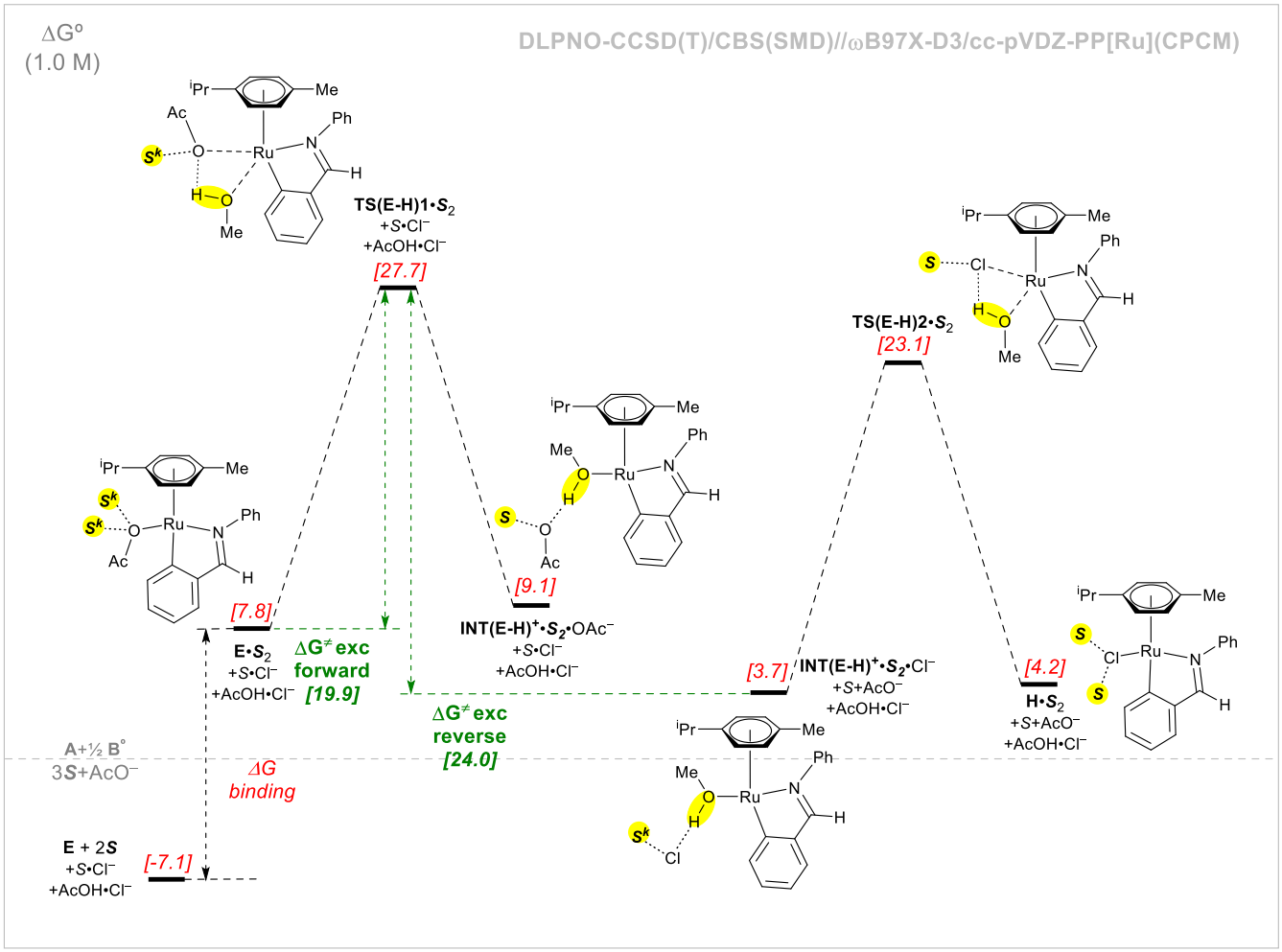


Figure S8b. Energy plot for the acetate/chloride exchange on cycloruthenates E and H in the S_2-reaction channel calculated at DLPNO-CCSD(T)/CBS(SMD) level in methanol (298 K, 1 M) after geometry optimizations at ωB97X-D3/cc-pVDZ-PP[Ru](CPCM) level. Quasi-harmonic Gibbs energies are shown between brackets, in italics and red colour, relative to separated reagents (**A**+½**B**^{0}+2AcO$^-$) plus three explicit MeOH molecules: two active MeOH molecule (close to the reaction center and shadowed in yellow) and one stoichiometric MeOH molecule required to monosolvate one chloride anion (bluish). Characteristic activation energies in the S_2-reaction channel are shown in green color. The hydrogen bonds are represented by dotted lines.



Computed cartesian coordinates (Å), lowest frequencies (cm^{-1}) and energies (a.u.) for all species

Data are tabulated in two columns. The left column includes cartesian coordinates, lowest frequencies and single-point energies calculated using the CPCM solvation model (MeOH) for the stationary points reported in the main text and this supplementary information that were located after geometry optimizations with the M06 functional. The right column includes the corresponding values calculated with either the CPCM or the SMD solvation models (in black and blue colours, respectively) after geometry optimization using the ωB97X-D3 functional. DZ, TZ, ATZ, and QZ are used as abbreviations for the basis sets cc-pVDZ-PP[Ru], cc-pVTZ-PP[Ru], aug-cc-pVTZ-PP[Ru] and cc-pVQZ-PP[Ru], respectively, which are described in the computational details.

A

CPCM (MeOH)

M06 SCF (DZ) = -556.338362

G (1 atm) = -556.175189

qh-G (1 mol/L) = -556.170593

qh-G (24.56 mol/L) = -556.167571

Lowest Frequency = 36.56

HF SCF energy (TZ) = -553.323387

HF SCF energy (QZ) = -553.357682

Correlation energy (DZ) = -1.999661

Correlation energy (TZ) = -2.396219

DLPNO-CCSD(T1)/CBS = -555.995957

PBE0+D3BJ (ATZ) = -556.304776

M06-2X (ATZ) = -556.714303

wB97M-V (ATZ) = -556.727447

B2GP-PLYP (ATZ) = -556.359743

B2K-PLYP (ATZ) = -556.281548

PWPB95 (ATZ) = -556.520809

PWPB95+D3BJ (ATZ) = -556.532185

PWPB95+D4 (ATZ) = -556.542117

* xyz 0 1

C	-0.394341	0.387316	-0.161724
C	-1.840318	0.174932	-0.079571
N	0.453965	-0.523584	0.132117
C	-2.705772	1.213713	-0.443127
C	-2.376706	-1.046231	0.354561
C	1.824324	-0.227067	0.077109
C	-4.085024	1.039010	-0.374921
C	-3.752129	-1.219613	0.421194
C	2.363192	0.991249	0.516830
C	2.690910	-1.221796	-0.397203
C	-4.609200	-0.177457	0.057035
C	3.736406	1.212433	0.455403
C	4.059122	-0.988376	-0.472240
C	4.588853	0.230452	-0.046522
H	-0.079648	1.391490	-0.514115
H	-2.286623	2.166481	-0.781691
H	-1.690795	-1.849499	0.634500
H	-4.753882	1.854605	-0.660000
H	-4.166032	-2.172824	0.759641
H	1.702483	1.753906	0.939370
H	2.260788	-2.175233	-0.715723

A

CPCM (MeOH)

wB97X-D3 SCF (DZ) = -556.638383

G (1 atm) = -556.470061

qh G-E (1 mol/L) = 0.173465

qh G-E (24.56 mol/L) = 0.176488

Lowest Frequency = 48.68

HF SCF energy (TZ) = -553.324306

HF SCF energy (QZ) = -553.357973

Correlation energy (DZ) = -2.000116

Correlation energy (TZ) = -2.396373

DLPNO-CCSD(T1)/CBS = -555.996039

PBE0+D3BJ (ATZ) = -556.304514

M06-2X (ATZ) = -556.718671

wB97M-V (ATZ) = -556.728137

B2GP-PLYP (ATZ) = -556.363482

B2K-PLYP (ATZ) = -556.286137

PWPB95 (ATZ) = -556.523008

PWPB95+D3BJ (ATZ) = -556.534375

PWPB95+D4 (ATZ) = -556.544276

SMD (MeOH)

HF SCF energy (TZ) = -553.329906

HF SCF energy (QZ) = -553.363579

Correlation energy (DZ) = -1.999246

Correlation energy (TZ) = -2.395775

DLPNO-CCSD(T1)/CBS = -556.001210

* xyz 0 1

C	-0.386124	0.375467	-0.174879
C	-1.843678	0.168034	-0.088743
N	0.450527	-0.528907	0.160407
C	-2.704062	1.199695	-0.481696
C	-2.382373	-1.038409	0.381276
C	1.830004	-0.229600	0.091445
C	-4.086241	1.031414	-0.406223
C	-3.760553	-1.205753	0.454630
C	2.367231	0.975191	0.565408
C	2.689078	-1.207317	-0.427496
C	-4.615145	-0.171015	0.061526
C	3.741385	1.202940	0.494150
C	4.058175	-0.968011	-0.508357
C	4.590579	0.238354	-0.047627

```
 H   -5.691834   -0.317348    0.111387
 H    4.145159    2.161955    0.811429
 H    4.720669   -1.768307   -0.858475
 H    5.666057    0.408472   -0.092087
*
---------------------------------------
```

AcO⁻

```
CPCM (MeOH)
M06 SCF (DZ) =             -228.489667
G (1 atm) =                -228.468780
qh-G (1 mol/L) =           -228.465292
qh-G (24.56 mol/L) =       -228.462270
Lowest Frequency =           59.09

HF SCF energy (TZ) =       -227.428657
HF SCF energy (QZ) =       -227.449100
Correlation energy (DZ) =    -0.677188
Correlation energy (TZ) =    -0.849914
DLPNO-CCSD(T1)/CBS =       -228.407144

PBE0+D3BJ (ATZ) =          -228.468326
M06-2X (ATZ) =             -228.635796
wB97M-V (ATZ) =            -228.647626
B2GP-PLYP (ATZ) =          -228.524276
B2K-PLYP (ATZ) =           -228.495969
PWPB95 (ATZ) =             -228.577108
PWPB95+D3BJ (ATZ) =        -228.578246
PWPB95+D4 (ATZ) =          -228.580712

*xyz -1 1
 C   -0.198859    0.000241   -0.003911
 C    1.340779   -0.053193   -0.001954
 O   -0.699107    1.151711    0.000733
 H   -0.807580   -1.096130    0.000823
 H    1.746985    0.581405   -0.807952
 H    1.724599    0.369189    0.943297
 O    1.730389   -1.077525   -0.112606
*
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```

AcOH

```
CPCM (MeOH)
M06 SCF (DZ) =             -228.978659
G (1 atm) =                -228.944284
qh-G (1 mol/L) =           -228.941066
qh-G (24.56 mol/L) =       -228.938043
Lowest Frequency =           90.03

HF SCF energy (TZ) =       -227.913634
HF SCF energy (QZ) =       -227.931207
Correlation energy (DZ) =    -0.681337
```

```
 H   -0.060305    1.360789   -0.554875
 H   -2.285560    2.140822   -0.848711
 H   -1.704232   -1.837599    0.685736
 H   -4.751627    1.841377   -0.712370
 H   -4.175209   -2.146796    0.822628
 H    1.709549    1.723840    1.013873
 H    2.262637   -2.150797   -0.775340
 H   -5.697626   -0.304522    0.122259
 H    4.150283    2.142359    0.873436
 H    4.716749   -1.732683   -0.926706
 H    5.666161    0.419805   -0.100572
*
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```

AcO⁻

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =        -228.557587
G (1 atm) =                -228.535538
qh G-E (1 mol/L) =            0.025811
qh G-E (24.56 mol/L) =        0.028834
Lowest Frequency =           53.83

HF SCF energy (TZ) =       -553.324306
HF SCF energy (QZ) =       -553.357974
Correlation energy (DZ) =    -2.000116
Correlation energy (TZ) =    -2.396373
DLPNO-CCSD(T1)/CBS =       -228.407396

PBE0+D3BJ (ATZ) =          -228.468592
M06-2X (ATZ) =             -228.632204
wB97M-V (ATZ) =            -228.644075
B2GP-PLYP (ATZ) =          -228.520688
B2K-PLYP (ATZ) =           -228.492208
PWPB95 (ATZ) =             -228.573373
PWPB95+D3BJ (ATZ) =        -228.574511
PWPB95+D4 (ATZ) =          -228.576973

SMD (MeOH)
HF SCF energy (TZ) =       -227.438035
HF SCF energy (QZ) =       -227.458181
Correlation energy (DZ) =    -0.674618
Correlation energy (TZ) =    -0.847594
DLPNO-CCSD(T1)/CBS =       -228.412921

* xyz -1 1
 C    0.191240   -0.027724    0.075343
 C   -1.349267   -0.025284   -0.006489
 O    0.772984    1.067356   -0.129474
 H   -1.724880    0.826127   -0.592967
 H   -1.765214    0.057371    1.012338
 H   -1.724238   -0.967961   -0.433330
 O    0.732314   -1.125085    0.364718
*
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```

AcOH

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =        -229.048486
G (1 atm) =                -229.013388
qh G-E (1 mol/L) =            0.038591
qh G-E (24.56 mol/L) =        0.041614
Lowest Frequency =          137.71

HF SCF energy (TZ) =       -227.913954
HF SCF energy (QZ) =       -227.931304
Correlation energy (DZ) =    -0.681429
```

```
Correlation energy (TZ) =    -0.847263
DLPNO-CCSD(T1)/CBS =       -228.880721

PBE0+D3BJ (ATZ) =          -228.940655
M06-2X (ATZ) =             -229.100780
wB97M-V (ATZ) =            -229.111994
B2GP-PLYP (ATZ) =          -228.990109
B2K-PLYP (ATZ) =           -228.962015
PWPB95 (ATZ) =             -229.044860
PWPB95+D3BJ (ATZ) =        -229.046146
PWPB95+D4 (ATZ) =          -229.048126

*xyz 0 1
 C   -0.091646    0.121378    0.000044
 C    1.384977   -0.098574    0.000048
 O   -0.761256   -1.043537   -0.000029
 O   -0.652173    1.192711   -0.000049
 H    1.673179   -0.686235    0.884165
 H    1.673181   -0.686320   -0.884012
 H    1.910037    0.862780    0.000004
 H   -1.708948   -0.820446   -0.000086
*
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```

```
Correlation energy (TZ) =    -0.847288
DLPNO-CCSD(T1)/CBS =       -228.880737

PBE0+D3BJ (ATZ) =          -228.940710
M06-2X (ATZ) =             -229.100081
wB97M-V (ATZ) =            -229.110933
B2GP-PLYP (ATZ) =          -228.989106
B2K-PLYP (ATZ) =           -228.961006
PWPB95 (ATZ) =             -229.043873
PWPB95+D3BJ (ATZ) =        -229.045158
PWPB95+D4 (ATZ) =          -229.047134

SMD (MeOH)
HF SCF energy (TZ) =       -227.915396
HF SCF energy (QZ) =       -227.932704
Correlation energy (DZ) =    -0.679753
Correlation energy (TZ) =    -0.845832
DLPNO-CCSD(T1)/CBS =       -228.880798

*xyz 0 1
 C   -0.092155    0.119565    0.000210
 C    1.391722   -0.108245    0.000036
 O   -0.774773   -1.037263   -0.000071
 O   -0.643484    1.196572   -0.000080
 H    1.675918   -0.693158    0.886312
 H    1.675726   -0.693290   -0.886216
 H    1.915794    0.852866   -0.000094
 H   -1.718787   -0.808811   -0.000267
*
---------------------------------------
```

AcOH•AcO$^-$

```
CPCM (MeOH)
M06 SCF (DZ) =             -457.502185
G (1 atm) =                -457.429534
qh-G (1 mol/L) =           -457.425008
qh-G (24.56 mol/L) =       -457.421985
Lowest Frequency =           46.07

HF SCF energy (TZ) =       -455.348140
HF SCF energy (QZ) =       -455.384075
Correlation energy (DZ) =    -1.372378
Correlation energy (TZ) =    -1.712634
DLPNO-CCSD(T1)/CBS =       -457.306359

PBE0+D3BJ (ATZ) =          -457.429410
M06-2X (ATZ) =             -457.755001
wB97M-V (ATZ) =            -457.775767
B2GP-PLYP (ATZ) =          -457.529071
B2K-PLYP (ATZ) =           -457.472991
PWPB95 (ATZ) =             -457.635496
PWPB95+D3BJ (ATZ) =        -457.639210
PWPB95+D4 (ATZ) =          -457.644745

*xyz -1 1
 C    1.766740    0.004695    0.156664
 C    3.230807    0.028502   -0.231153
 O    1.060045   -0.825225   -0.533012
 O    1.340189    0.736718    1.054896
 H    3.329893    0.278880   -1.299127
 H    3.668261   -0.974020   -0.102016
 H    3.792593    0.754985    0.370902
 H   -0.135225   -0.894021   -0.135839
 C   -2.026728   -0.072103   -0.010177
 C   -1.417256    1.131572   -0.691416
 O   -1.220834   -1.069216    0.210801
```

AcOH•AcO$^-$

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =        -457.638800
G (1 atm) =                -457.562525
qh G-E (1 mol/L) =            0.082408
qh G-E (24.56 mol/L) =        0.085430
Lowest Frequency =         22.25

HF SCF energy (TZ) =       -455.351730
HF SCF energy (QZ) =       -455.387455
Correlation energy (DZ) =    -1.370723
Correlation energy (TZ) =    -1.710766
DLPNO-CCSD(T1)/CBS =       -457.307685

PBE0+D3BJ (ATZ) =          -457.430078
M06-2X (ATZ) =             -457.753071
wB97M-V (ATZ) =            -457.773874
B2GP-PLYP (ATZ) =          -457.527279
B2K-PLYP (ATZ) =           -457.471171
PWPB95 (ATZ) =             -457.633672
PWPB95+D3BJ (ATZ) =        -457.637380
PWPB95+D4 (ATZ) =          -457.642810

SMD (MeOH)
HF SCF energy (TZ) =       -455.356570
HF SCF energy (QZ) =       -455.391748
Correlation energy (DZ) =    -1.366783
Correlation energy (TZ) =    -1.707262
DLPNO-CCSD(T1)/CBS =       -457.308563

*xyz -1 1
 C    1.805466    0.023444    0.138662
 C    3.284790    0.024529   -0.232315
 O    1.092494   -0.828637   -0.497939
 O    1.386301    0.824622    0.992716
```

```
 O   -3.209934   -0.090335    0.316653
 H   -0.948916    0.835032   -1.643455
 H   -0.606041    1.525132   -0.056919
 H   -2.177662    1.902471   -0.871762
*
---------------------------------------
```

AcOH•Cl$^-$

```
CPCM (MeOH)
M06 SCF (DZ) =             -689.348508
G (1 atm) =                -689.318052
qh-G (1 mol/L) =           -689.314583
qh-G (24.56 mol/L) =       -689.311561
Lowest Frequency =           73.00

HF SCF energy (TZ) =       -687.595253
HF SCF energy (QZ) =       -687.618072
Correlation energy (DZ) =    -0.836980
Correlation energy (TZ) =    -1.077866
DLPNO-CCSD(T1)/CBS =       -688.843573

PBE0+D3BJ (ATZ) =          -689.199269
M06-2X (ATZ) =             -689.498094
wB97M-V (ATZ) =            -689.499859
B2GP-PLYP (ATZ) =          -689.227255
B2K-PLYP (ATZ) =           -689.168414
PWPB95 (ATZ) =             -689.404594
PWPB95+D3BJ (ATZ) =        -689.406725
PWPB95+D4 (ATZ) =          -689.409408

*xyz -1 1
 O   -0.470535   -1.037237    0.017412
 C   -1.404213   -0.091669   -0.001022
 H    0.457581   -0.652676    0.017000
 C   -0.910539    1.326456    0.005780
 O   -2.580474   -0.391641   -0.016500
 Cl   2.361626   -0.020840   -0.005574
 H   -0.201681    1.489151   -0.820287
 H   -0.349170    1.521653    0.932846
 H   -1.757795    2.018456   -0.070645
*
---------------------------------------
```

B^0

```
CPCM (MeOH)
M06 SCF (DZ) =           -2808.636857
G (1 atm) =              -2808.270709
qh-G (1 mol/L) =         -2808.261688
qh-G (24.56 mol/L) =     -2808.258666
Lowest Frequency =           5.95

HF SCF energy (TZ) =     -2799.849316
```

```
 H    3.395921    0.316732   -1.288115
 H    3.699027   -0.989934   -0.133449
 H    3.853620    0.720319    0.397790
 C   -2.068404   -0.072964   -0.030663
 C   -1.431100    1.130627   -0.684881
 O   -1.271180   -1.088307    0.224912
 O   -3.256323   -0.116807    0.256624
 H   -0.997327    0.839765   -1.653261
 H   -0.599363    1.478398   -0.053399
 H   -2.177415    1.920110   -0.829933
 H   -0.270577   -0.908830   -0.071708
*
---------------------------------------
```

AcOH•Cl$^-$

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =        -689.432595
G (1 atm) =                -689.401220
qh G-E (1 mol/L) =            0.035173
qh G-E (24.56 mol/L) =        0.038196
Lowest Frequency =          71.1

HF SCF energy (TZ) =       -687.595798
HF SCF energy (QZ) =       -687.618431
Correlation energy (DZ) =    -0.836947
Correlation energy (TZ) =    -1.077819
DLPNO-CCSD(T1)/CBS =       -228.880737

PBE0+D3BJ (ATZ) =          -689.199438
M06-2X (ATZ) =             -689.496550
wB97M-V (ATZ) =            -689.498487
B2GP-PLYP (ATZ) =          -689.225933
B2K-PLYP (ATZ) =           -689.167088
PWPB95 (ATZ) =             -689.403170
PWPB95+D3BJ (ATZ) =        -689.405290
PWPB95+D4 (ATZ) =          -689.407963

SMD (MeOH)
HF SCF energy (TZ) =       -687.591537
HF SCF energy (QZ) =       -687.614395
Correlation energy (DZ) =    -0.835336
Correlation energy (TZ) =    -1.076439
DLPNO-CCSD(T1)/CBS =       -688.841535

*xyz -1 1
 O   -0.459942   -1.033698    0.012590
 C   -1.396282   -0.089851   -0.007965
 H   -0.916266    1.339513    0.000703
 C   -2.570567   -0.403696   -0.032278
 O    0.463726   -0.647916    0.029352
 Cl  -0.276515    1.524732   -0.874446
 H   -0.298795    1.522717    0.892053
 H   -1.776510    2.017858   -0.009765
 H    2.375950   -0.068007    0.048767
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B^0

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -2809.200467
G (1 atm) =               -2808.820780
qh G-E (1 mol/L) =            0.391637
qh G-E (24.56 mol/L) =        0.394660
Lowest Frequency =           13.84

HF SCF energy (TZ) =      -2799.852924
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```
HF SCF energy (QZ) =      -2799.913015
Correlation energy (DZ) =    -4.615789
Correlation energy (TZ) =    -5.832394
DLPNO-CCSD(T1)/CBS =      -2806.475507

PBE0+D3BJ (ATZ) =         -2808.175246
M06-2X (ATZ) =            -2809.018282
wB97M-V (ATZ) =           -2809.060377
B2GP-PLYP (ATZ) =         -2807.966640
B2K-PLYP (ATZ) =          -2807.723402
PWPB95 (ATZ) =            -2808.706555
PWPB95+D3BJ (ATZ) =       -2808.754580
PWPB95+D4 (ATZ) =         -2808.757637

*xyz 0 1
 C   -3.979983   -0.182404    0.126288
 C   -4.877559    1.026961    0.086793
 C   -3.747759   -0.930662   -1.072356
 C   -6.326937    0.554249    0.186643
 C   -4.561495    2.062203    1.152489
 C   -3.300562   -0.607430    1.295131
 C   -2.882749   -2.045176   -1.086525
 C   -2.439027   -1.743403    1.289248
 C   -2.218850   -2.482543    0.105563
 C   -1.256563   -3.620634    0.078676
 Ru  -1.841473   -0.341596   -0.263015
 Cl  -1.807797    1.639823   -1.688599
 H   -4.725494    1.490738   -0.905324
 H   -4.161008   -0.561334   -2.015435
 H   -7.015864    1.409816    0.108929
 H   -6.506493    0.059640    1.157046
 H   -6.580318   -0.162009   -0.611378
 H   -3.501912    2.364641    1.127376
 H   -4.794707    1.689201    2.164581
 H   -5.175992    2.961443    0.992919
 H   -3.347241    0.006205    2.198296
 H   -2.641367   -2.527497   -2.037601
 H   -1.852269   -1.978870    2.181423
 H   -0.433291   -3.455078    0.789687
 H   -1.779676   -4.549022    0.360914
 H   -0.832270   -3.760923   -0.925472
 C    1.256091    3.620505   -0.077996
 C    2.218572    2.482576   -0.105134
 C    2.882703    2.045034    1.086749
 C    2.438680    1.743743   -1.289026
 C    3.747879    0.930648    1.072172
 C    3.300331    0.607871   -1.295296
 C    3.980004    0.182666   -0.126662
 C    4.877610   -1.026699   -0.087465
 C    6.326998   -0.554016   -0.187212
 C    4.561508   -2.061702   -1.153383
 Ru   1.841536    0.341483    0.263069
 Cl   1.808062   -1.639798    1.688784
 H    0.432045    3.454218   -0.787957
 H    1.778698    4.548759   -0.361611
 H    0.832933    3.761532    0.926524
 H    2.641431    2.527114    2.037975
 H    1.851826    1.979417   -2.181084
 H    4.161310    0.561158    2.015109
 H    3.346926   -0.005557   -2.198605
 H    4.725532   -1.490701    0.904546
 H    7.015901   -1.409613   -0.109624
 H    6.506585   -0.059255   -1.157531
 H    6.580396    0.162105    0.610927
 H    3.501947   -2.364221   -1.128230
 H    4.794581   -1.688432   -2.165407
```

```
HF SCF energy (QZ) =      -2799.915306
Correlation energy (DZ) =    -4.614899
Correlation energy (TZ) =    -5.831790
DLPNO-CCSD(T1)/CBS =      -2806.476966

PBE0+D3BJ (ATZ) =         -2808.176306
M06-2X (ATZ) =            -2809.026902
wB97M-V (ATZ) =           -2809.067874
B2GP-PLYP (ATZ) =         -2807.978585
B2K-PLYP (ATZ) =          -2807.736773
PWPB95 (ATZ) =            -2808.716045
PWPB95+D3BJ (ATZ) =       -2808.763972
PWPB95+D4 (ATZ) =         -2808.766988

SMD (MeOH)
HF SCF energy (TZ) =      -2799.859088
HF SCF energy (QZ) =      -2799.921684
Correlation energy (DZ) =    -4.616808
Correlation energy (TZ) =    -5.833040
DLPNO-CCSD(T1)/CBS =      -2806.484273

*xyz 0 1
 C   -3.980964   -0.183264    0.108095
 C   -4.899958    1.019639    0.077352
 C   -3.742396   -0.926117   -1.093786
 C   -6.343814    0.528619    0.247331
 C   -4.545411    2.094584    1.101893
 C   -3.305470   -0.609022    1.274776
 C   -2.875776   -2.036282   -1.112076
 C   -2.440439   -1.744715    1.266187
 C   -2.216020   -2.476893    0.082344
 C   -1.270285   -3.639736    0.056840
 Ru  -1.840228   -0.338460   -0.276725
 Cl  -1.824303    1.640503   -1.704224
 H   -4.797822    1.458347   -0.928489
 H   -4.159823   -0.562768   -2.034440
 H   -7.045420    1.371505    0.160950
 H   -6.482325    0.065758    1.237941
 H   -6.609085   -0.216479   -0.518110
 H   -3.496851    2.413869    1.002742
 H   -4.709023    1.747271    2.134340
 H   -5.186095    2.975137    0.948655
 H   -3.367467   -0.011629    2.184865
 H   -2.645068   -2.519681   -2.062619
 H   -1.871195   -1.990597    2.163847
 H   -0.479372   -3.519669    0.808914
 H   -1.834578   -4.557532    0.283367
 H   -0.808787   -3.753528   -0.932162
 C    1.269807    3.639564   -0.055947
 C    2.215708    2.476863   -0.081846
 C    2.875848    2.036153    1.112321
 C    2.439901    1.744916   -1.265880
 C    3.742598    0.926095    1.093614
 C    3.305066    0.609337   -1.274877
 C    3.980923    0.183455   -0.108445
 C    4.900041   -1.019366   -0.078132
 C    6.343831   -0.528184   -0.248190
 C    4.545464   -2.094076   -1.102910
 Ru   1.840290    0.338328    0.276968
 Cl   1.824897   -1.640597    1.704508
 H    0.478490    3.519247   -0.807555
 H    1.833833    4.557410   -0.282934
 H    0.808851    3.753424    0.933299
 H    2.645352    2.519377    2.063005
 H    1.870373    1.990869   -2.163341
 H    4.160313    0.562643    2.034099
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 H    5.176078   -2.960945   -0.994104
 Cl   0.362668   -0.927698   -1.310703
 Cl  -0.362604    0.927185    1.311020
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B^{0+}

```
CPCM (MeOH)
M06 SCF (DZ) =            -2348.247695
G (1 atm) =               -2347.877346
qh-G (1 mol/L) =          -2347.869537
qh-G (24.56 mol/L) =      -2347.866515
Lowest Frequency =            9.36

HF SCF energy (TZ) =      -2340.165822
HF SCF energy (QZ) =      -2340.226362
Correlation energy (DZ) =    -4.447875
Correlation energy (TZ) =    -5.594326
DLPNO-CCSD(T1)/CBS =      -2346.508841

*xyz 1 1
 C   -3.502385    0.254739    0.617285
 C   -3.760145    1.428306    1.527066
 C   -3.527928    0.350723   -0.794771
 C   -5.210933    1.350599    2.001668
 C   -3.457995    2.776471    0.895494
 H   -3.099837    1.293989    2.404403
 C   -3.161117   -1.015493    1.185029
 C   -3.223086   -0.772639   -1.618275
 H   -3.667755    1.324816   -1.269315
 H   -5.428588    0.394344    2.503261
 H   -5.902010    1.453844    1.147588
 H   -5.422423    2.165126    2.711324
 H   -2.434062    2.822753    0.490073
 H   -4.166331    3.011540    0.083042
 H   -3.561071    3.570874    1.649989
 C   -2.859843   -2.128668    0.373648
 H   -3.023572   -1.090984    2.267845
 C   -2.889249   -2.027781   -1.053988
 H   -3.144695   -0.637433   -2.700005
 H   -2.497667   -3.050096    0.836737
 C   -2.486593   -3.177360   -1.912627
 H   -1.780849   -3.839477   -1.391607
 H   -3.379766   -3.770789   -2.167022
 H   -2.030697   -2.832709   -2.851686
 C    2.415056    3.410269   -1.450320
 C    2.855468    2.137498   -0.812243
 H    1.714768    3.958283   -0.803962
 H    3.293260    4.053721   -1.621555
 H    1.938129    3.226796   -2.423407
 C    3.168116    0.986507   -1.603971
 C    2.887921    1.996660    0.596563
 C    3.503555   -0.240967   -0.996553
 H    3.042724    1.034059   -2.688691
 C    3.228044    0.753756    1.206776
 H    2.547677    2.825230    1.222831
 C    3.541282   -0.386279    0.428141
 H    3.629687   -1.129338   -1.622807
 H    3.129771    0.658795    2.290715
 H    3.366873    0.012094   -2.185078
 H    4.798074   -1.458337    0.927613
 H    7.045519   -1.371032   -0.162103
 H    6.482165   -0.065083   -1.238712
 H    6.609148    0.216759    0.517387
 H    3.496938   -2.413477   -1.003754
 H    4.708939   -1.746471   -2.135280
 H    5.186232   -2.974619   -0.949976
 Cl   0.363924   -0.918606   -1.296608
 Cl  -0.363854    0.918166    1.297086
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 C    3.847419   -1.734142    1.028715
 C    3.239134   -1.948284    2.404109
 C    5.365584   -1.906734    1.060246
 H    3.425942   -2.486745    0.336133
 H    2.152456   -1.763780    2.408024
 H    3.707099   -1.295448    3.160401
 H    3.409257   -2.986279    2.727392
 H    5.812062   -1.797835    0.059234
 H    5.825531   -1.154477    1.723782
 H    5.626617   -2.904678    1.444614
 Ru  -1.612802   -0.459377   -0.212343
 Ru   1.618094    0.438583   -0.197214
 Cl   0.491634   -1.767211   -0.506300
 Cl  -0.169318    0.607659    1.525297
 Cl  -0.309514    1.113537   -1.630690
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B[1]

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CPCM (MeOH)
M06 SCF (DZ) =            -1172.476173
G (1 atm) =               -1172.257738
qh-G (1 mol/L) =          -1172.252182
qh-G (24.56 mol/L) =      -1172.249159
Lowest Frequency =           25.86

HF SCF energy (TZ) =      -1167.702638
HF SCF energy (QZ) =      -1167.747545
Correlation energy (DZ) =    -2.822811
Correlation energy (TZ) =    -3.530360
DLPNO-CCSD(T1)/CBS =      -1171.704881

PBE0+D3BJ (ATZ) =         -1172.319333
M06-2X (ATZ) =            -1172.770100
wB97M-V (ATZ) =           -1172.811090
B2GP-PLYP (ATZ) =         -1172.293525
B2K-PLYP (ATZ) =          -1172.174040
PWPB95 (ATZ) =            -1172.592978
PWPB95+D3BJ (ATZ) =       -1172.613533
PWPB95+D4 (ATZ) =         -1172.620329

*xyz 0 1
 Ru  -0.311540    0.101584   -0.145732
 O   -2.486014    0.033521   -0.233320
 O   -1.402935   -1.272948    1.120033
 C   -2.508442   -0.922740    0.601180
 Cl  -0.382311   -1.674273   -1.788724
 C   -3.772745   -1.636495    0.926884
 H   -4.635420   -0.966263    0.822473
 H   -3.895780   -2.466166    0.213006
 H   -3.731248   -2.059948    1.938425
 C    0.432742    1.888845   -1.115186
 C    1.463212    0.925996   -1.080470
 C   -0.256863    2.255775    0.084021
 H    0.091151    2.285226   -2.074352
 C    1.840242    0.268325    0.125851
 H    1.885378    0.568879   -2.024676
 C   -1.430656    3.173665    0.029401
 C    0.144552    1.653557    1.305118
 C    2.890728   -0.813767    0.099053
 C    1.156553    0.656219    1.312925
 H   -1.092424    4.219448    0.110263
 H   -1.968641    3.066709   -0.923919
 H   -2.129183    2.975533    0.854708
 H   -0.417583    1.862015    2.218741
 C    2.664151   -1.909235    1.128558
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B[1]

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1172.815540
G (1 atm) =               -1172.590581
qh G-E (1 mol/L) =            0.231997
qh G-E (24.56 mol/L) =        0.235020
Lowest Frequency =           20.60

HF SCF energy (TZ) =      -1167.704129
HF SCF energy (QZ) =      -1167.748386
Correlation energy (DZ) =    -2.822992
Correlation energy (TZ) =    -3.530291
DLPNO-CCSD(T1)/CBS =      -1171.705313

PBE0+D3BJ (ATZ) =         -1172.319786
M06-2X (ATZ) =            -1172.770408
wB97M-V (ATZ) =           -1172.811106
B2GP-PLYP (ATZ) =         -1172.294430
B2K-PLYP (ATZ) =          -1172.175112
PWPB95 (ATZ) =            -1172.593761
PWPB95+D3BJ (ATZ) =       -1172.614183
PWPB95+D4 (ATZ) =         -1172.620961

SMD (MeOH)
HF SCF energy (TZ) =      -1167.711868
HF SCF energy (QZ) =      -1167.756064
Correlation energy (DZ) =    -2.819917
Correlation energy (TZ) =    -3.527579
DLPNO-CCSD(T1)/CBS =      -1171.710473

*xyz 0 1
 Ru  -0.346583    0.147443    0.086890
 C    1.568222    0.780919    0.863672
 C    1.046074    0.550593   -1.501694
 C    1.777998    0.097788   -0.353684
 C    0.639418    1.860142    0.958552
 C    0.133461    1.619897   -1.415660
 C   -0.099946    2.285161   -0.168180
 Cl  -1.031679   -0.810646    2.206065
 C    2.699058   -1.098478   -0.481161
 C   -1.152022    3.349230   -0.056244
 C    4.071826   -0.608281   -0.958479
 C    2.806733   -1.931523    0.794458
 H    2.030560    0.412371    1.779167
 H    1.116470   -0.012310   -2.434591
 H    0.423383    2.292907    1.936097
 H   -0.483141    1.869373   -2.280878
 H    2.268979   -1.737108   -1.270891
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 C    4.265306   -0.171495    0.268678
 H    2.837451   -1.268924   -0.907682
 H    1.332041    0.101864    2.238934
 H    2.812770   -1.539318    2.157519
 H    3.388471   -2.723799    0.974397
 H    1.650021   -2.335642    1.056331
 H    4.455689    0.593039   -0.501579
 H    5.059664   -0.931409    0.201446
 H    4.343622    0.315231    1.256699
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 H   -2.004238    3.129427   -0.713382
 H   -0.724893    4.315171   -0.366304
 H   -1.510444    3.443535    0.976948
 H    3.994698   -0.057044   -1.907979
 H    4.525730    0.061495   -0.210265
 H    4.749718   -1.460882   -1.112357
 H    1.814984   -2.239805    1.159406
 H    3.317831   -1.382480    1.601233
 H    3.394819   -2.838936    0.594110
 O   -1.055871   -1.706453   -0.760533
 O   -2.416234   -0.044964   -0.476662
 C   -2.245157   -1.261161   -0.804495
 C   -3.396460   -2.137988   -1.173035
 H   -3.064837   -2.958379   -1.820186
 H   -3.806872   -2.565576   -0.245425
 H   -4.184195   -1.552028   -1.661679
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B[1]•*S*

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CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1288.528756
G (1 atm) =               -1288.256036
qh G-E (1 mol/L) =            0.282591
qh G-E (24.56 mol/L) =        0.285614
Lowest Frequency =           20.65

SMD (MeOH)
HF SCF energy (TZ) =      -1282.806174
HF SCF energy (QZ) =      -1282.858935
Correlation energy (DZ) =    -3.200154
Correlation energy (TZ) =    -3.999607
DLPNO-CCSD(T1)/CBS =      -1287.341590

*xyz 0 1
Ru  -0.356535   -0.090226    0.151894
 C    1.063583    0.577137   -1.321776
 C    0.144163    1.616063   -1.074126
 C    1.779169   -0.061304   -0.254490
 H    1.153869    0.179245   -2.334536
 C    0.611092    1.452880    1.314674
 C    1.546417    0.405732    1.057352
 C   -0.110232    2.062889    0.263728
 O   -2.437629   -0.176259   -0.402580
 O   -1.080009   -1.744825   -1.024222
 Cl  -1.029590   -1.426882    2.074247
 H   -0.456092    2.008859   -1.896538
 C    2.718093   -1.213767   -0.555055
 H    0.375291    1.713811    2.347209
 H    1.973557   -0.127263    1.909790
 C   -1.167727    3.091979    0.536613
 C   -2.270219   -1.302116   -0.968432
 H    0.912712   -1.616581    3.203199
 C    2.617935   -2.363554    0.447689
 C    4.147765   -0.666940   -0.652205
 H    2.429644   -1.599087   -1.546946
 H   -1.999409    2.999194   -0.174575
 H   -0.731773    4.096204    0.422067
 H   -1.555618    2.997710    1.559216
 C   -3.423242   -2.090639   -1.498222
 O    1.746106   -1.484474    3.690478
 H    1.592434   -2.760349    0.497368
 H    2.910342   -2.055040    1.463091
 H    3.286889   -3.181035    0.140354
 H    4.218041    0.144831   -1.392362
 H    4.479245   -0.272250    0.322030
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 H    4.842403   -1.465679   -0.952286
 H   -4.210291   -1.419211   -1.862390
 H   -3.833580   -2.690159   -0.671347
 H   -3.092391   -2.768879   -2.293436
 C    1.445858   -0.653113    4.796707
 H    0.707261   -1.115781    5.475394
 H    2.376892   -0.494700    5.359727
 H    1.059519    0.334659    4.485551
*
```

$B^1 \bullet S_2$

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1404.241013
G (1 atm) =               -1403.920305
qh G-E (1 mol/L) =            0.333096
qh G-E (24.56 mol/L) =        0.336119
Lowest Frequency =          13.2

SMD (MeOH)
HF SCF energy (TZ) =      -1397.892595
HF SCF energy (QZ) =      -1397.961126
Correlation energy (DZ) =    -3.580848
Correlation energy (TZ) =    -4.471754
DLPNO-CCSD(T1)/CBS =      -1402.974118

*xyz 0 1
Ru   -0.366441   -0.184297    0.175564
 C     1.047215    0.542356   -1.262415
 C     0.091487    1.553378   -1.020550
 C     1.778403   -0.080157   -0.199466
 C     0.539617    1.374921    1.374388
 C     1.512836    0.369488    1.113821
 C    -0.195501    1.967777    0.317671
 Cl   -0.867971   -1.788300    1.956200
 C     2.768759   -1.186162   -0.507243
 C    -1.306554    2.932804    0.608721
 C     2.794195   -2.296381    0.542674
 C     4.155953   -0.562490   -0.706045
 H     1.155640    0.151516   -2.276572
 H    -0.509120    1.935735   -1.847231
 H     0.276210    1.611694    2.405748
 H     1.944353   -0.149876    1.972901
 H     2.450862   -1.629857   -1.465485
 H    -2.075677    2.896421   -0.173857
 H    -0.897206    3.954052    0.643326
 H    -1.763001    2.702437    1.580564
 H     3.155546   -1.934299    1.517922
 H     1.793844   -2.730835    0.690252
 H     3.473035   -3.097982    0.216050
 H     4.139960    0.212054   -1.488017
 H     4.509173   -0.098025    0.229035
 H     4.882852   -1.333667   -1.001860
 O    -2.489565   -0.233345   -0.180741
 O    -1.191244   -1.677974   -1.138893
 C    -2.373051   -1.268889   -0.909210
 C    -3.569683   -1.997276   -1.427199
 H    -4.403909   -1.302280   -1.580371
 H    -3.868381   -2.739909   -0.671661
 H    -3.325891   -2.523793   -2.357509
 O    -1.818100    0.936132    3.443571
 C    -2.800657    0.630751    4.416940
 H    -1.564065    0.100347    3.014657
 H    -2.411290   -0.044180    5.199974
 H    -3.101262    1.573676    4.895312
 H    -3.698171    0.168259    3.970365
```

```
 O     1.725180   -1.383332    3.815836
 C     1.088933   -0.693661    4.878989
 H     1.015724   -1.738462    3.253268
 H     0.634505   -1.390251    5.607187
 H     0.302135   -0.008599    4.518290
 H     1.853467   -0.102116    5.403225
*
```

$B^1 \bullet S_3^k$

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1519.950272
G (1 atm) =               -1519.580256
qh G-E (1 mol/L) =            0.383935
qh G-E (24.56 mol/L) =        0.386958
Lowest Frequency =           11.81

SMD (MeOH)
HF SCF energy (TZ) =      -1512.996941
HF SCF energy (QZ) =      -1513.065938
Correlation energy (DZ) =    -3.960078
Correlation energy (TZ) =    -4.942582
DLPNO-CCSD(T1)/CBS =      -1518.603423

*xyz 0 1
Ru  -0.188594   -0.789463    0.187138
 Cl  -0.717069   -2.117012    2.173247
 C    1.086188    0.129704   -1.290081
 C   -0.054683    0.934204   -1.103970
 C    1.892282   -0.289566   -0.180005
 C   -0.441449    1.367129    0.206884
 C    3.061363   -1.224907   -0.419151
 C    1.526231    0.163663    1.106150
 C   -1.716116    2.128587    0.426551
 C    0.373915    0.984080    1.295214
 C    3.209090   -2.304011    0.653168
 C    4.336879   -0.385144   -0.561991
 H    1.290506   -0.298952   -2.272892
 H   -0.709015    1.139083   -1.953232
 H    2.865339   -1.721028   -1.383529
 H    2.034526   -0.219766    1.993509
 H   -2.102452    1.938869    1.436623
 H   -1.518210    3.206123    0.319264
 H   -2.475236    1.846175   -0.315339
 H    0.040700    1.216143    2.308101
 H    2.288957   -2.901005    0.748096
 H    3.441610   -1.877621    1.641356
 H    4.030497   -2.983763    0.382395
 H    4.231995    0.372222   -1.353914
 H    4.568538    0.135024    0.381682
 H    5.190955   -1.030419   -0.816396
 O   -0.404008   -2.663341   -0.871691
 C   -1.667710   -2.502871   -0.968488
 O   -2.136559   -1.416969   -0.515414
 C   -2.546961   -3.559164   -1.550125
 H   -3.026227   -4.099809   -0.719925
 H   -1.958991   -4.266659   -2.145873
 H   -3.335513   -3.099342   -2.158880
 O    1.186582   -2.536958   -3.169734
 C    0.169863   -2.217762   -4.100779
 H    0.734766   -2.760793   -2.337274
 H   -0.472956   -1.387497   -3.751303
 H   -0.478818   -3.084254   -4.324247
 H    0.654034   -1.902876   -5.036471
 O    1.960756   -1.419366    3.854455
 C    1.311517   -0.750103    4.922798
```

```
 H    1.263943   -1.864759    3.343160
 H    0.441277   -0.166315    4.576634
 H    0.969186   -1.454674    5.702628
 H    2.036713   -0.060460    5.378435
 O   -1.777630    0.611489    3.546438
 C   -2.602177    0.405151    4.679446
 H   -1.544392   -0.261347    3.182875
 H   -3.534039   -0.127995    4.422788
 H   -2.080964   -0.160439    5.472122
 H   -2.869451    1.392833    5.080794
*
```

B²

```
CPCM (MeOH)
M06 SCF (DZ) =              -940,635305
G (1 atm) =                 -940,373415
qh-G (1 mol/L) =            -940.366041
qh-G (24.56 mol/L) =        -940.363018
Lowest Frequency =            21.03

HF SCF energy (TZ) =        -935.468517
HF SCF energy (QZ) =        -935.526669
Correlation energy (DZ) =     -3.350250
Correlation energy (TZ) =     -4.157441
DLPNO-CCSD(T1)/CBS =        -940.173303

PBE0+D3BJ (ATZ) =           -940.551862
M06-2X (ATZ) =              -941.010042
wB97M-V (ATZ) =             -941.072758
B2GP-PLYP (ATZ) =           -940.581115
B2K-PLYP (ATZ) =            -940.464109
PWPB95 (ATZ) =              -940.810085
PWPB95+D3BJ (ATZ) =         -940.832472
PWPB95+D4 (ATZ) =           -940.842162

*xyz 0 1
 Ru   0.214373   -0.365967    0.082209
 O    1.376043    1.342619    0.077095
 O    2.146656   -1.242665   -0.404348
 C    1.206978    2.413165    0.797767
 O    0.913201   -0.393663   -1.981526
 C    2.015410   -0.912055   -1.623232
 C    2.224727    3.485672    0.481207
 O    0.339071    2.586314    1.649421
 C    3.130223   -1.095510   -2.593963
 H    2.139831    3.779555   -0.576234
 H    3.242959    3.092600    0.621551
 H    2.075570    4.365340    1.120141
 H    3.758960   -1.948191   -2.307185
 H    3.757103   -0.190266   -2.582337
 H    2.741481   -1.227913   -3.611735
 C   -0.309492   -1.536549    1.832600
 C    0.650205   -2.167935    2.785462
 C   -0.722793   -2.237121    0.655148
 C   -0.752003   -0.203137    2.008662
 H    1.362042   -2.818462    2.255434
 H    1.212294   -1.408011    3.346676
 H    0.104913   -2.792777    3.511506
 C   -1.513691   -1.598931   -0.319036
 H   -0.315899   -3.231741    0.453860
 C   -1.562795    0.435977    1.025636
 H   -0.370157    0.388082    2.842804
 C   -1.933207   -0.237299   -0.160806
 H   -1.708760   -2.107579   -1.268073
```

B²

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -941.0299423
G (1 atm) =                -940.757828
qh G-E (1 mol/L) =            0.280123
qh G-E (24.56 mol/L) =        0.283146
Lowest Frequency =          19.75

HF SCF energy (TZ) =        -935.469371
HF SCF energy (QZ) =        -935.526746
Correlation energy (DZ) =     -3.350462
Correlation energy (TZ) =     -4.158334
DLPNO-CCSD(T1)/CBS =        -940.174436

PBE0+D3BJ (ATZ) =           -940.552845
M06-2X (ATZ) =              -941.030346
wB97M-V (ATZ) =             -941.091302
B2GP-PLYP (ATZ) =           -940.599092
B2K-PLYP (ATZ) =            -940.482673
PWPB95 (ATZ) =              -940.827888
PWPB95+D3BJ (ATZ) =         -940.850396
PWPB95+D4 (ATZ) =           -940.860118

SMD (MeOH)
HF SCF energy (TZ) =        -935.481707
HF SCF energy (QZ) =        -935.538799
Correlation energy (DZ) =     -3.350462
Correlation energy (TZ) =     -4.153262
DLPNO-CCSD(T1)/CBS =        -940.178368

*xyz 0 1
 Ru  -0.159670   -0.465898    0.070185
 O   -1.089071    1.303978   -0.441674
 C   -1.197181    2.355218    0.315303
 C   -1.876669    3.518272   -0.382168
 O   -0.805104    2.444508    1.478814
 C    1.685338   -1.460198   -0.364682
 C    0.992142   -2.236262    0.595996
 C    1.966179   -0.074842   -0.168073
 C    0.496819   -1.620158    1.776293
 C    2.710750    0.711956   -1.229719
 C    1.507609    0.508028    1.042257
 C   -0.364016   -2.384170    2.738408
 C    0.776268   -0.238684    1.997138
 C    2.189496    2.137987   -1.407182
 C    4.209690    0.692408   -0.906045
 H   -1.278249    3.822262   -1.253888
 H   -2.862359    3.204980   -0.755125
 H   -1.988782    4.367333    0.302341
 H    1.931336   -1.912477   -1.328239
 H    0.734347   -3.272065    0.371963
 H    2.557838    0.173233   -2.179809
```

```
 H   -1.756087    1.502677    1.138391
 C   -2.673240    0.439215   -1.287546
 C   -2.407693    1.932991   -1.378788
 C   -4.164755    0.146455   -1.144161
 H   -2.313150   -0.034410   -2.221182
 H   -2.846715    2.476156   -0.524666
 H   -2.867053    2.341803   -2.291829
 H   -1.327486    2.153472   -1.408847
 H   -4.727578    0.582755   -1.984170
 H   -4.368099   -0.936271   -1.121337
 H   -4.553574    0.585235   -0.208795
*
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B^{+S}

```
CPCM (MeOH)
M06 SCF (DZ) =             -827.752645
G (1 atm) =                -827.483550
qh-G (1 mol/L) =           -827.477717
qh-G (24.56 mol/L) =       -827.474695
Lowest Frequency =           26.9

HF SCF energy (TZ) =       -823.112478
HF SCF energy (QZ) =       -823.162218
Correlation energy (DZ) =    -3.031128
Correlation energy (TZ) =    -3.758015
DLPNO-CCSD(T1)/CBS =       -827.359966

*xyz 1 1
 Ru  -0.282944    0.107309    0.054845
 O   -0.398289   -1.700224    1.285547
 O   -2.435718    0.043577    0.156909
 C   -1.022051   -1.637695    2.578310
 H   -0.764050   -2.449670    0.786684
 O   -1.362518   -1.128488   -1.315693
 C   -2.478203   -0.807255   -0.786188
 H   -0.891829   -2.598066    3.095260
 H   -2.090460   -1.391759    2.487647
 H   -0.506814   -0.848747    3.141090
 C   -3.750519   -1.432408   -1.223532
 H   -3.709484   -1.679274   -2.291838
 H   -3.889976   -2.369738   -0.662504
 H   -4.599345   -0.772186   -1.007686
 C    1.298600    0.741056   -1.255548
 C    1.896115    0.233544   -0.073692
 C    0.292323    1.747200   -1.210772
 H    1.515845    0.265306   -2.215436
 C    2.901316   -0.890577   -0.079446
 C    1.457495    0.790526    1.164029
 C   -0.153193    2.271275    0.031645
 H   -0.218395    2.040836   -2.130738
 C    4.303657   -0.290654   -0.152169
 C    2.672765   -1.905901   -1.187989
 H    2.792658   -1.407460    0.892655
 C    0.459887    1.784408    1.227430
 H    1.813040    0.338357    2.095766
 C   -1.307465    3.210347    0.099247
 H    5.064897   -1.084551   -0.104154
 H    4.439607    0.255187   -1.101905
 H    1.587538    1.584378    1.189354
 H   -0.888890   -3.205792    2.234017
 H    0.272524   -2.812657    3.527730
 H   -1.100802   -1.723236    3.213803
 H    0.342744    0.271096    2.856396
 H    2.695440    2.616546   -2.258729
 H    2.386615    2.758311   -0.518373
 H    1.106013    2.143855   -1.596846
 H    4.590308   -0.337491   -0.828475
 H    4.406607    1.202263    0.051199
 H    4.778861    1.210908   -1.692263
 O   -1.172210   -1.067354   -1.737409
 O   -2.201216   -1.154664    0.169631
 C   -2.248929   -1.272007   -1.095844
 C   -3.527765   -1.605744   -1.794963
 H   -4.055760   -2.400232   -1.252137
 H   -4.166242   -0.709822   -1.794898
 H   -3.335064   -1.910275   -2.829839
*
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B^{+S}

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =        -828.127823
G (1 atm) =                -827.851006
qh G-E (1 mol/L) =            0.285196
qh G-E (24.56 mol/L) =        0.288219
Lowest Frequency =          20.03

HF SCF energy (TZ) =       -823.113678
HF SCF energy (QZ) =       -823.162529
Correlation energy (DZ) =    -3.032013
Correlation energy (TZ) =    -3.758868
DLPNO-CCSD(T1)/CBS =       -827.360843

*xyz 1 1
 Ru  -0.293098    0.108331    0.054829
 C    1.291425    0.739160   -1.244220
 C    1.881881    0.224726   -0.063243
 C    0.290254    1.751923   -1.202251
 C    2.909328   -0.889707   -0.074103
 C    1.436513    0.777777    1.175058
 C   -0.159889    2.270415    0.038103
 C    2.663204   -1.936673   -1.159974
 C    4.308428   -0.272538   -0.189672
 C    0.440517    1.773254    1.237091
 C   -1.295547    3.244575    0.105308
 H    1.519451    0.277915   -2.206403
 H   -0.203284    2.058039   -2.125363
 H    2.832010   -1.388790    0.906012
 H    1.790830    0.331924    2.107333
 H    2.790843   -1.517263   -2.170352
 H    1.651750   -2.365632   -1.088687
 H    3.388586   -2.756262   -1.052736
 H    4.490433    0.463565    0.608044
 H    4.428335    0.236807   -1.159690
 H    5.078001   -1.055069   -0.115523
 H    0.062262    2.098101    2.207258
 H   -1.888043    3.091718    1.016827
 H   -0.885322    4.265699    0.129950
 H   -1.948885    3.154137   -0.771889
 O   -0.410578   -1.677510    1.273559
 C   -1.038747   -1.646549    2.571009
 H   -0.748418   -2.437424    0.773362
 H   -0.910373   -2.624063    3.053455
 H   -2.105255   -1.399923    2.476522
```

```
 H    4.489189    0.413598    0.674458
 H    2.869449   -1.474734   -2.184172
 H    1.643288   -2.302269   -1.179347
 H    3.363632   -2.753678   -1.064886
 H    0.073314    2.103242    2.198496
 H   -0.937652    4.248332    0.105277
 H   -1.889190    3.054267    1.018969
 H   -1.970348    3.089276   -0.768894
*
```

B⁺

```
CPCM (MeOH)
M06 SCF (DZ) =             -712.059019
G (1 atm) =                -711.839522
qh-G (1 mol/L) =           -711.833928
qh-G (24.56 mol/L) =       -711.830906
Lowest Frequency =           31.68

HF SCF energy (TZ) =       -707.989428
HF SCF energy (QZ) =       -708.030943
Correlation energy (DZ) =    -2.640219
Correlation energy (TZ) =    -3.277254
DLPNO-CCSD(T1)/CBS =       -711.692947

*xyz 1 1
 C    1.856771    0.185481    0.195250
 C    2.948108   -0.843480    0.353594
 C    1.195670    0.703063    1.334720
 C    2.794588   -2.041713   -0.573771
 C    4.294483   -0.150383    0.152609
 H    2.892728   -1.203547    1.396480
 C    1.419156    0.605468   -1.094947
 C    0.073211    1.556501    1.191583
 H    1.464230    0.329623    2.325669
 H    1.819224   -2.541260   -0.450812
 H    2.909516   -1.761251   -1.634003
 H    3.579513   -2.780553   -0.351109
 H    4.423892    0.696257    0.844681
 H    4.387929    0.232173   -0.878186
 H    5.115427   -0.863508    0.323711
 C    0.321200    1.477178   -1.236940
 H    1.856632    0.159337   -1.990738
 C   -0.395280    1.960011   -0.097560
 H   -0.516238    1.820745    2.073867
 H   -0.075706    1.678870   -2.235402
 C   -1.642883    2.760081   -0.250281
 H   -2.337937    2.568926    0.580356
 H   -1.398027    3.834478   -0.245354
 H   -2.145497    2.530934   -1.200622
 C   -2.648247   -1.067651    0.046264
 C   -3.975729   -1.724213    0.051923
 O   -1.984039   -0.875951    1.116926
 O   -2.094645   -0.686820   -1.037491
 H   -4.438172   -1.657271    1.043755
 H   -3.840648   -2.786707   -0.203315
 H   -4.622926   -1.276066   -0.712936
 Ru  -0.315699   -0.159115    0.005541
*
```

C¹

```
CPCM (MeOH)
M06 SCF (DZ) =            -1728.818310
G (1 atm) =               -1728.412044
```

```
 H   -0.521634   -0.874886    3.152542
 O   -2.431646    0.054937    0.138631
 O   -1.351840   -1.119200   -1.320328
 C   -2.472730   -0.805310   -0.797277
 C   -3.744028   -1.452669   -1.226161
 H   -3.708550   -1.685498   -2.297062
 H   -3.847610   -2.396429   -0.669340
 H   -4.599940   -0.809297   -0.992941
*
```

B⁺

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =        -712.379781
G (1 atm) =                -712.153891
qh G-E (1 mol/L) =            0.232811
qh G-E (24.56 mol/L) =        0.235833
Lowest Frequency =           26.5

HF SCF energy (TZ) =       -707.992095
HF SCF energy (QZ) =       -708.032931
Correlation energy (DZ) =    -2.642375
Correlation energy (TZ) =    -3.278904
DLPNO-CCSD(T1)/CBS =       -711.696086

* xyz 1 1
 Ru  -0.364091    0.011551    0.009573
 C    0.075120    1.706566    1.221705
 C    1.149061    0.798491    1.373787
 C   -0.353026    2.140698   -0.071181
 C    1.795467    0.255410    0.238088
 C   -1.540769    3.039417   -0.229428
 C    0.357645    1.645234   -1.207331
 C    2.834129   -0.840043    0.386913
 C    1.398054    0.712151   -1.056763
 C    2.473528   -2.098366   -0.407506
 C    4.206709   -0.282143   -0.005717
 H   -0.507165    1.998850    2.097602
 H    1.386772    0.409524    2.365020
 H   -2.260697    2.889206    0.585548
 H   -1.195718    4.084394   -0.197512
 H   -2.038532    2.870785   -1.192700
 H   -0.001934    1.887414   -2.208980
 H    2.859983   -1.106759    1.454971
 H    1.829144    0.256031   -1.949078
 H    2.435352   -1.907061   -1.491196
 H    1.500963   -2.508786   -0.089907
 H    3.233048   -2.874399   -0.233537
 H    4.462017    0.606340    0.590943
 H    4.232540   -0.002699   -1.071015
 H    4.980747   -1.044650    0.164351
 O   -2.009465   -0.691885   -1.063205
 O   -1.878685   -0.965904    1.080789
 C   -2.502407   -1.221097   -0.005611
 C   -3.698576   -2.098548   -0.045746
 H   -4.417407   -1.716564   -0.780572
 H   -3.371751   -3.097549   -0.372149
 H   -4.150664   -2.174139    0.948928
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C¹

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CPCM (•)
wB97X-D3 SCF (DZ) =       -1729.467635
G (1 atm) =               -1729.049089
```

qh-G (1 mol/L) = -1728.403452
qh-G (24.56 mol/L) = -1728.400429
Lowest Frequency = 27.97

HF SCF energy (TZ) = -1720.997419
HF SCF energy (QZ) = -1721.076143
Correlation energy (DZ) = -4.857403
Correlation energy (TZ) = -5.963957
DLPNO-CCSD(T1)/CBS = -1727.710420

*xyz 0 1

Ru	0.636253	0.047423	-0.212816
N	-1.450700	0.792678	0.004808
O	0.193609	-0.578618	1.741197
C	-2.578685	0.167408	0.086345
C	-1.596782	2.220973	0.065173
Cl	1.390545	2.087102	0.929026
C	1.020132	-1.136202	2.571135
C	-2.884189	-1.263074	0.085041
H	-3.484045	0.799209	0.106456
C	-1.318979	3.004861	-1.052541
C	-2.024718	2.814736	1.251527
C	0.367681	-1.469408	3.895514
O	2.202634	-1.394032	2.358634
C	-2.058429	-2.272109	0.601298
C	-4.129391	-1.612323	-0.465538
C	-1.465593	4.386230	-0.978384
H	-0.986847	2.529666	-1.978523
C	-2.157800	4.199295	1.323142
H	-2.223341	2.183299	2.122491
H	0.005159	-0.548967	4.377934
H	-0.512319	-2.111461	3.731342
H	1.076277	-1.977568	4.562209
C	-2.459774	-3.601424	0.525223
H	-1.121649	-1.991595	1.086231
C	-4.512994	-2.944146	-0.563215
H	-4.792504	-0.825015	-0.836989
C	-1.877112	4.988740	0.210396
H	-1.254989	4.997797	-1.859230
H	-2.481688	4.662382	2.258543
C	-3.674638	-3.942457	-0.069501
H	-1.817736	-4.382299	0.940421
H	-5.473789	-3.203499	-1.013350
H	-1.980586	6.074979	0.267266
H	-3.977506	-4.990619	-0.132182
C	1.682513	-1.779202	-0.716915
C	0.455281	-1.778207	-1.425240
C	2.622242	-0.719361	-0.835958
H	1.893145	-2.582841	-0.005390
C	0.102852	-0.670579	-2.241432
H	-0.255480	-2.596958	-1.295330
C	3.976022	-0.836642	-0.182366
C	2.235534	0.389765	-1.639193
C	-1.203285	-0.639204	-2.962632
C	1.009952	0.421002	-2.340948
C	4.633526	0.495355	0.135046
C	4.867360	-1.676730	-1.097059
H	3.809773	-1.380660	0.761274
H	2.863329	1.283960	-1.648968
H	-1.616782	0.378807	-3.017339
H	-1.048453	-0.986808	-3.997215
H	-1.943837	-1.303798	-2.494616
H	0.733994	1.308752	-2.914869
H	5.568255	0.326342	0.692671
H	4.905175	1.044435	-0.784188
H	3.974661	1.139474	0.738359

qh G-E (1 mol/L) = 0.430843
qh G-E (24.56 mol/L) = 0.433865
Lowest Frequency = 6.17

HF SCF energy (TZ) = -1721.003333
HF SCF energy (QZ) = -1721.080680
Correlation energy (DZ) = -4.861072
Correlation energy (TZ) = -5.968019
DLPNO-CCSD(T1)/CBS = -1727.718833

SMD (MeOH)
HF SCF energy (TZ) = -1721.017284
HF SCF energy (QZ) = -1721.094556
Correlation energy (DZ) = -4.858180
Correlation energy (TZ) = -5.965578
DLPNO-CCSD(T1)/CBS = -1727.730510

* xyz 0 1

Ru	-0.491575	-0.272451	-0.150400
O	0.649009	-1.856105	0.561571
C	1.127647	-2.866717	-0.092924
C	1.925272	-3.811496	0.787482
O	0.996508	-3.083379	-1.300071
C	-1.585365	-1.591739	-1.469457
C	-0.661763	-0.830887	-2.246018
C	-2.510973	-0.975806	-0.603229
C	-0.664602	0.579240	-2.184704
C	-3.470405	-1.756980	0.271287
C	-2.491574	0.457612	-0.542970
C	0.307825	1.389971	-2.988982
C	-1.610657	1.221120	-1.328193
C	-2.955018	-3.145117	0.647390
C	-4.836105	-1.829973	-0.422929
H	2.807956	-3.280682	1.174854
H	1.322103	-4.123303	1.652227
H	2.247909	-4.691839	0.218531
H	-1.474964	-2.674685	-1.470293
H	0.097506	-1.352484	-2.824570
H	-3.584398	-1.172077	1.198772
H	-3.123995	0.968027	0.186352
H	1.181310	0.792785	-3.280032
H	-0.193955	1.734550	-3.906256
H	0.642707	2.278839	-2.438882
H	-1.605108	2.306149	-1.232047
H	-1.946455	-3.091716	1.084879
H	-2.918331	-3.816259	-0.225666
H	-3.628067	-3.604207	1.386334
H	-5.226807	-0.826149	-0.649792
H	-4.762581	-2.388727	-1.370126
H	-5.566126	-2.342873	0.221212
N	1.339625	0.885676	0.242743
C	1.520172	2.154256	0.356332
C	2.565374	0.127170	0.340666
C	0.505385	3.225765	0.335269
C	3.207410	0.018520	1.572840
C	3.105234	-0.473554	-0.795131
C	0.787720	4.344609	-0.461086
C	-0.670518	3.192815	1.093747
C	4.401504	-0.697021	1.667086
C	4.300629	-1.180690	-0.694630
C	-0.131104	5.386664	-0.557667
C	-1.572090	4.251948	1.016844
C	4.952148	-1.296223	0.535040
C	-1.314076	5.339822	0.181085
H	2.558253	2.508706	0.439824
H	2.761055	0.483536	2.454512

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 H    4.433964   -2.670805   -1.294301
 H    5.015010   -1.172741   -2.068881
 H    5.859011   -1.822123   -0.639195
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 H    2.584198   -0.394528   -1.749969
 H    1.724208    4.386906   -1.023372
 H   -0.875241    2.334442    1.735476
 H    4.901203   -0.784589    2.634222
 H    4.724658   -1.647239   -1.586241
 H    0.083789    6.241909   -1.201437
 H   -2.488059    4.223779    1.610729
 H    5.886766   -1.856057    0.609160
 H   -2.031605    6.160601    0.114156
 Cl  -0.943294   -0.066027    2.273529
*
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C^1•*S*

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CPCM (•)
wB97X-D3 SCF (DZ) =       -1845.178202
G (1 atm) =               -1844.709891
qh G-E (1 mol/L) =            0.482187
qh G-E (24.56 mol/L) =        0.485210
Lowest Frequency =           24.22

SMD (MeOH)
HF SCF energy (TZ) =      -1836.108217
HF SCF energy (QZ) =      -1836.193420
Correlation energy (DZ) =    -5.237851
Correlation energy (TZ) =    -6.437681
DLPNO-CCSD(T1)/CBS =      -1843.357878

* xyz 0 1
Ru  -0.424199    0.699243    0.675256
 C    1.955395   -1.963114    0.064484
 C   -0.223217    2.445225    2.000889
 C    1.673482    1.246731    0.965771
 H    1.159531    1.187377    3.081067
 O   -0.550974   -0.416729    3.829049
 N   -0.742456   -0.678261   -1.019670
 Cl  -2.863875    0.620591    1.106221
 O   -0.459260   -1.126321    1.689594
 C    1.424810   -1.910449   -1.230244
 C    3.297236   -2.287728    0.249507
 C    0.915750    1.621920    2.112496
 H    1.301821   -1.762373    0.913167
 C   -1.037414    2.828929    3.200657
 C   -0.607454    2.858945    0.686195
 C    1.312891    1.700771   -0.324476
 H    2.528631    0.579563    1.079081
 C   -0.539450   -1.302486    2.973112
 C   -2.040406   -0.622882   -1.650443
 C    0.035379   -1.552329   -1.559575
 H   -3.236732    2.286787   -0.324153
 C    2.241725   -2.231000   -2.326488
 C    4.118764   -2.552670   -0.847263
 H    3.704936   -2.332772    1.261755
 H   -0.958540    2.054147    3.973112
 H   -0.666237    3.782712    3.606169
 H   -2.093193    2.956299    2.927030
 C    0.139941    2.504137   -0.451427
 H   -1.550728    3.389984    0.543337
 C    2.216019    1.391151   -1.502920
 C   -0.619927   -2.768765    3.359900
 C   -2.425666    0.518043   -2.350683
 C   -2.898838   -1.718828   -1.558604
 H   -0.354682   -2.077835   -2.443712
 C    3.588156   -2.528426   -2.138084
 H    1.820215   -2.222102   -3.335028
 H    5.172984   -2.794813   -0.694872
 H   -0.213757    2.815341   -1.433609
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 C    1.524657    1.403920   -2.864418
 C    3.370514    2.405342   -1.472295
 H    2.643412    0.391966   -1.329988
 H   -1.524502   -3.216424    2.922532
 H    0.245206   -3.312078    2.951569
 H   -0.645570   -2.880299    4.450577
 C   -3.676639    0.560285   -2.961854
 H   -1.753698    1.373742   -2.410923
 C   -4.152031   -1.667466   -2.167340
 H   -2.589475   -2.599167   -0.990743
 H    4.222162   -2.751260   -2.998506
 H    2.234527    1.077491   -3.638540
 H    1.182982    2.415245   -3.136471
 H    0.656645    0.731118   -2.897704
 H    3.925111    2.356985   -0.523365
 H    2.991698    3.432681   -1.597532
 H    4.074008    2.197676   -2.292325
 C   -4.544940   -0.528329   -2.870030
 H   -3.974421    1.456693   -3.509617
 H   -4.825484   -2.523468   -2.086108
 H   -5.527833   -0.487541   -3.344247
 C   -4.755042    3.403843   -0.761922
 H   -4.919303    4.381128   -1.238915
 H   -5.334453    2.647119   -1.322447
 H   -5.154449    3.451824    0.267349
 O   -3.367925    3.135089   -0.787699
*
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C¹•S₂ᵏ
CPCM (•)
wB97X-D3 SCF (DZ) =       -1960.885805
G (1 atm) =               -1960.370133
qh G-E (1 mol/L) =            0.532066
qh G-E (24.56 mol/L) =        0.535089
Lowest Frequency =           15.12

SMD (MeOH)
HF SCF energy (TZ) =      -1951.195822
HF SCF energy (QZ) =      -1951.288869
Correlation energy (DZ) =    -5.618718
Correlation energy (TZ) =    -6.909659
DLPNO-CCSD(T1)/CBS =      -1958.980907

* xyz 0 1
Ru  -0.557464    0.823896    0.730230
 C    1.195944    0.994842    2.016669
 C    1.642302    1.046063    0.686886
 C    0.185955    1.896722    2.482855
 H    1.559780    0.206890    2.673718
 C    0.085141    2.840015    0.188963
 C   -0.346893    2.810607    1.552076
 C    1.096719    1.969296   -0.258910
 C    1.833312   -2.124346    0.272611
 O    0.153079   -1.703902    2.913779
 Cl  -2.910190    1.521111    0.353121
 N   -0.801505   -0.730423   -0.842059
 O   -1.546152   -0.631508    1.892065
 H    2.398092    0.337325    0.353656
 C   -0.330238    1.817221    3.889960
 H   -0.429937    3.495998   -0.515540
 H   -1.188131    3.437019    1.850134
 C    1.688688    2.043250   -1.655095
 C    1.460474   -1.737905   -1.018204
 C    3.177012   -2.359125    0.559923
 H    1.083051   -2.211962    1.060795
 C   -1.045523   -1.537753    2.678763
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 H   -2.881551    0.237252    2.885702
 H   -2.435171    2.714128   -1.396454
 C   -2.135066   -0.905433   -1.381914
 C    0.044191   -1.533979   -1.381127
 H   -0.160165    0.815276    4.305639
 H    0.204382    2.545848    4.518075
 H   -1.405620    2.034150    3.930304
 C    0.670321    1.988899   -2.790540
 C    2.552723    3.310047   -1.730282
 H    2.358465    1.174352   -1.754768
 C    2.427515   -1.626404   -2.025140
 C    4.147598   -2.200032   -0.430003
 H    3.466915   -2.658416    1.569520
 C   -2.099266   -2.411617    3.330722
 O   -3.412524    0.595060    3.624091
 O   -2.265956    3.354196   -2.114412
 C   -2.584136   -0.109963   -2.433892
 C   -2.950071   -1.897410   -0.841952
 H   -0.313015   -2.156152   -2.215988
 H    1.184019    2.131414   -3.753208
 H   -0.107875    2.760731   -2.697031
 H    0.170355    1.011024   -2.821157
 H    3.285383    3.345870   -0.909460
 H    1.926644    4.215055   -1.670411
 H    3.102799    3.337060   -2.682758
 C    3.771840   -1.832608   -1.723576
 H    2.127370   -1.355411   -3.040790
 H    5.200564   -2.372806   -0.196499
 H   -2.729404   -1.780374    3.974270
 H   -2.750208   -2.855033    2.563460
 H   -1.629228   -3.201664    3.927931
 C   -4.774586    0.443752    3.284114
 C   -3.510911    3.937171   -2.444518
 C   -3.862490   -0.313976   -2.948604
 H   -1.951336    0.686652   -2.826155
 C   -4.232251   -2.089064   -1.356424
 H   -2.578898   -2.504382   -0.014604
 H    4.527224   -1.716699   -2.503410
 H   -5.378032    0.863701    4.102868
 H   -5.059464   -0.618728    3.165057
 H   -5.034431    0.975600    2.351803
 H   -3.975160    4.447918   -1.581704
 H   -4.229230    3.191520   -2.831502
 H   -3.336649    4.684638   -3.231981
 C   -4.691673   -1.299577   -2.410330
 H   -4.213912    0.308860   -3.774203
 H   -4.872375   -2.865306   -0.931202
 H   -5.695091   -1.452442   -2.813503
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C1•S3k
CPCM (•)
wB97X-D3 SCF (DZ) =       -2076.597612
G (1 atm) =               -2076.032783
qh G-E (1 mol/L) =            0.583262
qh G-E (24.56 mol/L) =        0.586285
Lowest Frequency =            6.17

SMD (MeOH)
HF SCF energy (TZ) =      -2066.290698
HF SCF energy (QZ) =      -2066.392366
Correlation energy (DZ) =    -6.001391
Correlation energy (TZ) =    -7.385115
DLPNO-CCSD(T1)/CBS =      -2074.616675

* xyz 0 1
```

Ru	-0.611784	0.719781	0.682513
C	1.177297	0.506031	1.931660
C	1.584422	0.922692	0.646369
C	0.199330	1.255304	2.649274
H	1.579948	-0.411609	2.358026
C	-0.352496	2.397589	2.023718
C	0.050341	2.779379	0.711823
C	1.030090	2.058299	-0.005732
Cl	-2.690235	1.723849	-0.203572
C	1.936294	-2.188397	0.126255
N	-0.760776	-0.868084	-0.904868
O	-0.654336	-2.256508	2.125252
O	-1.988280	-0.502205	1.681194
H	2.317592	0.326458	0.107549
C	-0.289039	0.809592	3.994753
H	-1.161873	2.939237	2.513634
H	-0.478093	3.601650	0.227695
C	1.504103	2.465197	-1.388245
H	-2.595710	2.494216	-2.311309
H	-4.770358	0.916988	-0.071187
H	-3.146258	0.595051	2.618240
C	1.577130	-1.659922	-1.118429
C	3.285588	-2.326247	0.448417
H	1.151116	-2.453607	0.839320
C	-2.079226	-1.250278	-1.379389
C	0.149077	-1.570449	-1.480006
C	-1.731547	-1.664663	2.205494
H	-1.362260	1.015335	4.106618
H	0.261154	1.363120	4.771094
H	-0.107472	-0.262885	4.140794
C	0.360901	2.672418	-2.380316
C	2.394143	3.707880	-1.270691
H	2.126241	1.633823	-1.758505
O	-2.837628	2.676738	-3.235724
O	-5.717480	0.739867	0.061240
O	-3.642725	0.965239	3.375588
C	2.558822	-1.313198	-2.052513
C	4.268791	-1.933261	-0.461365
H	3.570747	-2.732138	1.421407
C	-2.719616	-0.553493	-2.401220
C	-2.654569	-2.399744	-0.837441
H	-0.163054	-2.225466	-2.307709
C	-2.915577	-2.272505	2.928553
H	0.762924	2.942403	-3.368170
H	-0.317520	3.481116	-2.065963
H	-0.233123	1.753489	-2.490273
H	3.225673	3.538894	-0.569559
H	1.813383	4.572877	-0.910733
H	2.819545	3.968229	-2.251514
C	-4.247295	2.799068	-3.257816
C	-5.822533	-0.410401	0.878790
C	-4.280094	2.166097	2.985882
C	3.905254	-1.428245	-1.711560
H	2.268046	-0.928647	-3.033166
H	5.324742	-2.028851	-0.199099
C	-3.949972	-1.011827	-2.871200
H	-2.278148	0.348652	-2.824155
C	-3.886404	-2.848983	-1.310916
H	-2.121915	-2.944511	-0.055448
H	-3.690474	-2.525843	2.188669
H	-3.352330	-1.541337	3.622797
H	-2.614073	-3.180259	3.464183
H	-4.591682	3.740553	-2.791071
H	-4.748236	1.959423	-2.743156
H	-4.571666	2.800292	-4.308975
H	-6.885073	-0.550393	1.127589

C²

CPCM (MeOH)
M06 SCF (DZ) = -1496.983119
G (1 atm) = -1496.530667
qh-G (1 mol/L) = -1496.521466
qh-G (24.56 mol/L) = -1496.518444
Lowest Frequency = 25.86

HF SCF energy (TZ) = -1488.763330
HF SCF energy (QZ) = -1488.854520
Correlation energy (DZ) = -5.389370
Correlation energy (TZ) = -6.596748
DLPNO-CCSD(T1)/CBS = -1496.184258

*xyz 0 1

Ru	0.320991	-0.469503	-0.242077
N	-0.957556	1.327198	-0.016557
O	-0.287920	-0.651802	1.769634
C	-2.234328	1.461275	0.119920
C	-0.257005	2.582483	0.015037
O	1.722639	0.745385	0.726763
C	0.126244	-1.542643	2.615185
C	-3.290326	0.450146	0.160087
H	-2.618366	2.495962	0.157273
C	0.329244	3.084153	-1.143644
C	-0.200543	3.308869	1.204938
C	2.715386	1.377141	0.182431
C	-0.527649	-1.396229	3.973232
O	0.945598	-2.433040	2.395259
C	-3.157929	-0.828812	0.718018
C	-4.523003	0.834878	-0.393011
C	0.962921	4.323133	-1.113094
H	0.281414	2.501192	-2.066331
C	0.444079	4.542821	1.231313
H	-0.654439	2.888459	2.107225
C	3.526657	2.153561	1.197443
O	3.016379	1.388602	-1.011347
H	-0.322063	-0.397151	4.386611
H	-1.621596	-1.480488	3.872521
H	-0.163341	-2.164007	4.668060
C	-4.228514	-1.715844	0.673574
H	-2.218332	-1.098341	1.204929
C	-5.579615	-0.065176	-0.459697
H	-4.639988	1.846074	-0.794803
C	1.025836	5.054247	0.072189
H	1.412914	4.719365	-2.026737
H	0.489977	5.108034	2.165707
H	3.933206	1.466817	1.956897
H	2.874934	2.868657	1.724143
H	4.350218	2.692295	0.710328
C	-5.430545	-1.346217	0.070129
H	-4.124692	-2.708639	1.118770
H	-6.525679	0.236507	-0.914739
H	-5.467824	-1.321394	0.364117
H	-5.258628	-0.305022	1.822421
H	-4.909853	2.029755	2.090418
H	-3.557749	2.975731	2.774426
H	-4.921022	2.491113	3.819061
H	4.673799	-1.129064	-2.427125
C	-4.539438	-2.153874	-2.328239
H	-4.450604	-0.467440	-3.674844
H	-4.330884	-3.750654	-0.883816
H	-5.504268	-2.503720	-2.701510

*

C²

CPCM (MeOH)
wB97X-D3 SCF (DZ) = -1497.681977
G (1 atm) = -1488.855528
qh G-E (1 mol/L) = 0.479444
qh G-E (24.56 mol/L) = 0.482467
Lowest Frequency = 18.67

HF SCF energy (TZ) = -1488.765614
HF SCF energy (QZ) = -1721.080680
Correlation energy (DZ) = -5.389729
Correlation energy (TZ) = -6.596892
DLPNO-CCSD(T1)/CBS = -1496.184899

SMD (MeOH)
HF SCF energy (TZ) = -1488.787156
HF SCF energy (QZ) = -1488.876681
Correlation energy (DZ) = -5.383091
Correlation energy (TZ) = -6.591581
DLPNO-CCSD(T1)/CBS = -1496.201400

* xyz 0 1

Ru	0.136219	-0.758217	0.020059
C	2.048087	-1.250239	0.993316
C	1.253531	-0.453492	1.852451
C	1.513771	-2.430096	0.416686
C	-0.064887	-0.824382	2.231036
C	2.323064	-3.228499	-0.561704
C	0.180694	-2.801294	0.742255
C	-0.902678	-0.030845	3.217045
C	-0.583663	-2.003074	1.632768
C	-0.333604	1.353592	3.523891
C	-1.064663	-0.842355	4.509358
H	3.047944	-0.917978	0.718431
H	1.663638	0.498633	2.190867
H	3.053644	-2.590374	-1.076381
H	2.872735	-4.010837	-0.016120
H	1.671288	-3.700726	-1.305652
H	-0.278503	-3.658500	0.252226
H	-1.894058	0.076049	2.749603
H	-1.635511	-2.241548	1.786483
H	-0.132209	1.935862	2.611746
H	0.608332	1.284731	4.091572
H	-1.047382	1.924592	4.135734
H	-1.529307	-1.821423	4.318415
H	-0.086827	-1.016086	4.987980
H	-1.701705	-0.298359	5.223305
N	0.209176	1.395796	-0.427505
C	1.251560	2.143496	-0.494035
C	-1.021287	2.091398	-0.717390
C	2.658447	1.695487	-0.412414
C	-1.978773	2.293613	0.274607
C	-1.234829	2.567490	-2.011315

```
 H    1.528928    6.024061    0.092270
 H   -6.262470   -2.053823    0.030231
 C    0.232425   -2.606564   -0.589483
 C   -0.860499   -2.018801   -1.274258
 C    1.572160   -2.189607   -0.812898
 H    0.040563   -3.340943    0.196718
 C   -0.644370   -0.945019   -2.174772
 H   -1.881144   -2.336788   -1.052146
 C    2.731425   -2.886215   -0.144051
 C    1.768234   -1.122452   -1.733442
 C   -1.787291   -0.277779   -2.866140
 C    0.690427   -0.501656   -2.399756
 C    3.312776   -3.899861   -1.127666
 C    3.806673   -1.938373    0.364837
 H    2.312669   -3.419011    0.724519
 H    2.757218   -0.675894   -1.841072
 H   -1.856138   -0.659782   -3.897884
 H   -2.745200   -0.483828   -2.366557
 H   -1.641892    0.811576   -2.931339
 H    0.878464    0.361229   -3.043098
 H    2.547911   -4.610483   -1.481252
 H    3.733886   -3.389385   -2.012265
 H    4.123977   -4.477498   -0.655945
 H    4.607335   -2.512356    0.858312
 H    3.393940   -1.220194    1.089877
 H    4.276310   -1.365765   -0.453938
*
```

***para*-cymene (*p*-cym)**
CPCM (MeOH)
M06 SCF (DZ) = -389.193220
G (1 atm) = -389.020377
qh-G (1 mol/L) = -389.015737
qh-G (24.56 mol/L) = -389.012715
Lowest Frequency = 31.73

HF SCF energy (TZ) = -386.974197
HF SCF energy (QZ) = -386.998301
Correlation energy (DZ) = -1.508015
Correlation energy (TZ) = -1.800727
DLPNO-CCSD(T1)/CBS = -388.977333

PBE0+D3BJ (ATZ) = -389.186660
M06-2X (ATZ) = -389.457186
wB97M-V (ATZ) = -389.444198
B2GP-PLYP (ATZ) = -389.207334
B2K-PLYP (ATZ) = -389.154270
PWPB95 (ATZ) = -389.317116
PWPB95+D3BJ (ATZ) = -389.326375
PWPB95+D4 (ATZ) = -389.334867

```
*xyz 0 1
 C   -0.628170   -0.225827    0.003036
 C   -2.132314   -0.384330    0.005275
 C   -0.027731    1.040804   -0.006322
 C   -2.760720    0.199631   -1.256087
 C   -2.760439    0.224525    1.254888
 H   -2.339927   -1.471067    0.016079
 C    3.504031    2.267093    0.545473
 C    3.168123    0.775828   -1.336351
 C   -3.142897    2.995805   -0.026975
 C   -2.408028    3.260860   -2.309376
 C    4.841069    1.879519    0.611866
 C    4.513588    0.417844   -1.285731
 C   -3.362220    3.481877   -1.317389
 C    5.347859    0.957567   -0.305939
 H    1.101193    3.223603   -0.640973
 H   -1.818508    1.891156    1.273529
 H   -0.484693    2.380573   -2.782895
 H    3.109881    3.001627    1.252419
 H    2.493683    0.327145   -2.067668
 H   -3.889532    3.156425    0.753546
 H   -2.572627    3.628724   -3.324355
 H    5.492797    2.307230    1.376461
 H    4.908589   -0.298570   -2.009364
 H   -4.279036    4.027762   -1.549577
 H    6.399007    0.664088   -0.261142
 O    0.614924   -0.832590   -2.017587
 C    0.268545   -1.772967   -2.837096
 C    0.560838   -1.428225   -4.287986
 O   -0.244514   -2.852896   -2.532924
 H    1.616228   -1.140602   -4.402624
 H   -0.049242   -0.562208   -4.585921
 H    0.333709   -2.277851   -4.943355
 O   -1.754999   -0.617156   -0.832729
 C   -2.924038   -0.609571   -0.282249
 C   -4.047100   -0.469729   -1.294925
 O   -3.168484   -0.681575    0.926163
 H   -3.950478   -1.236011   -2.077442
 H   -3.964072    0.513402   -1.783122
 H   -5.025661   -0.551867   -0.806493
*
```

***para*-cymene (*p*-cym)**
CPCM (MeOH)
wB97X-D3 SCF (DZ) = -389.431305
G (1 atm) = -389.253700
qh G-E (1 mol/L) = 0.182803
qh G-E (24.56 mol/L) = 0.185825
Lowest Frequency = 36.43

HF SCF energy (TZ) = -386.975127
HF SCF energy (QZ) = -386.998766
Correlation energy (DZ) = -1.508306
Correlation energy (TZ) = -1.800653
DLPNO-CCSD(T1)/CBS = -388.977370

PBE0+D3BJ (ATZ) = -389.186613
M06-2X (ATZ) = -389.466654
wB97M-V (ATZ) = -389.451952
B2GP-PLYP (ATZ) = -389.214804
B2K-PLYP (ATZ) = -389.162007
PWPB95 (ATZ) = -389.324827
PWPB95+D3BJ (ATZ) = -389.334065
PWPB95+D4 (ATZ) = -389.342511

SMD (MeOH)
HF SCF energy (TZ) = -386.979465
HF SCF energy (QZ) = -387.003112
Correlation energy (DZ) = -1.507867
Correlation energy (TZ) = -1.800419
DLPNO-CCSD(T1)/CBS = -388.981605

```
 C    0.213192   -1.339444    0.006534
 C    1.355204    1.180155   -0.011036
 H   -0.653475    1.939944   -0.012515
 H   -2.330501   -0.247921   -2.166557
 H   -2.601138    1.290677   -1.310258
 H   -3.849163    0.024286   -1.269448
 H   -2.329343   -0.204054    2.174017
 H   -2.602266    1.316628    1.286986
 H   -3.848679    0.048348    1.272343
 C    1.601232   -1.199899    0.001913
 H   -0.227789   -2.342283    0.010903
 C    2.198704    0.061688   -0.005128
 H    1.798157    2.182172   -0.021060
 H    2.234730   -2.093323    0.002630
 C    3.688445    0.228621    0.004341
 H    4.019276    0.933995   -0.775114
 H    4.040302    0.635433    0.967590
 H    4.205406   -0.728368   -0.160093
*
```

Cl⁻

CPCM (MeOH)

M06 SCF (DZ) =	-460.353686
G (1 atm) =	-460.368709
qh-G (1 mol/L) =	-460.365690
qh-G (24.56 mol/L) =	-460.362667
HF SCF energy (TZ) =	-459.681515
HF SCF energy (QZ) =	-459.687835
Correlation energy (DZ) =	-0.147832
Correlation energy (TZ) =	-0.220866
DLPNO-CCSD(T1)/CBS =	-459.953281
PBE0+D3BJ (ATZ) =	-460.248399
M06-2X (ATZ) =	-460.388310
wB97M-V (ATZ) =	-460.379750
B2GP-PLYP (ATZ) =	-460.229838
B2K-PLYP (ATZ) =	-460.198810
PWPB95 (ATZ) =	-460.352737
PWPB95+D3BJ (ATZ) =	-460.352737
PWPB95+D4 (ATZ) =	-460.352737

***cis*-D⁺**

CPCM (MeOH)

M06 SCF (DZ) =	-1268.445316
G (1 atm) =	-1268.037024
qh-G (1 mol/L) =	-1268.028571
qh-G (24.56 mol/L) =	-1268.025549
Lowest Frequency =	25.86

```
*xyz 0 1
 C   -0.626276   -0.220788    0.008254
 C   -2.137970   -0.381134    0.008070
 C   -0.024994    1.046470    0.002921
 C   -2.764924    0.194954   -1.266768
 C   -2.773089    0.229730    1.262352
 C    0.214652   -1.336116    0.007127
 C    1.359781    1.186010   -0.003798
 C    1.604840   -1.196684   -0.000086
 C    2.203047    0.065451   -0.005001
 C    3.702659    0.226225   -0.000929
 H   -2.342939   -1.465222    0.022066
 H   -0.648301    1.945419    0.001551
 H   -2.327498   -0.262526   -2.167572
 H   -2.608571    1.284279   -1.330871
 H   -3.850846    0.011525   -1.283164
 H   -2.343021   -0.203670    2.178465
 H   -2.616711    1.320303    1.298249
 H   -3.859268    0.047680    1.275513
 H   -0.224675   -2.338061    0.009344
 H    1.798976    2.187989   -0.010368
 H    2.234742   -2.091053   -0.003667
 H    4.029955    0.931060   -0.780124
 H    4.055538    0.623082    0.964464
 H    4.207887   -0.734534   -0.173111
*
```

Cl⁻

CPCM (MeOH)

wB97X-D3 SCF (DZ) =	-460.370458
G (1 atm) =	-460.385500
qh G-E (1 mol/L) =	-0.012024
qh G-E (24.56 mol/L) =	-0.009001
HF SCF energy (TZ) =	-459.681518
HF SCF energy (QZ) =	-459.687834
Correlation energy (DZ) =	-0.147832
Correlation energy (TZ) =	-0.220866
DLPNO-CCSD(T1)/CBS =	-459.953279
PBE0+D3BJ (ATZ) =	-460.248393
M06-2X (ATZ) =	-460.386666
wB97M-V (ATZ) =	-460.378604
B2GP-PLYP (ATZ) =	-460.228600
B2K-PLYP (ATZ) =	-460.197558
PWPB95 (ATZ) =	-460.351461
PWPB95+D3BJ (ATZ) =	-460.351461
PWPB95+D4 (ATZ) =	-460.351461

SMD (MeOH)

HF SCF energy (TZ) =	-459.672863
HF SCF energy (QZ) =	-459.680069
Correlation energy (DZ) =	-0.147804
Correlation energy (TZ) =	-0.220905
DLPNO-CCSD(T1)/CBS =	-459.945862

***cis*-D⁺**

CPCM (MeOH)

wB97X-D3 SCF (DZ) =	-1269.080679
G (1 atm) =	-1268.659844
qh G-E (1 mol/L) =	0.433455
qh G-E (24.56 mol/L) =	0.436478
Lowest Frequency =	13.86

```
HF SCF energy (TZ) =      -1261.330526
HF SCF energy (QZ) =      -1261.405053
Correlation energy (DZ) =    -4.687907
Correlation energy (TZ) =    -5.722333
DLPNO-CCSD(T1)/CBS =      -1267.754294

*xyz 1 1
 Ru   0.423619   -0.465018    0.255641
 N   -1.450391    0.600011    0.005791
 O    0.365800   -0.609511   -1.903810
 C   -1.619531    1.858253   -0.238941
 C   -2.655476   -0.170478    0.132286
 O   -0.617365   -2.098198   -0.678451
 C   -0.355075   -1.656374   -1.841479
 C   -0.580901    2.836531   -0.545611
 H   -2.649154    2.250115   -0.184031
 C   -2.894034   -0.922141    1.282802
 C   -3.575306   -0.181583   -0.917693
 C   -0.875936   -2.330939   -3.056811
 C    0.496233    2.554129   -1.397883
 C   -0.700357    4.111659    0.026245
 C   -4.064706   -1.663264    1.390664
 H   -2.161604   -0.920772    2.093331
 C   -4.740760   -0.937447   -0.807242
 H   -3.360839    0.384457   -1.829110
 H   -0.511134   -3.368506   -3.080517
 H   -1.974071   -2.373212   -3.004335
 H   -0.562661   -1.805135   -3.966022
 C    1.462281    3.525972   -1.633175
 H    0.554282    1.583203   -1.895446
 C    0.286499    5.067329   -0.187336
 H   -1.560940    4.339821    0.662193
 C   -4.989993   -1.675522    0.346450
 H   -4.254271   -2.239805    2.298884
 H   -5.454670   -0.949467   -1.634073
 C    1.370117    4.773145   -1.014268
 H    2.293895    3.310125   -2.308114
 H    0.204472    6.049503    0.282994
 H   -5.903797   -2.267888    0.431790
 H    2.139045    5.528475   -1.193230
 C    2.423516    0.302674    0.441815
 C    1.603341    1.047882    1.315971
 C    2.499466   -1.125175    0.502357
 H    2.949326    0.824553   -0.364983
 C    0.784218    0.388414    2.278308
 H    1.534858    2.132632    1.201411
 C    3.367038   -1.862815   -0.486385
 C    1.675868   -1.765236    1.455022
 C   -0.135421    1.173316    3.151251
 C    0.823271   -1.024415    2.325812
 C    2.943186   -3.302465   -0.723702
 C    4.817682   -1.788779   -0.012886
 H    3.284221   -1.309157   -1.441304
 H    1.593857   -2.854592    1.454720
 H   -0.515659    2.068446    2.637243
 H    0.419493    1.517366    4.038945
 H   -0.983621    0.569904    3.503536
 H    0.144649   -1.561119    2.993169
 H    1.881939   -3.386929   -1.009399
 H    3.107293   -3.924264    0.172942
 H    3.547332   -3.739659   -1.532828
 H    5.156220   -0.748425    0.115699
 H    4.933232   -2.306961    0.954487
 H    5.482998   -2.276334   -0.741998
*
```

```
HF SCF energy (TZ) =      -1261.332736
HF SCF energy (QZ) =      -1261.406018
Correlation energy (DZ) =    -4.688373
Correlation energy (TZ) =    -5.722636
DLPNO-CCSD(T1)/CBS =      -1267.755092

SMD (MeOH)
HF SCF energy (TZ) =      -1261.350107
HF SCF energy (QZ) =      -1261.423275
Correlation energy (DZ) =    -4.684345
Correlation energy (TZ) =    -5.719272
DLPNO-CCSD(T1)/CBS =      -1267.769338

* xyz 1 1
 Ru   0.416169   -0.464418    0.253769
 C    2.374808    0.396774    0.455566
 C    1.526718    1.050227    1.369428
 C    2.522891   -1.029805    0.447711
 C    0.750416    0.301450    2.307139
 C    3.436300   -1.676512   -0.574923
 C    1.747480   -1.757650    1.372729
 C   -0.184065    1.006263    3.244784
 C    0.860406   -1.105423    2.284481
 C    3.063404   -3.118163   -0.913582
 C    4.883200   -1.575153   -0.074465
 H    2.872966    0.985213   -0.318178
 H    1.403355    2.131926    1.309941
 H    3.347238   -1.071737   -1.492889
 H    1.734221   -2.847190    1.330997
 H   -0.702073    1.834930    2.742775
 H    0.405221    1.430342    4.071805
 H   -0.924468    0.317333    3.670154
 H    0.218202   -1.709056    2.927355
 H    2.009328   -3.210619   -1.216281
 H    3.237857   -3.793801   -0.061328
 H    3.687174   -3.472925   -1.746670
 H    5.168321   -0.531733    0.128197
 H    5.012139   -2.152717    0.854815
 H    5.575331   -1.977959   -0.828538
 N   -1.448736    0.604548    0.029461
 C   -1.626542    1.858159   -0.206542
 C   -2.658276   -0.173159    0.142905
 C   -0.575111    2.841255   -0.509956
 C   -2.937091   -0.877075    1.314133
 C   -3.529449   -0.235710   -0.945321
 C    0.444862    2.574964   -1.432837
 C   -0.639533    4.090696    0.120664
 C   -4.104377   -1.631226    1.398314
 C   -4.692066   -1.001367   -0.855854
 C    1.415878    3.539874   -1.686949
 C    0.348870    5.042034   -0.118795
 C   -4.982683   -1.698953    0.314776
 C    1.378598    4.765611   -1.019806
 H   -2.655466    2.243865   -0.169623
 H   -2.249508   -0.829551    2.158899
 H   -3.284327    0.298191   -1.866318
 H    0.463444    1.620108   -1.959780
 H   -1.453527    4.306614    0.816985
 H   -4.327731   -2.173362    2.319329
 H   -5.368186   -1.053180   -1.711649
 H    2.205585    3.332186   -2.411890
 H    0.309836    6.006331    0.391259
 H   -5.891900   -2.299603    0.383274
 H    2.148052    5.515754   -1.214819
 O    0.341770   -0.601512   -1.889619
```

```
 O   -0.623104   -2.096054   -0.663330
 C   -0.374954   -1.652360   -1.829222
 C   -0.905969   -2.325625   -3.049146
 H   -0.496369   -3.344304   -3.101445
 H   -1.998701   -2.405906   -2.965085
 H   -0.634440   -1.766481   -3.950821
*
```

D⁺•Cl⁻

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CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1729.462944
G (1 atm) =               -1729.044486
qh G-E (1 mol/L) =            0.432279
qh G-E (24.56 mol/L) =        0.435301
Lowest Frequency =            5.55

HF SCF energy (TZ) =      -1721.009192
HF SCF energy (QZ) =      -1721.087232
Correlation energy (DZ) =    -4.847640
Correlation energy (TZ) =    -5.955552
DLPNO-CCSD(T1)/CBS =      -1727.713691

SMD (MeOH)
HF SCF energy (TZ) =      -1721.017651
HF SCF energy (QZ) =      -1721.096022
Correlation energy (DZ) =    -4.843942
Correlation energy (TZ) =    -5.952405
DLPNO-CCSD(T1)/CBS =      -1727.719755

*xyz 0 1
 Ru   0.014848    0.273348    0.929553
 C    1.699592    1.008311    2.037271
 C    2.063189    1.016245    0.669428
 C    0.537878    1.684441    2.509015
 C    1.258410    1.683651   -0.293826
 C    0.143879    1.647081    3.957526
 C   -0.268828    2.315658    1.528507
 C    1.720466    1.714057   -1.737506
 C    0.070566    2.317565    0.146630
 C    0.608612    1.712790   -2.782191
 C    2.620375    2.950115   -1.892526
 H    2.282074    0.398744    2.731520
 H    2.942440    0.459950    0.343895
 H    0.497218    0.722941    4.434215
 H    0.598033    2.499800    4.484166
 H   -0.946206    1.714418    4.070288
 H   -1.235613    2.728938    1.824752
 H    2.346359    0.820669   -1.890600
 H   -0.634874    2.773640   -0.556436
 H    0.004222    0.796322   -2.736680
 H   -0.067919    2.574101   -2.670048
 H    1.055528    1.767426   -3.785615
 H    3.444646    2.945145   -1.163576
 H    2.038160    3.874554   -1.749295
 H    3.055507    2.971471   -2.902484
 C    2.327097   -2.256999    0.372367
 N   -0.319186   -1.082504   -0.729020
 C    1.964177   -1.967496   -0.948973
 C    3.671328   -2.408045    0.702888
 C   -1.670329   -1.205250   -1.218282
 C    0.557773   -1.796844   -1.345686
 C    2.949625   -1.876198   -1.940793
 C    4.655298   -2.259939   -0.276097
 C   -2.411982   -0.064537   -1.529428
 C   -2.241352   -2.473499   -1.342541
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 C    4.293931   -1.998092   -1.598788
 C   -3.713838   -0.201389   -2.000809
 C   -3.551951   -2.600116   -1.804475
 C   -4.289124   -1.466399   -2.139677
 H    1.554295   -2.374093    1.133406
 H    3.951347   -2.637816    1.732801
 H    0.242070   -2.321680   -2.258534
 H    2.661627   -1.682366   -2.977289
 H    5.709524   -2.363088   -0.010088
 H   -1.988422    0.933669   -1.403677
 H   -1.668441   -3.357889   -1.054526
 H    5.061557   -1.895505   -2.368190
 H   -4.282842    0.696256   -2.252092
 H   -3.996623   -3.593382   -1.893402
 H   -5.315177   -1.565651   -2.499723
 O   -0.268754   -1.502707    2.122397
 O   -1.961431   -0.292505    1.537718
 C   -1.531613   -1.339467    2.114893
 C   -2.456737   -2.350321    2.704031
 H   -3.436743   -1.902979    2.903683
 H   -2.577983   -3.164453    1.973502
 H   -2.024938   -2.770644    3.620455
 Cl  -2.739596    3.681531   -1.519154
*
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```

D⁺•*S*•Cl⁻

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CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1845.159347
G (1 atm) =               -1844.694124
qh G-E (1 mol/L) =            0.482086
qh G-E (24.56 mol/L) =        0.485109
Lowest Frequency =           17.43

SMD (MeOH)
HF SCF energy (TZ) =      -1836.096877
HF SCF energy (QZ) =      -1836.182869
Correlation energy (DZ) =    -5.221944
Correlation energy (TZ) =    -6.423430
DLPNO-CCSD(T1)/CBS =      -1843.334281

*xyz 0 1
Ru   0.008581    0.468864    0.697069
 C    2.212555   -2.068766    0.379846
 C    0.557135    1.888262    2.273002
 C    2.027568    1.207310    0.391074
 H    2.291863    0.577091    2.451614
 O   -0.807520   -2.697978    1.663021
 N   -0.336351   -1.017516   -0.839199
 Cl  -3.899135    2.475356    1.403895
 O   -1.252314   -0.514883    1.894512
 C    1.929019   -1.876939   -0.979806
 C    3.537345   -2.159100    0.801020
 C    1.695143    1.191408    1.774259
 H    1.385356   -2.177410    1.087953
 C    0.182674    1.831613    3.723621
 C   -0.277877    2.508340    1.317476
 C    1.216437    1.874383   -0.557508
 H    2.884932    0.626157    0.048309
 C   -1.595610   -1.786675    1.878876
 C   -1.711696   -1.178007   -1.228178
 C    0.536179   -1.757763   -1.428621
 H   -3.088374    2.994436   -0.461703
 C    2.968472   -1.820574   -1.916914
 C    4.574602   -2.048298   -0.126522
 H    3.760079   -2.314858    1.858455
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 H    0.514029    0.888790    4.178808
 H    0.672835    2.661123    4.255089
 H   -0.902813    1.932875    3.851653
 C    0.033251    2.484868   -0.076192
 H   -1.254820    2.897233    1.620392
 C    1.606459    1.875567   -2.022233
 C   -3.057420   -2.014786    2.171706
 C   -2.521464   -0.052097   -1.388736
 C   -2.252881   -2.460315   -1.369043
 H    0.225234   -2.347192   -2.302383
 C    4.290510   -1.882828   -1.484440
 H    2.739287   -1.698309   -2.978381
 H    5.612775   -2.106438    0.207760
 H   -0.708402    2.895864   -0.767319
 C    0.425374    1.835282   -2.989729
 C    2.490516    3.106568   -2.267174
 H    2.222117    0.976230   -2.187162
 H   -3.328781   -1.531960    3.121092
 H   -3.654122   -1.538872    1.377972
 H   -3.281157   -3.086826    2.213473
 C   -3.866646   -0.211131   -1.713494
 H   -2.124968    0.958758   -1.272198
 C   -3.598518   -2.608740   -1.698381
 H   -1.631651   -3.337865   -1.180429
 H    5.103420   -1.809111   -2.209372
 H    0.800389    1.816286   -4.023255
 H   -0.222881    2.719464   -2.887679
 H   -0.192905    0.938299   -2.840897
 H    3.363351    3.113700   -1.596983
 H    1.919865    4.034035   -2.098095
 H    2.853496    3.110749   -3.305525
 C   -4.408633   -1.486421   -1.872058
 H   -4.491903    0.675824   -1.832756
 H   -4.017849   -3.611586   -1.801011
 H   -5.465413   -1.606601   -2.118984
 C   -3.624895    3.848358   -2.141168
 H   -3.156855    4.060879   -3.113426
 H   -4.509087    3.210087   -2.318314
 H   -3.969757    4.804963   -1.708825
 O   -2.664260    3.211902   -1.324638
*
```

D⁺•S_2•Cl⁻

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1960.896867
G (1 atm) =               -1960.381693
qh G-E (1 mol/L) =            0.533708
qh G-E (24.56 mol/L) =        0.536730
Lowest Frequency =           10.86

SMD (MeOH)
HF SCF energy (TZ) =      -1951.211649
HF SCF energy (QZ) =      -1951.305265
Correlation energy (DZ) =    -5.606170
Correlation energy (TZ) =    -6.899144
DLPNO-CCSD(T1)/CBS =      -1958.988147

*xyz 0 1
Ru  -0.198173    0.029951    0.850560
 C    1.361857    0.789684    2.111406
 C    1.756136    1.016113    0.770224
 C    0.120018    1.268378    2.618151
 H    1.988631    0.157609    2.744437
 C   -0.357296    2.154387    0.341844
 C   -0.731692    1.930490    1.696174
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C	0.904292	1.713219	-0.129496
C	2.391843	-2.139292	0.029266
O	-0.284047	-1.901937	1.803270
Cl	-4.915404	2.024426	0.704828
N	-0.353006	-1.124003	-0.983429
O	-2.102300	-0.837320	1.323813
H	2.699485	0.604783	0.410139
C	-0.315655	0.995567	4.029627
H	-1.077492	2.619331	-0.335453
H	-1.749682	2.166244	2.018178
C	1.388092	1.976613	-1.541905
C	2.014776	-1.734991	-1.257851
C	3.741630	-2.204773	0.365649
H	1.626403	-2.412495	0.757185
C	-1.557277	-1.887531	1.784955
H	-3.965638	1.865326	2.593790
H	-3.488732	2.717191	-0.684732
C	-1.677539	-1.333351	-1.514925
C	0.602680	-1.657081	-1.663161
H	0.035383	0.010015	4.365214
H	0.115095	1.756068	4.698811
H	-1.409762	1.047955	4.105467
C	0.297166	2.000858	-2.609117
C	2.162421	3.303566	-1.510827
H	2.102656	1.175258	-1.788909
C	2.996181	-1.440123	-2.213601
C	4.716043	-1.858354	-0.572076
H	4.033676	-2.525011	1.367798
C	-2.364386	-3.060143	2.230369
O	-3.492115	1.933675	3.450663
O	-2.832549	3.023557	-1.349901
C	-2.542425	-0.254374	-1.703445
C	-2.099439	-2.634268	-1.799193
H	0.355339	-2.090622	-2.642784
H	0.749229	2.226598	-3.586005
H	-0.465102	2.767928	-2.404779
H	-0.212955	1.031421	-2.693686
H	2.973383	3.280918	-0.767355
H	1.489858	4.139939	-1.261005
H	2.606138	3.502669	-2.497482
C	4.343199	-1.478372	-1.862701
H	2.699225	-1.156073	-3.226530
H	5.773175	-1.898709	-0.300297
H	-3.334219	-2.727808	2.619080
H	-2.541652	-3.702179	1.353851
H	-1.818317	-3.637800	2.985233
C	-3.690491	3.251457	3.921567
C	-3.539148	3.639882	-2.406228
C	-3.819599	-0.482332	-2.207503
H	-2.239818	0.764845	-1.457482
C	-3.384373	-2.852937	-2.296897
H	-1.430727	-3.476190	-1.605366
H	5.104796	-1.220845	-2.601269
H	-3.123483	3.366709	4.857343
H	-4.754159	3.461870	4.135810
H	-3.326501	4.011310	3.205572
H	-4.092036	4.535438	-2.069768
H	-4.256128	2.949768	-2.886246
H	-2.807214	3.953647	-3.164965
C	-4.245716	-1.777970	-2.506698
H	-4.492164	0.365922	-2.350902
H	-3.711381	-3.872611	-2.510855
H	-5.253321	-1.949103	-2.891267*

D^{+}•S_3•Cl^{-}

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -2076.607611
G (1 atm) =               -2076.044296
qh G-E (1 mol/L) =            0.583816
qh G-E (24.56 mol/L) =        0.586838
Lowest Frequency =           13.43

SMD (MeOH)
HF SCF energy (TZ) =      -2066.307633
HF SCF energy (QZ) =      -2066.408936
Correlation energy (DZ) =    -5.987585
Correlation energy (TZ) =    -7.372184
DLPNO-CCSD(T1)/CBS =      -2074.620713

*xyz 0 1
Ru  -0.115128    0.277583    0.793867
 C    1.503978    1.240674    1.828986
 C    1.821730    1.252727    0.450956
 C    0.280185    1.779177    2.324937
 H    2.175003    0.723822    2.518670
 C   -0.628650    2.282707    1.360675
 C   -0.328446    2.294224   -0.031727
 C    0.908578    1.789220   -0.499123
 Cl  -4.408528    2.369403    1.188703
 C    2.441046   -1.983853    0.287587
 N   -0.324754   -1.173959   -0.808750
 O   -0.198967   -1.432462    2.114416
 O   -2.005704   -0.475777    1.419952
 H    2.752108    0.798506    0.109088
 C   -0.082330    1.714419    3.781044
 H   -1.637393    2.567192    1.674055
 H   -1.091598    2.642009   -0.731604
 C    1.306689    1.826259   -1.961558
 H   -3.416412    2.685775   -0.692054
 H   -5.625729    1.569365   -0.451769
 H   -3.527267    1.051814    2.873222
 C    2.038302   -1.803412   -1.042056
 C    3.796543   -1.980370    0.605897
 H    1.690984   -2.137048    1.065377
 C   -1.663622   -1.482383   -1.248746
 C    0.617363   -1.803008   -1.422203
 C   -1.472220   -1.393811    2.115857
 H   -1.147090    1.464714    3.900061
 H    0.105703    2.690843    4.252622
 H    0.524004    0.960372    4.300641
 C    0.155750    1.667411   -2.951652
 C    2.057767    3.146990   -2.190643
 H    2.019706    1.001033   -2.119134
 O   -2.969862    2.818702   -1.554836
 O   -6.228675    1.330229   -1.183216
 O   -3.340687    0.742958    3.780089
 C    2.999994   -1.664197   -2.051349
 C    4.751344   -1.787994   -0.394377
 H    4.108648   -2.125325    1.642069
 C   -2.565696   -0.460631   -1.552614
 C   -2.064705   -2.818477   -1.315416
 H    0.350081   -2.393301   -2.310350
 C   -2.311330   -2.357339    2.882805
 H    0.545935    1.738824   -3.977442
 H   -0.608971    2.449501   -2.828128
 H   -0.337678    0.691040   -2.849763
 H    2.911408    3.250601   -1.503994
 H    1.386354    4.007133   -2.036937
 H    2.439070    3.188695   -3.221590
 C   -3.865537    3.511272   -2.403999
 C   -7.335020    2.204533   -1.102260
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 C   -4.104105    1.546204    4.657623
 C    4.353109   -1.633082   -1.723443
 H    2.682938   -1.555700   -3.091841
 H    5.813225   -1.773533   -0.139029
 C   -3.860449   -0.783078   -1.948761
 H   -2.281363    0.589706   -1.472492
 C   -3.365197   -3.133633   -1.711502
 H   -1.368148   -3.609871   -1.029301
 H   -2.924795   -2.934585    2.176129
 H   -2.984701   -1.771351    3.523948
 H   -1.691052   -3.033137    3.481365
 H   -4.065435    4.537392   -2.045941
 H   -4.824691    2.975136   -2.493799
 H   -3.402585    3.578542   -3.399170
 H   -8.048702    1.922507   -1.890518
 H   -7.853999    2.132989   -0.128990
 H   -7.050112    3.261379   -1.262478
 H   -5.189479    1.448595    4.474296
 H   -3.838318    2.616351    4.584626
 H   -3.898014    1.210174    5.684481
 H    5.099633   -1.497076   -2.508355
 C   -4.263823   -2.118174   -2.030298
 H   -4.572467    0.017354   -2.162370
 H   -3.674513   -4.180032   -1.755871
 H   -5.285428   -2.363709   -2.328507
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D⁺•AcO⁻

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CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1497.665811
G (1 atm) =               -1497.199547
qh G-E (1 mol/L) =            0.479598
qh G-E (24.56 mol/L) =        0.482621
Lowest Frequency =            8.69

HF SCF energy (TZ) =      -1488.757160
HF SCF energy (QZ) =      -1488.847555
Correlation energy (DZ) =    -5.383606
Correlation energy (TZ) =    -6.590971
DLPNO-CCSD(T1)/CBS =      -1496.171269

SMD (MeOH)
HF SCF energy (TZ) =      -1488.778992
HF SCF energy (QZ) =      -1488.868950
Correlation energy (DZ) =    -5.377186
Correlation energy (TZ) =    -6.585461
DLPNO-CCSD(T1)/CBS =      -1496.187555

*xyz 0 1
Ru   0.465596   -0.570270   -0.079354
 O   -0.321286   -0.641326   -1.887045
 C   -0.736002   -1.742072   -2.510036
 C   -2.209159   -1.745104   -2.815029
 O    0.014107   -2.661067   -2.795001
 C    2.162714   -1.212613    1.092479
 C    1.336101   -0.449483    1.945262
 C    1.656730   -2.336999    0.369547
 C   -0.044195   -0.733863    2.056339
 C    2.539336   -3.107667   -0.565022
 C    0.282177   -2.649006    0.507786
 C   -0.987235    0.068435    2.928939
 C   -0.562770   -1.833062    1.300246
 C   -0.533463    1.503966    3.185932
 C   -1.166949   -0.700766    4.246651
 H   -2.522182   -0.767428   -3.206619
```

```
H   -2.742707   -1.912008   -1.861558
H   -2.454828   -2.543684   -3.524982
H    3.199687   -0.908890    0.942003
H    1.752760    0.440712    2.417024
H    3.364958   -2.483540   -0.931481
H    2.969584   -3.961864   -0.019793
H    1.960291   -3.482538   -1.417698
H   -0.155052   -3.431699   -0.113799
H   -1.967170    0.076214    2.419639
H   -1.653865   -1.972579    1.228136
H   -0.334519    2.049786    2.250924
H    0.377915    1.540700    3.804082
H   -1.320741    2.046551    3.729508
H   -1.548077   -1.718049    4.069228
H   -0.212203   -0.781265    4.791578
H   -1.887047   -0.175468    4.891739
N    0.514896    1.566985   -0.490962
C    1.563558    2.307093   -0.399247
C   -0.727415    2.217563   -0.803086
C    2.926460    1.759152   -0.320796
C   -1.904236    1.777344   -0.196733
C   -0.770437    3.258681   -1.736040
C    3.810747    2.210533    0.666274
C    3.349748    0.813448   -1.264957
C   -3.111433    2.411610   -0.475075
C   -1.984126    3.884471   -2.017548
C    5.092799    1.671919    0.743057
C    4.645014    0.304107   -1.203679
C   -3.154913    3.470907   -1.382008
C    5.510226    0.721060   -0.191296
H    1.450038    3.400037   -0.407703
H   -1.902784    0.937421    0.499575
H    0.136290    3.562759   -2.263347
H    3.483156    2.963113    1.387242
H    2.669591    0.494679   -2.058936
H   -4.007668    2.050727    0.032513
H   -2.011532    4.694293   -2.749576
H    5.773882    2.002104    1.529782
H    4.977170   -0.423814   -1.946495
H   -4.103092    3.964202   -1.606043
H    6.521205    0.311778   -0.135910
O   -3.426129   -1.950763    0.299607
C   -4.140435   -0.923970    0.486294
C   -5.267260   -0.679689   -0.520438
O   -3.986199   -0.074929    1.401078
H   -5.666330   -1.627336   -0.908643
H   -4.855584   -0.115036   -1.373674
H   -6.075521   -0.080461   -0.078175
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***trans*-D⁺**
M CPCM (MeOH)
06 SCF (DZ) = -1268.442918
G (1 atm) = -1268.034830
qh-G (1 mol/L) = -1268.026232
qh-G (24.56 mol/L) = -1268.023209
Lowest Frequency = 19.38

HF SCF energy (TZ) = -1261.325967
HF SCF energy (QZ) = -1261.405053
Correlation energy (DZ) = -4.689071
Correlation energy (TZ) = -5.723637
DLPNO-CCSD(T1)/CBS = -1267.757054

*xyz 1 1

***trans*-D⁺**
CPCM (MeOH)
wB97X-D3 SCF (DZ) = -1269.080265
G (1 atm) = -1268.658501
qh G-E (1 mol/L) = 0.432697
qh G-E (24.56 mol/L) = 0.435720
Lowest Frequency = 15.49

HF SCF energy (TZ) = -1261.329005
HF SCF energy (QZ) = -1261.402327
Correlation energy (DZ) = -4.688828
Correlation energy (TZ) = -5.722976
DLPNO-CCSD(T1)/CBS = -1267.751686

SMD (MeOH)

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 Ru   0.423619   -0.465018    0.255641
 N   -1.450391    0.600011    0.005791
 O    0.365800   -0.609511   -1.903810
 C   -1.619531    1.858253   -0.238941
 C   -2.655476   -0.170478    0.132286
 O   -0.617365   -2.098198   -0.678451
 C   -0.355075   -1.656374   -1.841479
 C   -0.580901    2.836531   -0.545611
 H   -2.649154    2.250115   -0.184031
 C   -2.894034   -0.922141    1.282802
 C   -3.575306   -0.181583   -0.917693
 C   -0.875936   -2.330939   -3.056811
 C    0.496233    2.554129   -1.397883
 C   -0.700357    4.111659    0.026245
 C   -4.064706   -1.663264    1.390664
 H   -2.161604   -0.920772    2.093331
 C   -4.740760   -0.937447   -0.807242
 H   -3.360839    0.384457   -1.829110
 H   -0.511134   -3.368506   -3.080517
 H   -1.974071   -2.373212   -3.004335
 H   -0.562661   -1.805135   -3.966022
 C    1.462281    3.525972   -1.633175
 H    0.554282    1.583203   -1.895446
 C    0.286499    5.067329   -0.187336
 H   -1.560940    4.339821    0.662193
 C   -4.989993   -1.675522    0.346450
 H   -4.254271   -2.239805    2.298884
 H   -5.454670   -0.949467   -1.634073
 C    1.370117    4.773145   -1.014268
 H    2.293895    3.310125   -2.308114
 H    0.204472    6.049503    0.282994
 H   -5.903797   -2.267888    0.431790
 H    2.139045    5.528475   -1.193230
 C    2.423516    0.302674    0.441815
 C    1.603341    1.047882    1.315971
 C    2.499466   -1.125175    0.502357
 H    2.949326    0.824553   -0.364983
 C    0.784218    0.388414    2.278308
 H    1.534858    2.132632    1.201411
 C    3.367038   -1.862815   -0.486385
 C    1.675868   -1.765236    1.455022
 C   -0.135421    1.173316    3.151251
 C    0.823271   -1.024415    2.325812
 C    2.943186   -3.302465   -0.723702
 C    4.817682   -1.788779   -0.012886
 H    3.284221   -1.309157   -1.441304
 H    1.593857   -2.854592    1.454720
 H   -0.515659    2.068446    2.637243
 H    0.419493    1.517366    4.038945
 H   -0.983621    0.569904    3.503536
 H    0.144649   -1.561119    2.993169
 H    1.881939   -3.386929   -1.009399
 H    3.107293   -3.924264    0.172942
 H    3.547332   -3.739659   -1.532828
 H    5.156220   -0.748425    0.115699
 H    4.933232   -2.306961    0.954487
 H    5.482998   -2.276334   -0.741998
*
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HF SCF energy (TZ) =      -1261.345232
HF SCF energy (QZ) =      -1261.418391
Correlation energy (DZ) =    -4.685153
Correlation energy (TZ) =    -5.720315
DLPNO-CCSD(T1)/CBS =      -1267.765631

*xyz 1 1
 Ru   0.362131   -0.983433   -0.052211
 C    2.226297   -2.031826    0.045192
 C    0.333494   -2.495175    1.477188
 C    1.202952   -2.937211    0.447317
 C    2.403863   -0.773819    0.671915
 C    0.503314   -1.238800    2.122064
 C    1.550144   -0.366709    1.734791
 C    0.992886   -4.249032   -0.252032
 C    1.787732    0.975742    2.395138
 C    0.544673    1.614584    3.008810
 C    2.892382    0.788729    3.445662
 H    2.829749   -2.269150   -0.833423
 H   -0.543357   -3.096329    1.726921
 H    3.160321   -0.085382    0.292334
 H   -0.211293   -0.938171    2.887529
 H    1.548715   -5.039544    0.274006
 H    1.355936   -4.204223   -1.287205
 H   -0.070305   -4.523875   -0.257389
 H    2.177101    1.646676    1.612958
 H    0.798856    2.616017    3.385351
 H   -0.265670    1.729008    2.273901
 H    0.161318    1.030289    3.859812
 H    2.562502    0.100774    4.240222
 H    3.134635    1.756947    3.907581
 H    3.811374    0.382718    2.997498
 O   -1.538037   -1.524649   -0.888613
 O    0.173848   -1.242897   -2.172837
 C   -1.074025   -1.476397   -2.069011
 C   -1.952114   -1.623586   -3.264434
 H   -2.731779   -2.370383   -3.070940
 H   -2.440714   -0.653308   -3.442366
 H   -1.361564   -1.894337   -4.146795
 N   -0.194486    1.067390   -0.527084
 C    0.899410    1.896190   -0.974857
 C   -1.347008    1.650294   -0.535126
 C   -2.746342    0.287481    1.074715
 C    1.108382    3.138273   -0.369681
 C    1.755871    1.454189   -1.986459
 C   -2.627813    1.169373   -0.007276
 C   -4.002052   -0.083580    1.539625
 C    2.175027    3.939004   -0.777451
 C    2.813156    2.264631   -2.391892
 C   -3.787594    1.693591   -0.597597
 C   -5.152615    0.412806    0.922581
 C    3.029985    3.504719   -1.788046
 C   -5.045068    1.300851   -0.147676
 H   -1.394156    2.648136   -0.993630
 H   -1.852833   -0.100059    1.560322
 H    0.450410    3.467333    0.437752
 H    1.579090    0.488925   -2.461218
 H   -4.084385   -0.763829    2.389438
 H    2.336274    4.903888   -0.292496
 H    3.474740    1.921288   -3.189805
 H   -3.698231    2.406241   -1.421462
 H   -6.138190    0.113474    1.285765
 H    3.866974    4.130245   -2.104775
 H   -5.943171    1.699679   -0.622773
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E

CPCM (MeOH)

M06 SCF (DZ) =	-1267.994950
G (1 atm) =	-1267.600132
qh-G (1 mol/L) =	-1267.591512
qh-G (24.56 mol/L) =	-1267.588489
Lowest Frequency =	22.86

HF SCF energy (TZ) =	-1260.846696
HF SCF energy (QZ) =	-1260.921704
Correlation energy (DZ) =	-4.711725
Correlation energy (TZ) =	-5.750684
DLPNO-CCSD(T1)/CBS =	-1267.302090

PBE0+D3BJ (ATZ) =	-1267.926610
M06-2X (ATZ) =	-1268.634410
wB97M-V (ATZ) =	-1268.709277
B2GP-PLYP (ATZ) =	-1267.968880
B2K-PLYP (ATZ) =	-1267.804231
PWPB95 (ATZ) =	-1268.301321
PWPB95+D3BJ (ATZ) =	-1268.342096
PWPB95+D4 (ATZ) =	-1268.357382

*xyz 0 1

Ru	0.313856	0.224976	0.474590
C	1.624952	-0.422176	-0.984864
N	-0.980557	-0.204434	-1.155951
C	3.022474	-0.512636	-0.933238
C	1.019050	-0.772109	-2.219969
O	0.415426	2.088833	-0.528536
C	-0.408239	-0.615581	-2.245832
C	-2.389247	-0.061212	-1.106639
C	3.762492	-0.956544	-2.031257
H	3.558994	-0.224729	-0.022162
C	1.757250	-1.208891	-3.330223
C	1.360391	2.957339	-0.367099
H	-1.000235	-0.814294	-3.152227
C	-3.230882	-1.088522	-1.544840
C	-2.937795	1.114782	-0.583938
C	3.137588	-1.309847	-3.232247
H	4.851941	-1.026640	-1.951563
H	1.240728	-1.462196	-4.261891
C	1.181031	4.186487	-1.235347
O	2.320358	2.863475	0.399714
C	-4.613532	-0.930900	-1.473447
H	-2.796730	-2.019538	-1.920938
C	-4.318703	1.265669	-0.523684
H	-2.261703	1.905579	-0.246251
H	3.731275	-1.653344	-4.082724
H	0.231598	4.684796	-0.984640
H	1.118824	3.896544	-2.295189
H	2.010694	4.891110	-1.092816
C	-5.161417	0.244419	-0.965686
H	-5.265598	-1.740890	-1.809740
H	-4.742714	2.191648	-0.127147
H	-6.245916	0.364014	-0.907389
C	-0.896789	-0.944981	1.827915
C	0.395152	-1.537241	1.767862
C	-1.102541	0.403469	2.250540
H	-1.769806	-1.529028	1.520320
C	0.631705	-2.984430	1.411061
C	1.498979	-0.680161	2.057147
C	0.002613	1.239395	2.479126
H	-2.114440	0.815576	2.273022
C	-0.406435	-3.558301	0.460197

E

CPCM (MeOH)

wB97X-D3 SCF (DZ) =	-1268.618988
G (1 atm) =	-1268.210789
qh G-E (1 mol/L) =	0.419204
qh G-E (24.56 mol/L) =	0.422227
Lowest Frequency =	7.73

HF SCF energy (TZ) =	-1260.849780
HF SCF energy (QZ) =	-1260.923445
Correlation energy (DZ) =	-4.711580
Correlation energy (TZ) =	-5.750353
DLPNO-CCSD(T1)/CBS =	-1267.302987

PBE0+D3BJ (ATZ) =	-1267.927146
M06-2X (ATZ) =	-1268.645837
wB97M-V (ATZ) =	-1268.715353
B2GP-PLYP (ATZ) =	-1267.981722
B2K-PLYP (ATZ) =	-1267.818308
PWPB95 (ATZ) =	-1268.309998
PWPB95+D3BJ (ATZ) =	-1268.350725
PWPB95+D4 (ATZ) =	-1268.365924

SMD (MeOH)

HF SCF energy (TZ) =	-1260.866166
HF SCF energy (QZ) =	-1260.939589
Correlation energy (DZ) =	-4.707052
Correlation energy (TZ) =	-5.746743
DLPNO-CCSD(T1)/CBS =	-1267.315984

* xyz 0 1

Ru	0.301832	0.186173	0.465541
C	1.580454	-0.523039	-0.988870
N	-1.010408	-0.164247	-1.156598
C	2.971884	-0.711772	-0.940940
C	0.957529	-0.832655	-2.224415
C	-0.471439	-0.596994	-2.247234
C	-2.414817	0.071222	-1.113792
C	3.682470	-1.194007	-2.043085
C	1.660634	-1.311047	-3.339346
C	-3.316651	-0.941285	-1.447847
C	-2.880212	1.324755	-0.704883
C	3.034549	-1.498439	-3.246134
C	-4.688490	-0.690363	-1.391023
C	-4.249926	1.566971	-0.655423
C	-5.158124	0.561724	-0.998199
C	-0.920415	-0.993328	1.783359
C	0.373720	-1.575470	1.748484
C	-1.143722	0.359199	2.198081
C	0.624565	-3.031404	1.406730
C	1.468865	-0.712295	2.065548
C	-0.050920	1.197647	2.459452
C	-0.352492	-3.596354	0.376226
C	0.619874	-3.859321	2.697195
C	1.273311	0.645466	2.380909
C	-0.230055	2.658880	2.755768
H	3.525677	-0.474947	-0.027833
H	-1.077356	-0.761159	-3.148020
H	4.764349	-1.333959	-1.964532
H	1.128354	-1.531099	-4.269136
H	-2.942436	-1.926539	-1.735107
H	-2.154466	2.097514	-0.443364
H	3.602311	-1.873266	-4.100190
H	-5.391790	-1.484935	-1.649484
H	-4.611746	2.549564	-0.344844

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 C    0.714295   -3.809184    2.693026
 H    1.617356   -3.022766    0.907901
 C    1.320224    0.682051    2.375668
 H    2.514785   -1.072381    1.941388
 C   -0.168003    2.698050    2.749802
 H   -0.501569   -2.950420   -0.454404
 H   -1.400983   -3.625360    0.934572
 H   -0.123964   -4.580600    0.163853
 H    1.494403   -3.428168    3.371843
 H   -0.248627   -3.776810    3.232782
 H    0.941382   -4.863565    2.468154
 H    2.186403    1.334860    2.485114
 H    0.663787    3.268369    2.310906
 H   -0.171473    2.885878    3.836196
 H   -1.118130    3.072297    2.339102
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E⁺

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CPCM (MeOH)
M06 SCF (DZ) =            -1268.441301
G (1 atm) =               -1268.031236
qh-G (1 mol/L) =          -1268.023489
qh-G (24.56 mol/L) =      -1268.020467
Lowest Frequency =           22.26

HF SCF energy (TZ) =      -1260.846696
HF SCF energy (QZ) =      -1260.921704
Correlation energy (DZ) =    -4.711725
Correlation energy (TZ) =    -5.750685
DLPNO-CCSD(T1)/CBS =      -1267.302090

*xyz 1 1
 Ru  -0.313280    0.078288   -0.420143
 C    0.126074   -0.006176   -2.543623
 N    1.328166   -1.025761    0.361627
 C    0.719273   -1.166181   -3.274960
 C   -1.278119    0.119055   -2.351210
 C    0.951650    1.000351   -1.952873
 C   -1.141324   -1.806251   -0.099178
 O   -0.608998    0.577939    1.687111
 C    2.634623   -0.490185    0.509647
 C    1.089965   -2.260727    0.675886
 H    1.699674   -1.435711   -2.852072
 H    0.869798   -0.921611   -4.338690
 H    0.059751   -2.045276   -3.219204
 C   -1.830186    1.169313   -1.575601
 H   -1.934433   -0.668184   -2.733080
 C    0.418140    2.085221   -1.225302
 H    2.039457    0.887899   -2.013941
 C   -0.239245   -2.758748    0.442834
 C   -2.442917   -2.256533   -0.356254
 C   -1.627028    0.531600    2.385383
 C    3.741733   -1.171139   -0.004772
 C    2.801537    0.747000    1.139364
 H    1.878206   -2.890315    1.113757
 C   -0.978411    2.145641   -0.980221
 H   -2.906855    1.202331   -1.385539
 H    1.096668    2.801552   -0.759248
 H   -6.232024    0.754637   -0.953237
 H   -1.782731   -1.583398    1.467707
 H   -2.157634    0.761482    2.202527
 H    1.637274   -3.076709    0.971160
 H    2.487844   -1.094950    1.979695
 H   -0.362025   -2.988682   -0.541035
 H   -1.380658   -3.644021    0.769541
 H   -0.059007   -4.621154    0.103967
 H    1.361476   -3.482662    3.418363
 H   -0.371429   -3.819994    3.177882
 H    0.854936   -4.913129    2.483569
 H    2.134244    1.297179    2.517115
 H    0.574561    3.242502    2.288428
 H   -0.181206    2.824570    3.843091
 H   -1.199843    3.023486    2.391918
 O    0.448036    2.055286   -0.505238
 C    1.374723    2.939495   -0.337798
 C    1.120672    4.227610   -1.105081
 O    2.374632    2.821560    0.377450
 H    0.272484    4.754843   -0.641788
 H    0.844379    4.008395   -2.145864
 H    2.003971    4.877311   -1.078003
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CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1269.072786
G (1 atm) =               -1268.651014
qh G-E (1 mol/L) =            0.432851
qh G-E (24.56 mol/L) =        0.435873
Lowest Frequency =           10.79

HF SCF energy (TZ) =      -1261.312142
HF SCF energy (QZ) =      -1261.385289
Correlation energy (DZ) =    -4.705054
Correlation energy (TZ) =    -5.739564
DLPNO-CCSD(T1)/CBS =      -1267.751395

SMD (MeOH)
HF SCF energy (TZ) =      -1261.327085
HF SCF energy (QZ) =      -1261.400192
Correlation energy (DZ) =    -4.702289
Correlation energy (TZ) =    -5.737377
DLPNO-CCSD(T1)/CBS =      -1267.764435

*xyz 1 1
 Ru  -0.398494   -0.008555   -0.434807
 C   -0.239089   -0.170552   -2.598032
 N    1.299085   -0.944186    0.407583
 C    0.092208   -1.380868   -3.423945
 C   -1.584016    0.158230   -2.249916
 C    0.775089    0.691590   -2.101634
 C   -1.074989   -1.944108   -0.107209
 C    2.555023   -0.290591    0.589013
 C    1.166089   -2.181485    0.750325
 C   -1.879486    1.272708   -1.437895
 C    0.486878    1.867377   -1.347114
 C   -0.116601   -2.802738    0.487745
 C   -2.325664   -2.515684   -0.384129
 C    3.710491   -0.809791    0.001873
 C    2.606866    0.895289    1.325961
 C   -0.838820    2.148045   -0.976112
 C   -0.376895   -4.145395    0.786755
 C   -2.596319   -3.857299   -0.092247
 C    4.924584   -0.141274    0.164625
```

```
 C   -0.613536   -4.079533    0.717223
 C   -2.822585   -3.576058   -0.082665
 H   -3.194983   -1.581147   -0.783840
 C   -1.710856    1.203736    3.704398
 O   -2.727323   -0.078968    2.013643
 C    5.014175   -0.619534    0.126575
 H    3.598391   -2.120277   -0.529095
 C    4.076565    1.285701    1.270294
 H    1.925339    1.266741    1.536542
 C   -1.600083    3.210922   -0.109155
 C   -1.914962   -4.489860    0.452774
 H    0.118712   -4.777479    1.134755
 H   -3.846457   -3.893868   -0.298929
 H   -2.209044    0.553528    4.435197
 H   -2.331533    2.107099    3.590181
 H   -0.712857    1.494428    4.048866
 H   -2.560005   -0.545513    1.163572
 C    5.185656    0.606591    0.764089
 H    5.875902   -1.151368   -0.283735
 H    4.205638    2.246862    1.773602
 C   -0.646616    3.836482    0.896289
 C   -2.204438    4.280747   -1.019143
 H   -2.428279    2.722448    0.441139
 H   -2.223693   -5.516830    0.658689
 H    6.184169    1.038899    0.861520
 H   -0.150174    3.081070    1.526343
 H    0.131456    4.435877    0.393863
 H   -1.200995    4.520532    1.557180
 H   -2.945690    3.859552   -1.715961
 H   -1.413270    4.767363   -1.614923
 H   -2.701690    5.056675   -0.416853
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 C    3.822749    1.553476    1.485405
 C   -1.214705    3.332487   -0.106718
 C   -1.628404   -4.677476    0.492088
 C    4.984129    1.038501    0.904558
 C   -0.153358    3.714908    0.922948
 C   -1.564356    4.511453   -1.025483
 H    1.086548   -1.767810   -3.162472
 H    0.095915   -1.116534   -4.492179
 H   -0.649841   -2.175590   -3.268274
 H   -2.392556   -0.510109   -2.550333
 H    1.820128    0.424595   -2.275121
 H    1.993902   -2.724565    1.224047
 H   -2.912510    1.462054   -1.141177
 H    1.311088    2.481614   -0.985944
 H   -3.119742   -1.920591   -0.847160
 H    3.651678   -1.722754   -0.595110
 H    1.692031    1.287248    1.773040
 H    0.399778   -4.764209    1.244027
 H   -3.580735   -4.268347   -0.330972
 H    5.827482   -0.546231   -0.297122
 H    3.862006    2.476672    2.067410
 H   -2.130058    3.043330    0.436975
 H   -1.851094   -5.723007    0.713165
 H    5.935344    1.560838    1.025456
 H    0.076858    2.871658    1.589723
 H    0.781494    4.049923    0.447003
 H   -0.521023    4.546235    1.541966
 H   -2.356791    4.243093   -1.740385
 H   -0.679454    4.830715   -1.599189
 H   -1.914446    5.367222   -0.429554
 O   -0.800378    0.420658    1.647020
 C   -1.872492    0.436853    2.260938
 C   -1.981454    0.967420    3.647032
 O   -3.001942    0.019507    1.736891
 H   -2.637291    0.327079    4.249390
 H   -2.439768    1.966430    3.588646
 H   -0.986431    1.049762    4.094869
 H   -2.827386   -0.319013    0.835891
*
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E•S

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CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1384.330915
G (1 atm) =               -1383.872643
qh G-E (1 mol/L) =            0.470491
qh G-E (24.56 mol/L) =        0.473514
Lowest Frequencies =          7.73

HF SCF energy (TZ) =      -1375.937311
HF SCF energy (QZ) =      -1376.019293
Correlation energy (DZ) =    -5.097822
Correlation energy (TZ) =    -6.228596
DLPNO-CCSD(T1)/CBS =      -1382.933343

SMD (MeOH)
HF SCF energy (TZ) =      -1375.952054
HF SCF energy (QZ) =      -1376.033840
Correlation energy (DZ) =    -5.093118
Correlation energy (TZ) =    -6.224699
DLPNO-CCSD(T1)/CBS =      -1382.944407


* xyz 0 1
 Ru   0.439587    0.244849   -0.466760
 C    1.668410    1.177747    0.902659
```

N	-0.676975	0.074772	1.338212
C	1.212146	1.120644	2.241756
C	2.874295	1.868522	0.695293
C	-2.007261	-0.428215	1.441500
C	-0.079183	0.489987	2.406886
C	1.916178	1.684443	3.317169
C	3.574230	2.449670	1.753197
C	-2.352114	-1.615807	0.789844
C	-2.976373	0.286536	2.153420
C	3.107290	2.354307	3.070628
C	-3.656472	-2.095588	0.877436
C	-4.281261	-0.200316	2.231757
C	-4.624937	-1.393286	1.597939
C	0.488629	1.993236	-1.707036
C	1.340139	1.013637	-2.306121
C	-0.868442	1.708854	-1.413973
C	0.842901	-0.279367	-2.581705
C	-1.815211	2.720601	-0.795194
C	-1.365602	0.410132	-1.770801
C	1.735171	-1.364150	-3.114585
C	-0.543403	-0.561925	-2.346589
C	-1.144807	3.680571	0.185776
C	-2.537846	3.475448	-1.917839
H	3.291690	1.954951	-0.312156
H	-0.553392	0.388366	3.391556
H	1.519690	1.603421	4.333116
H	4.505615	2.985937	1.550756
H	-1.603689	-2.156311	0.206843
H	-2.713143	1.237498	2.622364
H	3.667908	2.808771	3.889929
H	-3.918812	-3.026906	0.370589
H	-5.034112	0.366048	2.784223
H	-5.648137	-1.770427	1.654761
H	0.913820	2.955037	-1.418622
H	2.392435	1.238884	-2.482862
H	-2.567985	2.138111	-0.236573
H	-2.394233	0.151029	-1.508383
H	2.792182	-1.154457	-2.905814
H	1.607090	-1.434462	-4.205781
H	1.461934	-2.334671	-2.678536
H	-0.918817	-1.573142	-2.507817
H	-0.626889	3.137014	0.990151
H	-0.411701	4.331976	-0.316100
H	-1.902255	4.333465	0.644446
H	-3.057242	2.782655	-2.597550
H	-1.821564	4.064184	-2.514107
H	-3.284931	4.167750	-1.500947
O	1.205933	-1.670352	0.119079
C	2.383745	-2.222569	0.193506
C	3.612567	-1.338893	0.160013
O	2.506726	-3.443905	0.306265
H	3.536401	-0.574549	-0.623997
H	4.504381	-1.957488	0.004197
H	3.704725	-0.809737	1.119656
O	-0.365101	-3.483540	-1.196947
C	-0.461564	-4.731985	-0.541621
H	0.218879	-2.903329	-0.656955
H	-0.898549	-5.458570	-1.242861
H	0.526927	-5.096135	-0.217899
H	-1.117742	-4.681722	0.348762

*

E•S_2

CPCM (MeOH)

wB97X-D3 SCF (DZ) = -1500.043858

```
G (1 atm) =               -1499.536104
qh G-E (1 mol/L) =            0.521804
qh G-E (24.56 mol/L) =        0.524827
Lowest Frequencies =          7.73

SMD (MeOH)
HF SCF energy (TZ) =      -1491.047108
HF SCF energy (QZ) =      -1491.136739
Correlation energy (DZ) =    -5.475863
Correlation energy (TZ) =    -6.700137
DLPNO-CCSD(T1)/CBS =      -1498.579269

* xyz 0 1
Ru   0.597491    0.135510   -0.716077
 C    1.741177    0.925769    0.810334
 C    2.968818    1.603239    0.746403
 C    1.221808    0.703659    2.109230
 C    3.628377    2.027735    1.902937
 C    1.879524    1.113365    3.277471
 C   -0.061145    0.034766    2.132873
 C    3.093549    1.782131    3.172745
 N   -0.582014   -0.287929    0.994778
 C   -1.889707   -0.856796    0.963451
 C   -2.933842   -0.250355    1.668164
 C   -2.133800   -1.995852    0.189779
 C   -4.216766   -0.795550    1.616636
 C   -3.416257   -2.535082    0.149283
 C   -4.461512   -1.939471    0.859444
 C    0.604721    2.017809   -1.747097
 C    1.506468    1.156551   -2.443689
 C   -0.745833    1.647430   -1.528045
 C    1.072461   -0.108989   -2.892503
 C   -1.751795    2.541390   -0.827800
 C   -1.174201    0.378590   -2.041561
 C    2.006471   -1.060681   -3.582641
 C   -0.297333   -0.485508   -2.705150
 C   -1.164717    3.362974    0.318263
 C   -2.429819    3.439077   -1.870121
 H    3.433185    1.809003   -0.222547
 H    4.580330    2.558664    1.814011
 H    1.436332    0.907394    4.255784
 H   -0.583985   -0.182219    3.072996
 H    3.623183    2.113710    4.068098
 H   -2.745175    0.663327    2.236586
 H   -1.318468   -2.465354   -0.361556
 H   -5.029183   -0.312319    2.163553
 H   -3.601374   -3.431257   -0.446821
 H   -5.466459   -2.364440    0.814601
 H    0.983648    2.956243   -1.340945
 H    2.548904    1.449724   -2.574914
 H   -2.519132    1.870093   -0.406196
 H   -2.193960    0.046816   -1.833247
 H    1.855457   -2.083594   -3.211520
 H    1.780542   -1.056464   -4.660203
 H    3.055147   -0.768986   -3.449784
 H   -0.628992   -1.477645   -3.012976
 H   -1.966832    3.921393    0.823433
 H   -0.428288    4.099305   -0.041117
 H   -0.671695    2.721846    1.063812
 H   -2.885463    2.845000   -2.676958
 H   -1.698271    4.127310   -2.324423
 H   -3.222008    4.042278   -1.401412
 O    1.529228   -1.736440   -0.184565
 C    2.764401   -1.926792    0.224137
 C    3.883056   -1.421370   -0.658759
 O    3.012548   -2.564342    1.242858
```

```
 H    3.643367   -0.450430   -1.106140
 H    4.020453   -2.147199   -1.476083
 H    4.816928   -1.359518   -0.087122
 O    0.170303   -3.681763    1.432429
 C    0.092190   -3.366068    2.802393
 H    0.671146   -2.968048    0.991209
 H   -0.131109   -4.287111    3.363073
 H    1.041360   -2.950069    3.183885
 H   -0.716627   -2.640764    3.019264
 O    0.330739   -3.529623   -1.900519
 C    0.883173   -4.793721   -1.578082
 H    0.751735   -2.874340   -1.307909
 H    1.953052   -4.858247   -1.849618
 H    0.341335   -5.558816   -2.153320
 H    0.778586   -5.019248   -0.503741
*
```

F

```
CPCM (MeOH)
M06 SCF (DZ) =            -1107.746206
G (1 atm) =               -1107.494428
qh-G (1 mol/L) =          -1107.486330
qh-G (24.56 mol/L) =      -1107.483307
Lowest Frequency =           22.62

HF SCF energy (TZ) =      -1101.839189
HF SCF energy (QZ) =      -1101.906698
Correlation energy (DZ) =    -3.774798
Correlation energy (TZ) =    -4.687417
DLPNO-CCSD(T1)/CBS =      -1107.147733

*xyz 0 1
 Ru  -0.269489    0.914599    0.933559
 N   -0.259882   -0.350453   -0.583596
 O   -1.901706   -0.115676    1.870376
 C   -1.575157   -0.640029   -1.091994
 C    0.702535   -1.023764   -1.149999
 O    1.340339    2.049246    0.066117
 O    0.143766   -0.709336    2.273922
 O   -0.718620    2.624732   -0.281980
 C   -1.098770   -0.894971    2.469755
 C   -2.327377    0.356023   -1.714842
 C   -2.092142   -1.927674   -0.941648
 C    2.119730   -1.097850   -0.834976
 H    0.402738   -1.639849   -2.011188
 C    0.518677    2.855736   -0.465693
 C   -1.592621   -2.002008    3.334431
 C   -3.597034    0.050864   -2.196495
 H   -1.907453    1.359510   -1.807987
 C   -3.367737   -2.220396   -1.418708
 H   -1.492720   -2.690070   -0.434787
 C    2.730135   -0.593381    0.326261
 C    2.918887   -1.776229   -1.774823
 C    0.981700    4.039239   -1.242126
 H   -2.527981   -1.713908    3.831819
 H   -1.804560   -2.878011    2.700673
 H   -0.833453   -2.287704    4.073522
 C   -4.122074   -1.233321   -2.048711
 H   -4.183943    0.827636   -2.693248
 H   -3.773147   -3.227518   -1.293602
 C    4.095048   -0.758189    0.524608
 H    2.122239   -0.078050    1.070911
 C    4.284553   -1.929770   -1.576671
 H    2.451517   -2.184243   -2.676341
 H    1.936451    3.823984   -1.739200
```

F

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1108.208048
G (1 atm) =               -1107.946166
qh G-E (1 mol/L) =            0.273302
qh G-E (24.56 mol/L) =        0.276325
Lowest Frequency =           14.21

HF SCF energy (TZ) =      -1101.844987
HF SCF energy (QZ) =      -1101.911849
Correlation energy (DZ) =    -3.770871
Correlation energy (TZ) =    -4.682115
DLPNO-CCSD(T1)/CBS =      -1107.146580

SMD (MeOH)
HF SCF energy (TZ) =      -1101.856541
HF SCF energy (QZ) =      -1101.923213
Correlation energy (DZ) =    -3.765024
Correlation energy (TZ) =    -4.677340
DLPNO-CCSD(T1)/CBS =      -1107.153740

* xyz 0 1
 Ru  -0.216051    0.860766    0.911808
 N   -0.282885   -0.462760   -0.599876
 O   -1.933526   -0.020156    1.872096
 C   -1.615723   -0.753640   -1.071142
 C    0.667890   -1.080338   -1.216924
 O    1.488218    1.868064    0.061987
 O    0.059783   -0.712227    2.368028
 O   -0.519004    2.555505   -0.382487
 C   -1.197947   -0.813122    2.538406
 C   -2.346248    0.230503   -1.736125
 C   -2.162004   -2.014000   -0.831560
 C    2.102043   -1.066401   -0.898153
 H    0.381320   -1.679907   -2.091308
 C    0.737019    2.693603   -0.544069
 C   -1.783534   -1.845771    3.448037
 C   -3.636848   -0.060546   -2.172542
 H   -1.898144    1.211866   -1.898179
 C   -3.457043   -2.293123   -1.267333
 H   -1.576713   -2.762231   -0.292193
 C    2.598153   -1.036855    0.412132
 C    2.996182   -1.160802   -1.974547
 C    1.304822    3.791593   -1.386197
 H   -2.714228   -1.475239    3.894687
 H   -2.023099   -2.735759    2.845706
 H   -1.062967   -2.130030    4.223865
 C   -4.195433   -1.318882   -1.938500
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```
 H    1.143596    4.878996   -0.548133
 H    0.223906    4.343214   -1.975338
 H   -5.122426   -1.463072   -2.423574
 C    4.877602   -1.419385   -0.422848
 H    4.556912   -0.365923    1.434110
 H    4.887947   -2.453653   -2.321677
 H    5.951114   -1.541614   -0.258002
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F*

```
CPCM (MeOH)
M06 SCF (DZ) =            -1107.740132
G (1 atm) =               -1107.490631
qh-G (1 mol/L) =          -1107.481454
qh-G (24.56 mol/L) =      -1107.478431
Lowest Frequency =           21.17

HF SCF energy (TZ) =      -1101.841709
HF SCF energy (QZ) =      -1101.908350
Correlation energy (DZ) =    -3.770337
Correlation energy (TZ) =    -4.681250
DLPNO-CCSD(T1)/CBS =      -1107.141958

*xyz 0 1
 Ru  -0.304015    1.091981    0.153767
 N   -0.600305   -0.837508   -0.430589
 O   -0.961183    0.366982    2.076785
 O    1.124257    0.571649    1.545361
 O    0.672529    2.156613   -1.406880
 O    0.162484    3.196315    0.438576
 C   -2.007728   -1.083973   -0.518073
 C    0.170455   -1.870283   -0.588689
 C    0.250199    0.225515    2.412444
 C    0.676244    3.232870   -0.717440
 C   -2.646881   -1.926797    0.393399
 C   -2.742430   -0.441987   -1.518027
 C    1.623876   -1.908936   -0.617506
 H   -0.325218   -2.839436   -0.759535
 C    0.661872   -0.338287    3.724593
 C    1.265233    4.480230   -1.280461
 C   -4.022296   -2.121935    0.301397
 H   -2.059681   -2.407157    1.180644
 C   -4.117361   -0.643291   -1.601722
 H   -2.222602    0.199304   -2.236555
 C    2.229274   -3.174995   -0.539730
 C    2.436280   -0.774935   -0.783667
 H   -0.153803   -0.253096    4.453183
 H    0.905859   -1.404211    3.593353
 H    1.563468    0.168268    4.093852
 H    2.287050    4.280468   -1.634257
 H    1.275530    5.281856   -0.532372
 H    0.677238    4.801014   -2.153565
 C   -4.760889   -1.482050   -0.692925
 H   -4.522043   -2.778218    1.018268
 H   -4.687687   -0.145734   -2.389902
 C    3.611488   -3.306298   -0.588733
 H    1.598274   -4.062801   -0.433385
 C    3.816491   -0.913893   -0.850521
 H    1.974546    0.211449   -0.871445
 H   -4.210407    0.704196   -2.700391
 H   -3.888837   -3.278265   -1.078624
 C    3.972417   -1.063626    0.632773
 H    1.905772   -1.020145    1.253727
 C    4.370110   -1.167617   -1.749372
 H    2.607934   -1.217214   -2.994715
 H    2.204344    3.438320   -1.905261
 H    1.594053    4.623293   -0.726446
 H    0.559065    4.152241   -2.103701
 H   -5.210322   -1.538827   -2.276224
 C    4.859859   -1.116407   -0.443688
 H    4.354778   -1.045666    1.655485
 H    5.059645   -1.224828   -2.593942
 H    5.937094   -1.131997   -0.263208
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CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1108.204259
G (1 atm) =               -1107.943608
qh G-E (1 mol/L) =            0.270931
qh G-E (24.56 mol/L) =        0.273953
Lowest Frequency =            5.75

HF SCF energy (TZ) =      -1101.844579
HF SCF energy (QZ) =      -1101.911009
Correlation energy (DZ) =    -3.769567
Correlation energy (TZ) =    -4.680407
DLPNO-CCSD(T1)/CBS =      -1107.143670

SMD (MeOH)
HF SCF energy (TZ) =      -1101.855977
HF SCF energy (QZ) =      -1101.922220
Correlation energy (DZ) =    -3.763217
Correlation energy (TZ) =    -4.675170
DLPNO-CCSD(T1)/CBS =      -1107.150236

* xyz 0 1
 Ru  -0.281227   -0.790363   -0.633892
 N    0.941213    0.846385   -0.830999
 O   -0.787429   -0.432401   -2.690936
 O    0.687948   -1.889697   -2.080877
 O    0.104625   -1.656798    1.258878
 O   -1.450920   -2.507528   -0.006815
 C    0.093835    2.004092   -0.805152
 C    2.191902    1.040123   -1.068791
 C    0.068037   -1.302073   -3.031914
 C   -0.809045   -2.535469    1.085970
 C   -0.065737    2.803899   -1.938347
 C   -0.621937    2.274276    0.364456
 C    3.244810    0.020173   -1.110723
 H    2.520592    2.072201   -1.254030
 C    0.385168   -1.608496   -4.458207
 C   -1.118328   -3.532391    2.157850
 C   -0.941775    3.886140   -1.892938
 H    0.481943    2.561943   -2.851368
 C   -1.498320    3.358789    0.397420
 H   -0.470366    1.651288    1.250807
 C    4.414756    0.341440   -1.815484
 C    3.154942   -1.213267   -0.448114
 H   -0.457167   -1.335915   -5.104476
 H    1.264416   -1.014073   -4.750107
 H    0.634406   -2.670714   -4.572004
 H   -0.209497   -3.780684    2.719526
 H   -1.566111   -4.434314    1.724319
 H   -1.841781   -3.081945    2.854511
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```
 H   -5.840163   -1.637926   -0.760282
 C    4.408966   -2.173393   -0.743835
 H    4.068405   -4.295893   -0.514354
 H    4.441684   -0.028227   -0.988534
 H    5.496464   -2.272097   -0.790501
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CPCM (MeOH)
M06 SCF (DZ) =            -1664.109143
G (1 atm) =               -1663.667688
qh-G (1 mol/L) =          -1663.656956
qh-G (24.56 mol/L) =      -1663.653934
Lowest Frequency =           21.43

HF SCF energy (TZ) =      -1655.136388
HF SCF energy (QZ) =      -1655.235195
Correlation energy (DZ) =    -5.837156
Correlation energy (TZ) =    -7.146596
DLPNO-CCSD(T1)/CBS =      -1663.168096

*xyz 0 1
 Ru  -0.381062   -0.411227    0.160683
 N   -1.375709    1.382681   -0.187429
 N    2.398526   -1.279680    0.823363
 C   -0.690518    2.545116    0.304196
 C   -2.554401    1.613135   -0.679076
 O   -1.846182   -0.777082    1.684064
 O    1.028516    0.067815   -1.397450
 O   -0.837027   -0.902441   -1.893768
 O   -0.059942    0.353416    2.132330
 C    1.206690   -1.997762    1.035881
 C    3.102478   -1.496151   -0.221851
 C    0.583426    2.870034   -0.165929
 C   -1.297708    3.331916    1.285966
 C   -3.592039    0.698064   -1.135912
 H   -2.837325    2.674202   -0.774322
 C   -1.165916   -0.123971    2.533406
 C    0.248810   -0.382367   -2.292937
 C    0.926626   -2.337862    2.396177
 C    0.401528   -2.584328    0.022809
 C    4.282147   -0.692144   -0.544549
 H    2.859943   -2.295630   -0.950799
 C    1.231798    3.994411    0.335725
 H    1.051628    2.233334   -0.919193
 C   -0.636420    4.450173    1.788416
 H   -2.279898    3.043796    1.673334
 C   -3.608875   -0.694617   -0.944254
 C   -4.684104    1.301782   -1.786210
 C   -1.623910    0.066019    3.936819
 C    0.600731   -0.295259   -3.737071
 C   -0.075253   -3.216816    2.716170
 H    1.562584   -1.893387    3.166610
 C   -0.626240   -3.500390    0.385890
 H    0.726653   -2.573756   -1.019970
 C    4.630018    0.429614    0.222558
 C    5.067461   -1.032869   -1.652494
 C    0.628572    4.786861    1.312869
 H    2.225385    4.251810   -0.040592
 C   -1.659741    4.165454   -0.728835
 H   -1.068437    4.512282   -2.778596
 H   -2.051396    3.576877    1.313169
 C    5.462139   -0.571840   -1.898282
 H    4.495612    1.313545   -2.308787
 C    4.212930   -2.114075   -0.516026
 H    2.262013   -1.460505    0.128272
 H   -2.345319    5.014710   -0.700144
 C    5.360950   -1.802090   -1.248270
 H    6.361567   -0.319090   -2.463315
 H    4.142123   -3.070332    0.006407
 H    6.184216   -2.517848   -1.304165
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CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1664.884297
G (1 atm) =               -1664.426995
qh G-E (1 mol/L) =            0.471486
qh G-E (24.56 mol/L) =        0.474509
Lowest Frequency =           16.69

HF SCF energy (TZ) =      -1655.150380
HF SCF energy (QZ) =      -1655.249005
Correlation energy (DZ) =    -5.832736
Correlation energy (TZ) =    -7.142223
DLPNO-CCSD(T1)/CBS =      -1663.186125

SMD (MeOH)
HF SCF energy (TZ) =      -1655.167649
HF SCF energy (QZ) =      -1655.266123
Correlation energy (DZ) =    -5.826426
Correlation energy (TZ) =    -7.137156
DLPNO-CCSD(T1)/CBS =      -1663.198857

* xyz 0 1
 Ru   0.019646   -1.358928   -0.160150
 N   -1.272689    0.074633   -0.957331
 C   -0.595596    1.193353   -1.566592
 C   -2.559334    0.139063   -0.983062
 C   -0.675869    1.368896   -2.948230
 C    0.153303    2.070610   -0.781162
 C   -3.520374   -0.874780   -0.527883
 C    0.003146    2.428398   -3.549942
 C    0.818065    3.133198   -1.390529
 C   -3.268843   -2.253080   -0.561283
 C   -4.764383   -0.410979   -0.075984
 C    0.752592    3.311668   -2.773814
 C   -4.238674   -3.146162   -0.117169
 C   -5.724892   -1.306771    0.386922
 C   -5.461111   -2.676473    0.368348
 H   -3.006691    1.063752   -1.375060
 H   -1.256338    0.664301   -3.548325
 H    0.211112    1.907343    0.295326
 H   -0.053765    2.558900   -4.632684
 H    1.397883    3.825490   -0.775743
 H   -2.316587   -2.620062   -0.943510
 H   -4.972122    0.662266   -0.074570
 H    1.284200    4.140608   -3.245847
 H   -4.038259   -4.219207   -0.147223
 H   -6.682985   -0.935258    0.755882
 H   -6.215008   -3.382805    0.723318
 N    3.359189   -0.864194    2.012662
 C    2.409292   -1.897289    1.890807
 C    3.350344    0.054429    1.122202
 C    1.882858   -2.444164    3.043092
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 H   -1.113303    5.056037    2.562950
 C   -4.682674   -1.446914   -1.401068
 H   -2.778619   -1.180687   -0.431150
 C   -5.750961    0.543782   -2.251345
 H   -4.687290    2.386937   -1.927346
 H   -0.998516   -0.551277    4.601264
 H   -1.487457    1.114885    4.237405
 H   -2.673439   -0.230275    4.054502
 H   -0.051508   -0.938011   -4.340648
 H    1.653795   -0.575762   -3.881982
 H    0.488211    0.746550   -4.074427
 C   -0.871703   -3.803580    1.701307
 H   -0.255828   -3.475135    3.763535
 H   -1.210681   -3.970800   -0.410766
 C    5.744015    1.187544   -0.112351
 H    4.004605    0.691247    1.079903
 C    6.185196   -0.272902   -1.986675
 H    4.793104   -1.904603   -2.255453
 H    1.148732    5.662815    1.708000
 C   -5.751953   -0.836162   -2.058197
 H   -4.687113   -2.528045   -1.241376
 H   -6.586175    1.031051   -2.759460
 H   -1.667532   -4.502816    1.969045
 C    6.525301    0.837828   -1.217050
 H    6.008875    2.061957    0.487784
 H    6.792866   -0.547105   -2.852587
 H   -6.590958   -1.438786   -2.415274
 H    7.400608    1.437653   -1.479307
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CPCM (MeOH)
M06 SCF (DZ) =            -1664.135237
G (1 atm) =               -1663.692534
qh-G (1 mol/L) =          -1663.681708
qh-G (24.56 mol/L) =      -1663.678686
Lowest Frequency =           18.77

HF SCF energy (TZ) =      -1655.177792
HF SCF energy (QZ) =      -1655.278105
Correlation energy (DZ) =    -5.820469
Correlation energy (TZ) =    -7.130914
DLPNO-CCSD(T1)/CBS =      -1663.204986

*xyz 0 1
 Ru  -0.000046    0.000073    0.000000
 C   -3.415809    0.121730   -0.268764
 N    0.887258   -1.868374   -0.250695
 C   -4.647852   -0.507439   -0.392024
 C   -3.349076    1.470584    0.120696
 H   -2.493670   -0.423015   -0.474180
 N   -0.887337    1.868375    0.250703
 O   -1.231483   -0.822021    1.569331
 O    1.231381    0.822092   -1.569425
 O    0.740549   -0.055645    2.030506
 O   -0.740549    0.055434   -2.030564
 C   -0.068402   -2.936225   -0.299153
 C    2.127490   -2.251668   -0.265318
 C    1.984615   -2.391966    0.614476
 C    4.287553    1.190044    1.142383
 C    0.911134   -3.469797    2.975990
 C    1.017446   -3.412356    0.556268
 C    5.260119    1.335675    2.142469
 C    4.185148    2.157465    0.135328
 C    0.486122   -3.951506    1.760522
 C    6.111273    2.435550    2.132490
 C    5.037836    3.260197    0.126597
 C    6.000204    3.400816    1.126323
 H    2.614470    0.061259    0.300103
 H    2.226659   -2.066579    4.008421
 H    2.592041   -2.159442   -0.261608
 H    0.510396   -3.884898    3.903505
 H    0.841982   -3.942659   -0.380370
 H    5.334779    0.578226    2.925141
 H    3.426920    2.041294   -0.644006
 H   -0.242686   -4.762536    1.707023
 H    6.866304    2.548150    2.913700
 H    4.947787    4.011971   -0.660318
 H    6.666493    4.266473    1.125245
 O   -1.290279   -1.541496    1.525422
 O    0.254317   -0.033478    1.502729
 C   -0.723249   -0.571952    2.111647
 C   -1.200205   -0.065964    3.435784
 H   -0.407763    0.501186    3.938129
 H   -2.062660    0.596781    3.268005
 H   -1.528155   -0.905217    4.062207
 O    1.266406   -1.070539   -1.895148
 O   -0.310467   -2.553056   -1.946049
 C    0.629255   -1.949111   -2.552435
 C    0.947579   -2.236132   -3.985536
 H    0.715670   -3.280515   -4.226968
 H    2.001179   -2.015278   -4.194199
 H    0.322602   -1.585337   -4.615905
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CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1664.906023
G (1 atm) =               -1664.449012
qh G-E (1 mol/L) =            0.473362
qh G-E (24.56 mol/L) =        0.476384
Lowest Frequency =           14.86

HF SCF energy (TZ) =      -1655.184063
HF SCF energy (QZ) =      -1655.282847
Correlation energy (DZ) =    -5.817148
Correlation energy (TZ) =    -7.126107
DLPNO-CCSD(T1)/CBS =      -1663.203591

SMD (MeOH)
HF SCF energy (TZ) =      -1655.201273
HF SCF energy (QZ) =      -1655.299838
Correlation energy (DZ) =    -5.810870
Correlation energy (TZ) =    -7.121386
DLPNO-CCSD(T1)/CBS =      -1663.216703

*xyz 0 1
 Ru   0.000169    0.000246    0.000364
 C   -3.340421    0.305660   -0.674917
 N    0.846929   -1.913953   -0.151819
 C   -4.511381   -0.445293   -0.715244
 C   -3.272250    1.452219    0.129012
 N   -0.847091    1.914253    0.152474
```

C	-5.830648	0.185610	-0.130000
H	-4.688448	-1.555931	-0.698711
C	-4.549868	2.161136	0.367267
C	-2.127548	2.251759	0.265287
C	0.068400	2.936154	0.299371
C	-0.327803	-0.614460	2.432290
C	0.327790	0.614201	-2.432410
C	-0.060655	-3.919232	0.693245
C	-1.025120	-2.976446	-1.315898
C	3.348973	-1.470400	-0.120885
H	2.308877	-3.328986	-0.414660
C	-5.779396	1.525477	0.250783
H	-6.794858	-0.319754	-0.228167
H	-4.508428	3.215327	0.658500
H	-2.308851	3.329081	0.414701
C	1.024836	2.976387	1.316370
C	0.060954	3.919094	-0.693091
C	-0.495652	-1.041867	3.850332
C	0.496205	1.041114	-3.850534
C	-1.005319	-4.943470	0.665779
H	0.676732	-3.860413	1.499742
C	-1.957226	-4.009206	-1.341429
H	-1.024827	-2.190562	-2.074373
C	4.549778	-2.160860	-0.367617
C	3.415642	-0.121559	0.268628
H	-6.700420	2.077270	0.452723
C	1.957019	4.009078	1.342051
H	1.024293	2.190554	2.074899
C	1.005678	4.943267	-0.665466
H	-0.676246	3.860257	-1.499754
H	-1.551139	-0.986461	4.147446
H	-0.173466	-2.090982	3.946239
H	0.124643	-0.430526	4.518170
H	-0.134219	0.439000	-4.517180
H	1.549975	0.972076	-4.151074
H	0.188567	2.094821	-3.943866
C	-1.954372	-4.993642	-0.352077
H	-0.999188	-5.703912	1.450873
H	-2.697740	-4.043915	-2.144954
C	5.779273	-1.525112	-0.251253
H	4.508379	-3.215043	-0.658886
C	4.647653	0.507697	0.391769
H	2.493476	0.423098	0.474186
C	1.954490	4.993434	0.352618
H	2.697374	4.043755	2.145726
H	0.999775	5.703683	-1.450589
H	-2.694969	-5.796870	-0.373811
C	5.830469	-0.185261	0.129577
H	6.700313	-2.076831	-0.453316
H	4.688207	1.556175	0.698506
H	2.695155	5.796597	0.374465
H	6.794657	0.320162	0.227659

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***cis*-F^A**
CPCM (MeOH)
M06 SCF (DZ) = -1663.691961
G (1 atm) = -1664.131748

C	-0.134159	-2.965670	-0.196658
C	2.073633	-2.301064	-0.226456
C	-5.619998	-0.066678	0.045082
C	-4.401792	1.850468	0.858559
C	-2.073965	2.300659	0.228109
C	0.133398	2.966568	0.195051
C	-0.202904	-3.894476	0.842140
C	-1.041634	-3.021524	-1.256616
C	3.272468	-1.453553	-0.126291
C	-5.565645	1.085531	0.830442
C	1.044363	3.022194	1.252039
C	0.198177	3.896103	-0.843352
C	-1.184383	-4.886239	0.818709
C	-2.011955	-4.020180	-1.275996
C	4.402841	-1.853963	-0.853428
C	3.340430	-0.305748	0.675861
C	2.014163	4.021382	1.268820
C	1.179173	4.888401	-0.822558
C	-2.090040	-4.952406	-0.238619
C	5.567402	-1.090134	-0.824589
C	4.512075	0.444088	0.716977
C	2.088266	4.954365	0.231812
C	5.621595	0.063235	-0.040905
H	-2.478028	0.014212	-1.273995
H	-4.556747	-1.338063	-1.343165
H	2.264742	-3.368661	-0.408610
H	-6.533421	-0.665260	0.016966
H	-4.360345	2.760132	1.463781
H	-2.265531	3.368187	0.410165
H	0.498496	-3.821503	1.676573
H	-0.975976	-2.275277	-2.049594
H	-6.433524	1.392851	1.417623
H	0.981611	2.275452	2.044800
H	-0.505916	3.823156	-1.675521
H	-1.241878	-5.606899	1.637362
H	-2.716337	-4.069051	-2.109548
H	4.361528	-2.764524	-1.457308
H	2.477378	-0.012573	1.273131
H	2.721349	4.070125	2.100000
H	1.233590	5.609543	-1.640993
H	-2.858793	-5.727835	-0.255373
H	6.435945	-1.399228	-1.409853
H	4.557261	1.337759	1.343631
H	2.856674	5.730176	0.246459
H	6.535537	0.660995	-0.012191
O	-1.419886	-0.761753	1.435001
O	0.484970	0.019314	2.111756
C	-0.635203	-0.513691	2.396400
C	-0.998162	-0.867300	3.806126
H	-2.089398	-0.901811	3.917476
H	-0.601416	-1.869870	4.027419
H	-0.561979	-0.149306	4.510466
O	1.420630	0.761999	-1.433764
O	-0.484475	-0.017793	-2.111323
C	0.635993	0.514823	-2.395460
C	0.999548	0.869034	-3.804879
H	0.563526	0.151542	-4.509815
H	2.090857	0.903249	-3.915755
H	0.603345	1.871915	-4.025710

*

***cis*-F^A**
CPCM (MeOH)
wB97X-D3 SCF (DZ) = -1664.899239
G (1 atm) = -1664.441320

```
qh-G (1 mol/L) =          -1663.679762
qh-G (24.56 mol/L) =      -1663.676741
Lowest Frequency =           22.62

HF SCF energy (TZ) =      -1654.774653
HF SCF energy (QZ) =      -1655.163581
Correlation energy (DZ) =    -5.831585
Correlation energy (TZ) =    -7.142172
DLPNO-CCSD(T1)/CBS =      -1663.198062

*xyz 0 1
 Ru   0.027970   -0.664330   -0.756968
 C   -3.375924   -0.629801   -0.200285
 N    1.420606    0.830908   -0.577834
 C   -4.687571   -0.736079   -0.647237
 C   -3.081482   -0.802334    1.163151
 H   -2.577260   -0.401449   -0.907618
 O   -1.026625   -2.545567   -0.943008
 N   -0.593679   -0.533341    1.213751
 O    0.355952   -0.739318   -2.888013
 O    1.007527   -2.483147   -0.172961
 O   -1.071754    0.678931   -2.063445
 C    2.750211    0.283609   -0.619086
 C    1.384570    2.124125   -0.441839
 C   -5.722712   -1.024186    0.242683
 H   -4.905866   -0.593007   -1.708511
 C   -4.137141   -1.076432    2.052251
 C   -1.762707   -0.674103    1.767166
 C   -0.017532   -3.166725   -0.490820
 C    0.454751   -0.316054    2.181910
 C   -0.505158    0.172718   -3.081981
 C    3.236538   -0.307799   -1.786734
 C    3.546702    0.339293    0.525586
 C    0.252179    3.018530   -0.239034
 H    2.356956    2.641504   -0.465988
 C   -5.443921   -1.195213    1.597945
 H   -6.749801   -1.110780   -0.120856
 H   -3.918319   -1.198929    3.117501
 H   -1.781661   -0.674984    2.868947
 C   -0.034419   -4.644929   -0.298609
 C    1.262285   -1.371841    2.606142
 C    0.622683    0.958008    2.726597
 C   -0.868611    0.619771   -4.456746
 C    4.521789   -0.841344   -1.799848
 H    2.596358   -0.343763   -2.670527
 C    4.826665   -0.210897    0.506301
 H    3.146338    0.796774    1.435486
 C   -1.057672    2.614377    0.069036
 C    0.527937    4.395406   -0.310709
 H   -6.248686   -1.415555    2.303172
 H   -0.335275   -4.863110    0.738574
 H    0.967599   -5.066459   -0.452695
 H   -0.759479   -5.117741   -0.973164
 C    2.243781   -1.143843    3.567191
 H    1.114546   -2.361952    2.172858
 C    1.614645    1.179471    3.680083
 H   -0.030392    1.772052    2.398184
 H   -0.087951    0.344033   -5.176551
 H   -1.808288    0.127985   -4.753430
 H   -1.042184    1.704035   -4.474219
 C    5.318937   -0.801316   -0.655144
 H    4.904991   -1.295563   -2.717381
 H    5.440496   -0.175848    1.410577
 C   -2.052546    3.557329    0.288073
 H   -1.283275    1.551629    0.136780
 C   -0.472077    5.338176   -0.104022
```

```
qh G-E (1 mol/L) =            0.472467
qh G-E (24.56 mol/L) =        0.475490
Lowest Frequencies =         23.68

HF SCF energy (TZ) =      -1654.778159
HF SCF energy (QZ) =      -1655.168244
Correlation energy (DZ) =    -5.825477
Correlation energy (TZ) =    -7.136409
DLPNO-CCSD(T1)/CBS =      -1663.197541

SMD (MeOH)
HF SCF energy (TZ) =      -1655.186618
HF SCF energy (QZ) =      -1655.285442
Correlation energy (DZ) =    -5.818777
Correlation energy (TZ) =    -7.131141
DLPNO-CCSD(T1)/CBS =      -1663.213221

* xyz 0 1
  Ru     0.214356   -0.587188    0.239488
  N      1.009016    0.979204   -0.939845
  N     -1.685762    0.329176    0.427570
  C      0.144980    1.641932   -1.887362
  C      2.247753    1.335142   -1.030847
  O      0.378801   -1.743497   -1.591809
  O      0.386473   -0.148741    2.355036
  O      1.994355   -1.747983   -0.137045
  O     -0.395911   -2.065456    1.689917
  C     -1.763127    1.764471    0.559093
  C     -2.820908   -0.265664    0.596685
  C     -0.721777    0.900814   -2.694990
  C      0.165008    3.035742   -1.983079
  C      3.357521    0.946557   -0.149801
  H      2.528476    1.998382   -1.860682
  C      1.530650   -2.155699   -1.243875
  C     -0.068312   -1.302160    2.646003
  C     -2.739169    2.467403   -0.153167
  C     -0.861137    2.457807    1.370580
  C     -3.132211   -1.686169    0.385312
  H     -3.670707    0.343601    0.934122
  C     -1.552004    1.557994   -3.599808
  H     -0.718616   -0.185593   -2.622397
  C     -0.672419    3.685778   -2.887863
  H      0.811288    3.614981   -1.320264
  C      4.630414    0.841219   -0.728027
  C      3.205584    0.733251    1.225699
  C      2.323763   -3.080101   -2.117147
  C     -0.211689   -1.729169    4.075409
  C     -2.823235    3.854021   -0.043853
  H     -3.411149    1.927533   -0.823573
  C     -0.952864    3.843702    1.475086
  H     -0.111418    1.902378    1.931259
  C     -2.534767   -2.455834   -0.620154
  C     -4.129514   -2.256028    1.189505
  C     -1.534040    2.950349   -3.699147
  H     -2.219166    0.970872   -4.235009
  H     -0.659205    4.776377   -2.943681
  C      5.727986    0.471636    0.045826
  H      4.755104    1.033440   -1.796951
  C      4.308955    0.387746    2.000613
  H      2.223712    0.826891    1.688122
  H      1.744358   -3.378519   -2.998164
  H      3.243800   -2.568502   -2.435033
  H      2.617220   -3.968074   -1.540211
  H     -0.930194   -1.067651    4.579987
  H      0.755550   -1.625275    4.586521
  H     -0.559160   -2.766658    4.136755
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 H    1.547318    4.724070   -0.535681
 C    2.429137    0.130328    4.102587
 H    2.868674   -1.975369    3.903328
 H    1.741979    2.179678    4.102090
 H    6.323883   -1.230516   -0.670651
 C   -1.767358    4.920928    0.197265
 H   -3.064687    3.223131    0.531700
 H   -0.238433    6.403313   -0.171533
 H    3.202094    0.303534    4.855374
 H   -2.555532    5.658610    0.367606
*
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F[c]

```
CPCM (MeOH)
M06 SCF (DZ) =            -1496.971413
G (1 atm) =               -1496.520099
qh-G (1 mol/L) =          -1496.509795
qh-G (24.56 mol/L) =      -1496.506772
Lowest Frequency =           11.12

HF SCF energy (TZ) =      -1488.788639
HF SCF energy (QZ) =      -1488.878856
Correlation energy (DZ) =    -5.347938
Correlation energy (TZ) =    -6.553782
DLPNO-CCSD(T1)/CBS =      -1496.164438

*xyz 0 1
 Ru   0.111322   -0.359672    0.453782
 C    2.353593   -0.498488    1.074401
 C    1.725774   -1.748394    1.290208
 C    3.337553   -0.352359    0.040925
 H    2.340827    0.255695    1.869074
 N   -1.815105    0.273050   -0.124515
 O    0.736564    0.037588   -1.552594
 O    0.151691    1.248438    1.887428
 O   -0.668794   -0.670997    2.448677
 O   -0.141649   -1.869662   -1.044647
 H    1.238467   -1.957217    2.248390
 C    4.100200    0.950984   -0.042421
 C    3.584202   -1.433105   -0.772985
 C   -2.733633   -0.817818   -0.303405
 C   -2.309281    1.435100   -0.418245
 C    0.348448   -1.110135   -1.933814
 C   -0.425712    0.535422    2.762791
 C    5.245000    0.939296   -1.041109
 C    3.168349    2.126440   -0.325761
 H    4.533140    1.116415    0.966501
 C    2.932985   -2.679358   -0.572992
 H    4.328644   -1.362640   -1.570640
 C   -3.267022   -1.057144   -1.571930
 C   -3.073869   -1.645380    0.767595
 C   -1.662012    2.736469   -0.492302
 H   -3.386639    1.463753   -0.652040
 C    0.472017   -1.553585   -3.349491
 C   -0.830867    1.090696    4.083792
 H    5.794180    1.893313   -1.001445
 H    4.871076    0.819560   -2.073290
 H    5.964682    0.128642   -0.844983
 C   -1.930908    4.547947    0.770761
 H   -3.583281    4.392867   -0.613700
 H   -0.250351    4.378903    2.117930
 C   -2.911149   -3.784674   -0.794527
 H   -1.778999   -2.013289   -1.267188
 C   -4.488092   -3.591938    1.027322
 H   -4.617557   -1.648169    1.955806
 H   -2.194901    3.460520   -4.403266
 C    5.567660    0.242969    1.412849
 H    6.711420    0.369194   -0.417636
 H    4.183640    0.224323    3.073309
 H   -1.991751    5.635282    0.852547
 C   -3.878074   -4.358549    0.033568
 H   -2.445654   -4.377216   -1.585261
 H   -5.252322   -4.032791    1.670809
 H    6.427878   -0.039680    2.023973
 H   -4.165201   -5.403587   -0.103752
*
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F[c]

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1497.674330
G (1 atm) =               -1497.208238
qh G-E (1 mol/L) =            0.479226
qh G-E (24.56 mol/L) =        0.482249
Lowest Frequency =          8.16

HF SCF energy (TZ) =      -1488.799691
HF SCF energy (QZ) =      -1488.888333
Correlation energy (DZ) =    -5.339361
Correlation energy (TZ) =    -6.544600
DLPNO-CCSD(T1)/CBS =      -1496.163906

SMD (MeOH)
HF SCF energy (TZ) =      -1488.816062
HF SCF energy (QZ) =      -1488.904545
Correlation energy (DZ) =    -5.333610
Correlation energy (TZ) =    -6.540115
DLPNO-CCSD(T1)/CBS =      -1496.176325

* xyz 0 1
 Ru   0.091499   -0.296238    0.413237
 N   -1.824583    0.286392   -0.214878
 C   -2.713807   -0.820163   -0.474679
 C   -2.355600    1.447598   -0.390080
 C   -3.108602   -1.664695    0.563444
 C   -3.155185   -1.046858   -1.778923
 C   -1.703878    2.762486   -0.323288
 C   -3.952625   -2.738471    0.287590
 C   -3.995871   -2.127211   -2.046003
 C   -0.358940    2.974320   -0.652871
 C   -2.510541    3.855638    0.026132
 C   -4.395780   -2.976377   -1.014960
 C    0.171711    4.259776   -0.606455
 C   -1.969938    5.137046    0.094004
 C   -0.626390    5.339793   -0.223207
 H   -3.431503    1.477472   -0.614509
 H   -2.747283   -1.471962    1.573588
 H   -2.823295   -0.385786   -2.582653
 H   -4.265605   -3.396603    1.101172
 H   -4.334763   -2.305143   -3.068850
 H    0.259204    2.131307   -0.959810
 H   -3.567454    3.694659    0.254368
 H   -5.052889   -3.822881   -1.225006
 H    1.218205    4.422060   -0.873205
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```
 H    3.731974    3.074362   -0.331419
 H    2.685308    2.003028   -1.311214
 H    2.371706    2.207830    0.431388
 C    2.037577   -2.864786    0.450317
 H    3.179167   -3.519572   -1.231766
 C   -4.143057   -2.121870   -1.768678
 H   -2.968041   -0.417901   -2.408465
 C   -3.957332   -2.701503    0.562871
 H   -2.642672   -1.446828    1.750505
 C   -0.274318    2.940227   -0.517948
 C   -2.514928    3.849763   -0.590287
 H    0.697029   -0.707556   -4.010440
 H   -0.453387   -2.053358   -3.670250
 H    1.287271   -2.290985   -3.421214
 H   -0.235001    1.977448    4.333177
 H   -1.890774    1.385495    4.035262
 H   -0.731445    0.327431    4.866860
 C    1.365858   -4.170738    0.718490
 C   -4.492146   -2.946673   -0.701913
 H   -4.550013   -2.308332   -2.765746
 H   -4.231644   -3.341574    1.405424
 C    0.238479    4.226228   -0.622536
 H    0.394465    2.081039   -0.464670
 C   -1.998393    5.136199   -0.682161
 H   -3.598220    3.694930   -0.589157
 H    0.269830   -4.060717    0.640331
 H    1.684840   -4.951097    0.011596
 H    1.575738   -4.526989    1.741815
 H   -5.178698   -3.782789   -0.855567
 C   -0.617478    5.326199   -0.698282
 H    1.321889    4.372215   -0.647285
 H   -2.673443    5.992373   -0.749059
 H   -0.205096    6.335181   -0.778186
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CPCM (MeOH)
M06 SCF (DZ) =            -1223.438642
G (1 atm) =               -1223.138393
qh-G (1 mol/L) =          -1223.129016
qh-G (24.56 mol/L) =      -1223.125994
Lowest Frequency =           18.08

HF SCF energy (TZ) =      -1216.960319
HF SCF energy (QZ) =      -1217.035943
Correlation energy (DZ) =    -4.163223
Correlation energy (TZ) =    -5.165577
DLPNO-CCSD(T1)/CBS =      -1222.810017

*xyz 0 1
 Ru  -0.410891   -0.910482    0.200278
 N    0.055561    0.980529   -0.325485
 O   -0.958442   -2.923743    0.825799
 C   -1.112838    1.776410   -0.587617
 C    1.175375    1.639923   -0.390698
 O   -1.110104   -1.453983   -1.760210
 O    0.229487   -0.502503    2.213120
 O    0.960509   -1.785176   -1.215784
 H   -2.600331    5.980432    0.382690
 H   -0.201430    6.345289   -0.183533
 C    1.789867   -1.556296    1.460388
 C    2.412422   -0.369086    1.040475
 C    2.049734   -2.789641    0.787792
 C    3.349687   -0.382042   -0.041711
 C    1.363943   -4.039669    1.261961
 C    2.908844   -2.771589   -0.284427
 C    4.119938    0.891977   -0.357190
 C    3.558931   -1.577559   -0.692721
 C    5.164156    0.725125   -1.459549
 C    3.188350    2.065827   -0.679511
 H    1.288085   -1.593725    2.428803
 H    2.373537    0.511256    1.685534
 H    1.576371   -4.230547    2.325878
 H    0.270965   -3.936866    1.164448
 H    1.679212   -4.918613    0.682953
 H    3.117975   -3.698408   -0.826064
 H    4.659475    1.153070    0.573031
 H    4.262338   -1.635999   -1.525350
 H    5.897839   -0.059833   -1.221717
 H    4.691421    0.469927   -2.422470
 H    5.714887    1.667339   -1.600115
 H    3.768353    2.994584   -0.795684
 H    2.637470    1.877053   -1.613335
 H    2.447079    2.227143    0.116751
 O    0.072159    1.294863    1.868866
 O   -0.807994   -0.621804    2.350977
 C   -0.572871    0.580224    2.693458
 C   -1.073409    1.134099    3.990322
 H   -1.021499    0.369988    4.776040
 H   -2.127803    1.421006    3.857534
 H   -0.498434    2.022384    4.277234
 O    0.784726    0.077742   -1.585734
 O   -0.033678   -1.851153   -1.053200
 C    0.469638   -1.100457   -1.942053
 C    0.695169   -1.589844   -3.337802
 H   -0.150929   -2.211941   -3.657436
 H    1.601553   -2.214118   -3.345088
 H    0.835961   -0.748812   -4.026622
*
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CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1223.951610
G (1 atm) =               -1223.638811
qh G-E (1 mol/L) =            0.324576
qh G-E (24.56 mol/L) =        0.327598
Lowest Frequency =          24.04

HF SCF energy (TZ) =      -1216.965341
HF SCF energy (QZ) =      -1217.039852
Correlation energy (DZ) =    -4.160127
Correlation energy (TZ) =    -5.162068
DLPNO-CCSD(T1)/CBS =      -1222.809842

SMD (MeOH)
HF SCF energy (TZ) =      -1216.978585
HF SCF energy (QZ) =      -1217.052895
Correlation energy (DZ) =    -4.154473
Correlation energy (TZ) =    -5.157454
DLPNO-CCSD(T1)/CBS =      -1222.818817


*xyz 0 1
```

```
 O   -1.837082   -0.204215    1.631561
 C   -2.318865   -3.315422    0.619331
 H   -0.374913   -3.576792    0.410333
 C   -1.844201    1.582926   -1.759763
 C   -1.510564    2.740506    0.339837
 C    2.534711    1.193249   -0.125202
 H    1.101742    2.692938   -0.705363
 C    0.039599   -1.887773   -2.083362
 C   -0.947541   -0.152207    2.536210
 H   -2.491945   -4.318676    1.036361
 H   -2.577207   -3.296652   -0.450811
 H   -2.936277   -2.583668    1.155393
 C   -2.969132    2.365412   -2.003184
 H   -1.523166    0.813318   -2.463632
 C   -2.643751    3.512531    0.092366
 H   -0.932200    2.864401    1.260661
 C    2.892404   -0.044755    0.435690
 C    3.556637    2.105634   -0.448036
 C    0.283810   -2.517061   -3.412221
 C   -1.267351    0.337159    3.906988
 C   -3.374350    3.329321   -1.079608
 H   -3.535662    2.220491   -2.926721
 H   -2.955938    4.262929    0.823318
 C    4.229892   -0.352831    0.652182
 H    2.109170   -0.756779    0.699817
 C    4.892442    1.790388   -0.236434
 H    3.288274    3.076648   -0.875826
 H   -0.309979   -2.016768   -4.188647
 H   -0.036364   -3.570097   -3.373848
 H    1.350814   -2.488744   -3.666469
 H   -2.288443    0.048543    4.189354
 H   -1.215634    1.437739    3.914069
 H   -0.543065   -0.045989    4.636941
 H   -4.261012    3.937839   -1.273987
 C    5.233499    0.556237    0.315143
 H    4.494693   -1.317781    1.092003
 H    5.670952    2.510469   -0.499522
 H    6.282822    0.303225    0.487095
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 Ru  -0.413316   -0.861510    0.335944
 N    0.050190    1.051386   -0.235340
 C   -1.117657    1.823274   -0.584640
 C    1.168462    1.656184   -0.455758
 C   -1.553312    1.863489   -1.909163
 C   -1.800886    2.524976    0.408510
 C    2.533736    1.177074   -0.202566
 C   -2.685159    2.608872   -2.238162
 C   -2.930396    3.268228    0.070937
 C    2.858540    0.094995    0.629072
 C    3.568460    1.895761   -0.822895
 C   -3.377920    3.309434   -1.250458
 C    4.189716   -0.263942    0.817225
 C    4.898435    1.526425   -0.642147
 C    5.211148    0.443174    0.179332
 H    1.113582    2.661163   -0.896813
 H   -1.006957    1.303618   -2.669721
 H   -1.445018    2.482804    1.438602
 H   -3.025005    2.642002   -3.275682
 H   -3.462843    3.819861    0.848855
 H    2.064994   -0.451742    1.136479
 H    3.322174    2.750894   -1.457931
 H   -4.264315    3.891774   -1.510877
 H    4.433130   -1.104457    1.470693
 H    5.692600    2.087608   -1.138617
 H    6.253736    0.154457    0.330817
 O   -0.903541   -2.902322    0.888199
 C   -2.255746   -3.348090    0.711352
 H   -0.310444   -3.518308    0.433970
 H   -2.363453   -4.369599    1.103071
 H   -2.543442   -3.314388   -0.349606
 H   -2.885690   -2.662370    1.289325
 O   -1.102321   -1.279029   -1.648904
 O    0.961028   -1.676260   -1.111741
 C    0.042664   -1.712192   -1.989034
 C    0.284729   -2.272303   -3.357321
 H   -0.278738   -1.700226   -4.105294
 H   -0.078054   -3.311180   -3.378901
 H    1.355068   -2.266529   -3.594650
 O    0.205977   -0.561699    2.377114
 O   -1.855196   -0.222009    1.793786
 C   -0.975198   -0.232140    2.708770
 C   -1.308949    0.172040    4.111699
 H   -2.346789   -0.091920    4.349256
 H   -1.204412    1.265121    4.191292
 H   -0.618135   -0.295728    4.823342
*
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F[25]

```
CPCM (MeOH)
M06 SCF (DZ) =            -1339.118736
G (1 atm) =               -1338.766181
qh-G (1 mol/L) =          -1338.757489
qh-G (24.56 mol/L) =      -1338.754467
Lowest Frequency =           34.40

HF SCF energy (TZ) =      -1332.055648
HF SCF energy (QZ) =      -1332.139588
Correlation energy (DZ) =    -4.549922
Correlation energy (TZ) =    -5.644693
DLPNO-CCSD(T1)/CBS =      -1338.449287

*xyz 0 1
 Ru   0.395948    0.580333    0.134426
 C   -3.076500   -0.386072    0.827147
```

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 O    1.871050    0.185022   -1.419954
 C   -2.719226   -1.303098   -0.171153
 C   -4.375420    0.109340    0.883778
 H   -2.330531   -0.067173    1.557577
 O   -0.772597    1.134883   -1.630931
 O   -0.637896    1.107330    1.936678
 N   -0.246344   -1.376151    0.010421
 O    1.393009    0.344528    1.997474
 O    1.121397    2.585540    0.136582
 C    3.199711    0.019488   -0.932775
 H    1.835964    1.055820   -1.893153
 C   -3.690271   -1.724016   -1.092973
 C   -1.396597   -1.918010   -0.249506
 C   -5.324337   -0.283407   -0.059978
 H   -4.650073    0.813599    1.673335
 C   -1.907048    1.971555   -1.417325
 H   -0.087097    1.706102   -2.061180
 C    0.395465    0.822597    2.621466
 C    0.858971   -2.290540   -0.087569
 C    1.427260    3.202844   -0.929239
 H    3.515762    0.896997   -0.342369
 H    3.215202   -0.869005   -0.286771
 H    3.894036   -0.130632   -1.774854
 C   -4.977663   -1.200618   -1.051936
 H   -3.421708   -2.460693   -1.856487
 H   -1.393881   -2.973501   -0.568924
 H   -6.340556    0.116448   -0.015474
 H   -2.244363    2.398287   -2.375128
 H   -1.669240    2.787592   -0.712404
 H   -2.711420    1.356096   -0.993901
 C    0.441049    1.065048    4.090137
 C    1.582738   -2.619548    1.059268
 C    1.202233   -2.848568   -1.319858
 C    1.905774    4.620583   -0.795939
 O    1.353664    2.706869   -2.092630
 H   -5.718948   -1.520156   -1.788468
 H    1.173575    0.403672    4.570049
 H    0.748713    2.107059    4.270016
 H   -0.553036    0.926420    4.534967
 C    2.646550   -3.513023    0.968315
 H    1.306838   -2.161481    2.011148
 C    2.274890   -3.733080   -1.404045
 H    0.634049   -2.566102   -2.210591
 H    1.236322    5.281081   -1.367667
 H    2.903476    4.710504   -1.251291
 H    1.943090    4.947129    0.250367
 C    2.998673   -4.069517   -0.261586
 H    3.205960   -3.777116    1.869465
 H    2.545844   -4.161869   -2.372258
 H    3.838180   -4.765795   -0.328812
*
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```

***cis*-G^A**

```
CPCM (MeOH)
M06 SCF (DZ) =            -1664.127413
G (1 atm) =               -1663.688223
qh-G (1 mol/L) =          -1663.676636
qh-G (24.56 mol/L) =      -1663.673613
Lowest Frequency =           10.70

HF SCF energy (TZ) =      -1655.127323
HF SCF energy (QZ) =      -1655.226565
Correlation energy (DZ) =    -5.864154
Correlation energy (TZ) =    -7.176307
DLPNO-CCSD(T1)/CBS =      -1663.201885
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***cis*-G^A**

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1664.892088
G (1 atm) =               -1664.435048
qh G-E (1 mol/L) =            0.471283
qh G-E (24.56 mol/L) =        0.474305
Lowest Frequency =          0.84

HF SCF energy (TZ) =      -1655.134819
HF SCF energy (QZ) =      -1655.233846
Correlation energy (DZ) =    -5.857696
Correlation energy (TZ) =    -7.168244
DLPNO-CCSD(T1)/CBS =      -1663.197728
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*xyz 0 1
 Ru  -0.194783    0.394988    0.449568
 C   -0.739236    1.564586   -1.063185
 N    1.618507    0.693347   -0.544276
 H    0.027141    3.156230   -0.078093
 C    0.260651    1.823013   -2.055668
 C   -1.972361    2.229829   -1.252424
 N   -0.506908   -1.413359   -0.513559
 O   -0.136314   -0.958770    2.384898
 O    0.234084    1.945901    1.869876
 O   -1.946059    0.038737    1.642946
 C    2.877344    0.256407   -0.056241
 C    1.551375    1.322521   -1.690076
 O    0.384851    3.785272    0.594680
 C    0.013402    2.608214   -3.194675
 C   -2.213784    3.015896   -2.376294
 H   -2.760948    2.117822   -0.498103
 C    0.711668   -2.099768   -0.862189
 C   -1.547612   -2.183952   -0.587884
 C   -1.368522   -0.714618    2.492363
 C    0.492683    3.143740    1.738898
 C    3.912689   -0.145266   -0.908955
 C    3.077029    0.213587    1.328909
 H    2.449871    1.532189   -2.286286
 C   -1.231884    3.193875   -3.364155
 H    0.810521    2.767318   -3.928902
 H   -3.185002    3.508268   -2.490700
 C    1.123580   -2.120574   -2.193103
 C    1.440884   -2.766857    0.120776
 C   -2.947757   -1.803513   -0.425117
 H   -1.366906   -3.251648   -0.798853
 C   -2.179339   -1.335778    3.589430
 C    0.961881    3.989213    2.865591
 C    5.129174   -0.567441   -0.381583
 H    3.755890   -0.165214   -1.990453
 C    4.297049   -0.205571    1.848344
 H    2.260133    0.516401    1.988398
 H   -1.440774    3.809514   -4.242382
 C    2.275356   -2.823121   -2.543016
 H    0.531708   -1.588039   -2.943863
 C    2.585599   -3.472839   -0.240653
 H    1.091568   -2.718857    1.155911
 C   -3.470769   -0.655137   -1.026715
 C   -3.800231   -2.657860    0.286834
 H   -1.625959   -1.309125    4.538680
 H   -2.352897   -2.395616    3.341662
 H   -3.152372   -0.839744    3.700793
 H    1.974355    4.357311    2.641401
 H    0.972512    3.415033    3.797568
 H    0.312231    4.870556    2.964032
 C    5.329312   -0.599696    0.997141
 H    5.924329   -0.889964   -1.059128
 H    4.441496   -0.226616    2.931700
 C    3.005128   -3.503944   -1.569864
 H    2.597893   -2.845394   -3.587357
 H    3.155820   -4.003902    0.526420
 C   -4.815190   -0.337582   -0.874604
 H   -2.812047   -0.020746   -1.622149
 C   -5.140045   -2.325698    0.458255
 H   -3.398886   -3.576120    0.727347
 H    6.284161   -0.937623    1.407499
 H    3.904519   -4.059101   -1.848262
 C   -5.649149   -1.162190   -0.119043
 H   -5.216092    0.561613   -1.351151
 H   -5.794573   -2.983097    1.035895

SMD (MeOH)
HF SCF energy (TZ) =      -1655.152198
HF SCF energy (QZ) =      -1655.250979
Correlation energy (DZ) =    -5.851727
Correlation energy (TZ) =    -7.163822
DLPNO-CCSD(T1)/CBS =      -1663.211269

* xyz 0 1
 Ru  -0.238928   -0.221166   -0.126167
 C    0.696199   -0.131300    1.646953
 N   -1.752322   -0.844071    1.189823
 C   -0.044105   -0.631502    2.762509
 C    1.969694    0.396708    1.969983
 N    0.290272   -2.205063   -0.570610
 C   -3.098358   -1.118976    0.810028
 C   -1.404393   -0.990047    2.431878
 C    0.464154   -0.677957    4.070819
 C    2.480627    0.359000    3.266463
 C   -0.810855   -3.142147   -0.530641
 C    1.333885   -2.705857   -1.135842
 C   -3.821029   -2.178455    1.367148
 C   -3.690834   -0.315821   -0.170107
 C    1.741126   -0.194210    4.323076
 C   -0.883846   -4.065538    0.510332
 C   -1.760959   -3.140621   -1.551488
 C    2.657276   -2.071157   -1.272069
 C   -5.127352   -2.425705    0.949687
 C   -4.998266   -0.565745   -0.579422
 C   -1.911130   -5.009152    0.519285
 C   -2.780098   -4.091045   -1.536517
 C    3.352074   -1.606674   -0.154224
 C    3.261589   -2.027237   -2.534435
 C   -5.720900   -1.623879   -0.024626
 C   -2.857147   -5.027746   -0.505195
 C    4.623215   -1.054757   -0.303231
 C    4.523376   -1.458048   -2.683788
 C    5.205046   -0.967176   -1.567761
 H    2.578483    0.845395    1.178861
 H   -2.126626   -1.305068    3.195120
 H   -0.150323   -1.078909    4.882282
 H    3.474464    0.771204    3.464430
 H    1.244274   -3.713569   -1.567579
 H   -3.348286   -2.838718    2.096237
 H   -3.114865    0.504424   -0.601060
 H    2.156264   -0.220791    5.332678
 H   -0.131904   -4.043241    1.302287
 H   -1.679985   -2.395174   -2.344336
 H   -5.676402   -3.266738    1.379167
 H   -5.454370    0.069633   -1.341933
 H   -1.967751   -5.736809    1.331907
 H   -3.520199   -4.098895   -2.339804
 H    2.894965   -1.687438    0.831597
 H    2.732646   -2.424856   -3.404368
 H   -6.741713   -1.826651   -0.355752
 H   -3.658518   -5.769605   -0.497166
 H    5.160604   -0.691343    0.575669
 H    4.981310   -1.403307   -3.673725
 H    6.198484   -0.528130   -1.683961
 O   -1.003878    1.793168   -0.159954
 O   -0.606382    2.526901    1.916989
 C   -1.116787    2.656669    0.711703
 C   -1.857695    3.930533    0.484143
 H   -0.119789    1.669081    1.955153
 H   -2.758633    3.929247    1.115038
 H   -2.142903    4.015070   -0.568913
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 H   -6.704477   -0.906825    0.006469
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G[4]

```
CPCM (MeOH)
M06 SCF (DZ) =            -1664.127788
G (1 atm) =               -1663.687978
qh-G (1 mol/L) =          -1663.676564
qh-G (24.56 mol/L) =      -1663.673541
Lowest Frequency =           14.41

HF SCF energy (TZ) =      -1655.134382
HF SCF energy (QZ) =      -1655.233309
Correlation energy (DZ) =    -5.855773
Correlation energy (TZ) =    -7.166994
DLPNO-CCSD(T1)/CBS =      -1663.196304

*xyz 0 1
 Ru  -0.290684    0.029198   -0.025789
 C    0.336692   -0.506837    1.786015
 N   -2.078909   -0.657707    0.808742
 H    0.549053    1.466608    2.359781
 C   -0.691735   -1.020188    2.646921
 C    1.623722   -0.425567    2.374263
 N    1.564824    0.617611   -0.797301
 O   -1.100896   -0.011780   -2.208918
 O   -0.802786    2.019224    0.559486
 O   -0.253367   -1.750562   -1.178447
 C   -3.298472   -0.800397    0.105367
 C   -1.983801   -1.096302    2.034565
 O    0.290927    2.412835    2.480917
 C   -0.447521   -1.421656    3.968576
 C    1.860496   -0.819294    3.690364
 H    2.464553   -0.040433    1.783949
 C    1.580314    2.033172   -1.044333
 C    2.675109    0.030124   -1.131910
 C   -0.831586   -1.240610   -2.198785
 C   -0.489289    2.771643    1.484350
 C   -4.004834   -2.008062    0.119592
 C   -3.777702    0.273277   -0.652205
 H   -2.861148   -1.498169    2.562688
 C    0.830932   -1.321295    4.498119
 H   -1.273681   -1.809567    4.574549
 H    2.871820   -0.733045    4.100709
 C    0.823721    2.570747   -2.086496
 C    2.328113    2.866724   -0.212102
 C    3.101293   -1.355373   -0.975492
 H    3.438664    0.667313   -1.608308
 C   -1.228729   -2.130593   -3.333276
 C   -0.961462    4.177668    1.560234
 C   -5.192091   -2.129371   -0.599731
 H   -3.604957   -2.859875    0.677079
 C   -4.967174    0.147564   -1.359858
 H   -3.202475    1.202476   -0.667530
 H    1.034021   -1.625873    5.527410
 C    0.816814    3.947782   -2.286879
 H    0.237835    1.895136   -2.714555
 C    2.307455    4.246246   -0.414963
 H    2.910579    2.426537    0.603434
 H   -1.235002    4.782052    0.788504
 O   -0.815910   -0.158912   -2.384373
 O    1.140879    0.476840   -1.623767
 C    0.351090    0.276834   -2.601718
 C    0.834803    0.512657   -4.006907
 H    0.011514    0.851697   -4.648121
 H    1.204763   -0.444691   -4.406115
 H    1.660040    1.235037   -4.022870
*
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G[4]

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1664.894932
G (1 atm) =               -1664.439146
qh G-E (1 mol/L) =            0.471990
qh G-E (24.56 mol/L) =        0.475012
Lowest Frequency =           8.61

HF SCF energy (TZ) =      -1655.140565
HF SCF energy (QZ) =      -1655.239440
Correlation energy (DZ) =    -5.851070
Correlation energy (TZ) =    -7.160702
DLPNO-CCSD(T1)/CBS =      -1663.195199

SMD (MeOH)
HF SCF energy (TZ) =      -1655.156675
HF SCF energy (QZ) =      -1655.255365
Correlation energy (DZ) =    -5.845527
Correlation energy (TZ) =    -7.156383
DLPNO-CCSD(T1)/CBS =      -1663.207464

* xyz 0 1
  Ru    -0.268766    0.001568   -0.008803
  C      0.354644   -0.472695    1.838580
  N     -2.045523   -0.706512    0.821898
  H      0.322004    1.498220    2.298327
  C     -0.650717   -1.080967    2.657516
  C      1.618936   -0.328013    2.464532
  N      1.599967    0.641564   -0.788212
  O     -1.028119   -0.183113   -2.181225
  O     -0.892600    2.004173    0.421136
  O     -0.119440   -1.838796   -1.072715
  C     -3.288864   -0.788368    0.134412
  C     -1.947595   -1.181751    2.024171
  O      0.039015    2.437914    2.407608
  C     -0.412882   -1.527854    3.965098
  C      1.858642   -0.764481    3.768130
  H      2.442912    0.132538    1.908566
  C      1.583042    2.058733   -1.049418
  C      2.699156    0.072161   -1.151961
  C     -0.684169   -1.395578   -2.127888
  C     -0.678196    2.775200    1.358528
  C     -3.945558   -2.011365   -0.023417
  C     -3.828968    0.375050   -0.422725
  H     -2.817966   -1.616108    2.533700
  C      0.849079   -1.371343    4.527230
  H     -1.221554   -1.993108    4.537041
  H      2.853200   -0.632674    4.204355
  C      0.910552    2.547602   -2.169878
  C      2.203320    2.931833   -0.156266
  C      3.139234   -1.323439   -1.003049
  H      3.448834    0.712151   -1.639970
  C     -0.962778   -2.341199   -3.262667
  C     -1.225876    4.161707    1.393983
  C     -5.152177   -2.064508   -0.723629
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 C    2.436550   -2.336427   -0.221255
 C    4.309685   -1.698509   -1.609171
 H   -1.116793   -1.605433   -4.291524
 H   -2.295725   -2.383519   -3.215958
 H   -0.649491   -3.062810   -3.336423
 H   -1.482414    4.344448    2.514332
 H   -1.623357    4.406332    0.718284
 H   -0.088207    4.847755    1.543950
 C   -5.678853   -1.053414   -1.338222
 H   -5.734077   -3.078565   -0.589083
 H   -5.342054    0.995048   -1.939577
 C    1.551677    4.790257   -1.451146
 H    0.228865    4.369222   -3.106478
 H    2.889467    4.897457    0.242588
 C    2.966978   -3.616196   -0.118226
 H    1.506600   -2.080517    0.284802
 C    4.830795   -2.982640   -1.513851
 H    4.842516   -0.937307   -2.187738
 H   -6.608064   -1.151414   -1.904948
 H    1.536417    5.871240   -1.610537
 C    4.158429   -3.947160   -0.765161
 H    2.443488   -4.368509    0.477291
 H    5.767237   -3.230308   -2.019335
 H    4.565829   -4.957898   -0.680330
*
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G[c]

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CPCM (MeOH)
M06 SCF (DZ) =            -1496.968066
G (1 atm) =               -1496.517267
qh-G (1 mol/L) =          -1496.507182
qh-G (24.56 mol/L) =      -1496.504160
Lowest Frequency =           17.33

HF SCF energy (TZ) =      -1488.743687
HF SCF energy (QZ) =      -1488.834119
Correlation energy (DZ) =    -5.388829
Correlation energy (TZ) =    -6.595755
DLPNO-CCSD(T1)/CBS =      -1496.162372

*xyz 0 1
 Ru   0.034410    0.502772   -0.278309
 C   -1.372176   -0.812798   -1.506755
 C   -0.058537   -1.364895   -1.564533
 C   -2.415795   -1.514415   -0.822231
 H   -1.659158   -0.065857   -2.250720
 C   -0.923130    0.004576    1.380414
 N    1.515554   -0.555718    0.756833
 O   -1.171831    2.031483   -1.194159
 O    1.010850    2.208236    0.581003
 O    0.663589    1.582233   -2.312576
 C    0.207894   -2.635788   -0.959376
 H    0.630472   -1.016107   -2.344197
 C   -3.865303   -1.073877   -0.892835
 C   -2.081569   -2.658322   -0.132318
 C   -0.156229   -0.677926    2.370169
 C   -2.253843    0.314086    1.732876
 H   -3.499174   -2.920964    0.385077
 C   -5.036471    0.315202   -1.111926
 H   -3.288289    1.316710   -0.306855
 H    1.050222   -1.711131    5.545299
 C    0.856817    3.922228   -2.390993
 H    0.422089    1.842648   -2.844964
 C    2.137853    4.307687   -0.381418
 H    2.716650    2.530064    0.720221
 C    2.570765   -2.260345   -0.127925
 C    4.274175   -1.688866   -1.745928
 H   -1.042739   -1.794434   -4.210076
 H   -1.923020   -2.843334   -3.066622
 H   -0.181327   -3.108995   -3.326989
 H   -2.019461    4.208594    2.154409
 H   -1.634550    4.426932    0.413777
 H   -0.433798    4.863082    1.687235
 C   -5.702281   -0.904130   -1.265528
 H   -5.659823   -3.023520   -0.849475
 H   -5.460695    1.227736   -1.536876
 C    1.464082    4.806255   -1.496282
 H    0.332123    4.306034   -3.268868
 H    2.616906    4.991928    0.322493
 C    3.119478   -3.534029   -0.016265
 H    1.700390   -1.984500    0.461234
 C    4.814145   -2.967830   -1.642023
 H    4.740127   -0.954491   -2.408622
 H   -6.645562   -0.948924   -1.814144
 H    1.412681    5.883250   -1.669586
 C    4.235209   -3.894551   -0.774796
 H    2.671256   -4.253135    0.673002
 H    5.697946   -3.234334   -2.225320
 H    4.661273   -4.896057   -0.679662
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G[c]

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CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1497.664307
G (1 atm) =               -1497.197771
qh G-E (1 mol/L) =            0.479183
qh G-E (24.56 mol/L) =        0.482206
Lowest Frequency =          0.95

HF SCF energy (TZ) =      -1488.757140
HF SCF energy (QZ) =      -1488.846130
Correlation energy (DZ) =    -5.376615
Correlation energy (TZ) =    -6.583484
DLPNO-CCSD(T1)/CBS =      -1496.161645

SMD (MeOH)
HF SCF energy (TZ) =      -1488.770487
HF SCF energy (QZ) =      -1488.859330
Correlation energy (DZ) =    -5.372058
Correlation energy (TZ) =    -6.579916
DLPNO-CCSD(T1)/CBS =      -1496.171812

* xyz 0 1
 Ru   0.033138    0.523409   -0.271299
 C   -0.937411    0.023549    1.399776
 N    1.515810   -0.553756    0.757200
 C   -0.170629   -0.686236    2.366542
 C   -2.263530    0.325345    1.782079
 C    2.854112   -0.731129    0.296046
 C    1.188230   -0.937112    1.952973
 C   -0.682778   -1.087383    3.608854
 C   -2.780427   -0.067631    3.018220
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C	2.839480	-0.735751	0.282019
C	1.190470	-0.924775	1.967884
C	-0.368657	2.282873	-2.157699
C	0.566111	3.080614	1.332054
C	1.495495	-3.346727	-1.242500
C	-0.783877	-3.218842	-0.205238
C	-4.078935	0.299202	-1.512551
C	-4.698913	-2.107064	-1.651658
H	-4.239123	-1.043955	0.151086
H	-2.855585	-3.185674	0.438340
C	-0.688696	-1.050011	3.614762
C	-2.781096	-0.052777	2.970093
H	-2.891435	0.850874	1.019665
C	3.275682	0.057942	-0.785230
C	3.707709	-1.702049	0.811386
H	1.925833	-1.363014	2.655610
C	-0.667911	3.439082	-3.061460
C	1.323923	4.317997	1.645726
O	-0.606183	3.008377	1.917576
H	1.792415	-4.000386	-0.406319
H	1.393025	-3.990722	-2.134444
H	2.321809	-2.648698	-1.446645
H	-0.587342	-4.175999	0.290835
H	-5.134285	0.599798	-1.412958
H	-3.849115	0.284864	-2.593211
H	-3.446840	1.077136	-1.057631
H	-5.759882	-1.807218	-1.683195
H	-4.342388	-2.194391	-2.693544
H	-4.641732	-3.106589	-1.193438
C	-2.007812	-0.743726	3.914254
H	-0.057977	-1.574860	4.340221
H	-3.818892	0.202208	3.207834
C	4.556531	-0.106624	-1.305548
H	2.592915	0.799397	-1.208534
C	4.985459	-1.858197	0.286998
H	3.373453	-2.371476	1.607827
H	-0.191114	3.301897	-4.040576
H	-0.259749	4.356649	-2.608285
H	-1.751170	3.577162	-3.177817
H	2.319160	4.285823	1.191191
H	1.399933	4.439500	2.735362
H	0.765323	5.184603	1.261390
H	-1.021603	2.139303	1.701405
H	-2.439005	-1.026809	4.877347
C	5.418826	-1.062440	-0.773579
H	4.881091	0.521137	-2.139390
H	5.644699	-2.624637	0.702608
H	6.421364	-1.194728	-1.187561

*

G^S

CPCM (MeOH)

M06 SCF (DZ) = -1223.435119

G (1 atm) = -1223.136104

qh-G (1 mol/L) = -1223.126798

qh-G (24.56 mol/L) = -1223.123776

Lowest Frequency = 27.32

C	3.320985	0.117824	-0.712258
C	3.695791	-1.736879	0.791046
C	-1.998768	-0.781181	3.936398
C	4.615878	-0.026942	-1.208154
C	4.987979	-1.874516	0.291836
C	5.456321	-1.020837	-0.708506
H	-2.912192	0.877204	1.094338
H	1.917382	-1.396245	2.630546
H	-0.047009	-1.633667	4.311881
H	-3.814010	0.184618	3.272332
H	2.657094	0.887483	-1.108954
H	3.336428	-2.442291	1.542215
H	-2.416683	-1.085275	4.898262
H	4.966654	0.644464	-1.995090
H	5.629404	-2.669069	0.679590
H	6.468417	-1.137401	-1.101851
C	-1.407454	-0.842428	-1.543940
C	-0.103467	-1.384019	-1.616157
C	-2.443179	-1.540135	-0.849451
C	0.185299	-2.644989	-1.008276
C	-3.895695	-1.080011	-0.887104
C	-2.100913	-2.690952	-0.172022
C	1.496018	-3.335632	-1.280909
C	-0.799879	-3.241444	-0.252845
C	-4.100301	0.301585	-1.509148
C	-4.770940	-2.114664	-1.609739
H	-1.690141	-0.054095	-2.240056
H	0.592009	-0.997305	-2.365764
H	-4.236440	-1.031980	0.162897
H	-2.862841	-3.226346	0.402783
H	1.854664	-3.885480	-0.398375
H	1.378591	-4.065582	-2.099157
H	2.275972	-2.624139	-1.583740
H	-0.594348	-4.192253	0.248030
H	-5.145485	0.621300	-1.379695
H	-3.893380	0.285830	-2.592338
H	-3.443971	1.061881	-1.062873
H	-5.827981	-1.804377	-1.598854
H	-4.457946	-2.218112	-2.662145
H	-4.704004	-3.106669	-1.138814
O	-1.164059	2.036862	-1.230033
O	0.700701	1.561626	-2.281713
C	-0.336440	2.270736	-2.174153
C	-0.598571	3.415332	-3.113429
H	-0.112378	3.240254	-4.080892
H	-0.173220	4.329331	-2.670761
H	-1.676884	3.568251	-3.246440
O	1.004348	2.223015	0.562089
C	0.565016	3.099505	1.312341
C	1.310771	4.361798	1.581023
O	-0.584387	3.000466	1.938302
H	2.232637	4.388046	0.992382
H	1.539779	4.421774	2.654555
H	0.668985	5.217241	1.327883
H	-0.972276	2.112739	1.757988

*

G^S

CPCM (MeOH)

wB97X-D3 SCF (DZ) = -1223.941314

G (1 atm) = -1223.629658

qh G-E (1 mol/L) = 0.322728

qh G-E (24.56 mol/L) = 0.325751

Lowest Frequency = 18.66

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HF SCF energy (TZ) =      -1216.921817
HF SCF energy (QZ) =      -1216.997688
Correlation energy (DZ) =    -4.195928
Correlation energy (TZ) =    -5.198125
DLPNO-CCSD(T1)/CBS =      -1222.804294

*xyz 0 1
 Ru  -0.364871    0.617190    0.012776
 C   -1.705541   -0.831663   -0.162788
 H   -1.237785   -1.184598    1.720154
 C   -1.185262   -2.085930   -0.626147
 C   -3.107889   -0.779255    0.017360
 N    0.847837   -0.957199   -0.516965
 O    1.210830    2.336175   -0.122166
 O   -1.101614    1.433061   -1.806589
 O   -1.836317    2.233548    0.081882
 O    0.340495    0.425758    2.008880
 O   -0.875986   -1.342795    2.632881
 C   -2.006301   -3.195142   -0.887232
 C    0.235889   -2.085866   -0.786759
 C   -3.918026   -1.879901   -0.246893
 H   -3.568487    0.150715    0.371374
 C    2.250829   -0.873018   -0.710483
 C    1.255934    3.289415    0.933374
 H    1.002840    2.799562   -0.946821
 C   -1.874062    2.236072   -1.182955
 C    0.035026   -0.424876    2.852811
 C   -3.376047   -3.094175   -0.698695
 H   -1.557988   -4.130474   -1.240009
 H    0.801493   -2.973461   -1.102696
 H   -4.999950   -1.800121   -0.097481
 C    3.049374   -0.285592    0.277063
 C    2.844004   -1.350722   -1.884548
 H    1.994116    4.078440    0.719781
 H    1.563036    2.749171    1.838649
 H    0.266440    3.744518    1.107713
 C   -2.814323    3.115730   -1.934949
 C    0.667647   -0.483671    4.193406
 H   -4.028704   -3.947766   -0.897804
 C    4.426305   -0.207503    0.100553
 H    2.573322    0.095510    1.183606
 C    4.223410   -1.261423   -2.056805
 H    2.214409   -1.772543   -2.672985
 H   -2.401697    3.377993   -2.917921
 H   -3.754386    2.564645   -2.098675
 H   -3.045956    4.020912   -1.359021
 H    1.165478   -1.456760    4.317798
 H    1.394179    0.326812    4.311926
 H   -0.108338   -0.416667    4.969847
 C    5.019993   -0.694513   -1.064830
 H    5.044489    0.240325    0.883042
 H    4.676052   -1.632014   -2.980181
 H    6.101872   -0.623955   -1.201706
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HF SCF energy (TZ) =      -1216.928306
HF SCF energy (QZ) =      -1217.002861
Correlation energy (DZ) =    -4.191499
Correlation energy (TZ) =    -5.193294
DLPNO-CCSD(T1)/CBS =      -1222.804004

* xyz 0 1
 Ru  -0.351102    0.603311    0.022111
 C   -1.705811   -0.871747   -0.126069
 C   -1.171609   -2.106106   -0.612054
 C   -3.109099   -0.853110    0.055071
 N    0.862746   -0.960918   -0.545494
 C   -1.965783   -3.227368   -0.893938
 C    0.261469   -2.084300   -0.803651
 C   -3.904005   -1.964760   -0.225619
 C    2.271561   -0.874631   -0.747867
 C   -3.340476   -3.158465   -0.698664
 C    3.089317   -0.470845    0.311731
 C    2.831503   -1.160332   -1.995549
 C    4.465570   -0.378139    0.125837
 C    4.211701   -1.057316   -2.176055
 C    5.032020   -0.669771   -1.117845
 H   -3.588033    0.060655    0.421742
 H   -1.504603   -4.145672   -1.269783
 H    0.827586   -2.961009   -1.143001
 H   -4.986098   -1.905979   -0.074995
 H   -3.975093   -4.020871   -0.913530
 H    2.630884   -0.236287    1.273508
 H    2.182184   -1.447617   -2.825771
 H    5.102145   -0.073057    0.959467
 H    4.644246   -1.278127   -3.154440
 H    6.111616   -0.588710   -1.261288
 O    0.394501    0.405837    2.017892
 O   -1.122707   -1.052937    2.747678
 C   -0.062000   -0.302500    2.922099
 C    0.559379   -0.376334    4.274677
 H   -1.408532   -0.929745    1.802735
 H    1.009708   -1.372451    4.396909
 H    1.331087    0.392840    4.378288
 H   -0.213020   -0.258251    5.045887
 O    1.247983    2.224492   -0.120675
 C    1.343607    3.233472    0.887277
 H    1.139064    2.659532   -0.978031
 H    2.202122    3.891707    0.687088
 H    1.496210    2.713908    1.840349
 H    0.419271    3.829316    0.940647
 O   -1.116665    1.412305   -1.796071
 O   -1.839193    2.211591    0.099352
 C   -1.883833    2.213400   -1.166397
 C   -2.834718    3.097480   -1.916230
 H   -2.391130    3.418719   -2.866951
 H   -3.742473    2.516373   -2.140382
 H   -3.115726    3.966365   -1.309221
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G[2S]

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CPCM (MeOH)
M06 SCF (DZ) =            -1339.120407
G (1 atm) =               -1338.769325
qh-G (1 mol/L) =          -1338.759917
qh-G (24.56 mol/L) =      -1338.756894
Lowest Frequency =            6.77

HF SCF energy (TZ) =      -1332.025720
HF SCF energy (QZ) =      -1332.109802
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Correlation energy (DZ) =    -4.579345
Correlation energy (TZ) =    -5.674714
DLPNO-CCSD(T1)/CBS =      -1338.449915

*xyz 0 1
 Ru   0.246369   -0.258138   -0.120639
 C    1.256707    1.441956    0.060239
 N   -1.296339    1.086434    0.037430
 C    2.652387    1.662512    0.007038
 C    0.446534    2.621655    0.141210
 H    1.893367    0.499913    1.763868
 O   -0.921050   -2.253883   -0.641314
 O    0.246048   -0.092498   -2.278865
 O    1.984621   -1.521396   -0.261288
 O    0.066187   -0.855170    1.894028
 C   -2.664397    0.729382   -0.042004
 C   -0.959828    2.348109    0.123570
 C    3.192812    2.946913    0.043920
 H    3.326843    0.801013   -0.078989
 C    0.993046    3.912632    0.173684
 O    1.922281    0.114305    2.677635
 C   -1.043024   -3.272906    0.335043
 H   -0.265241   -2.558064   -1.307161
 C    1.057503    0.855085   -2.961621
 H    0.611722   -0.999892   -2.471681
 C    2.153783   -2.332474   -1.222008
 C    0.870429   -0.656755    2.811670
 C   -3.525725    1.347177   -0.953870
 C   -3.147456   -0.283957    0.792556
 H   -1.724573    3.135575    0.184787
 C    2.371023    4.079420    0.128970
 H    4.279480    3.074697   -0.000513
 H    0.327742    4.781750    0.224506
 H   -1.469687   -4.190655   -0.102961
 H   -1.721403   -2.913136    1.121345
 H   -0.070202   -3.513328    0.800446
 H    0.913133    0.754096   -4.048881
 H    2.125029    0.719782   -2.715107
 H    0.749448    1.862165   -2.647273
 C    3.406133   -3.164714   -1.217703
 O    1.342683   -2.489168   -2.181453
 C    0.714482   -1.268970    4.153979
 C   -4.863233    0.960597   -1.017865
 H   -3.134769    2.115941   -1.626562
 C   -4.484512   -0.658412    0.728249
 H   -2.456475   -0.755040    1.496923
 H    2.810711    5.079507    0.153690
 H    4.004696   -2.918327   -2.108223
 H    3.136756   -4.228087   -1.302557
 H    4.008369   -3.001805   -0.315512
 H    1.624280   -1.832134    4.407489
 H   -0.158805   -1.928893    4.176840
 H    0.606599   -0.473962    4.906594
 C   -5.347554   -0.039490   -0.177849
 H   -5.529375    1.442274   -1.738373
 H   -4.858177   -1.442317    1.392318
 H   -6.396174   -0.342115   -0.232098
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H

```
CPCM (MeOH)
M06 SCF (DZ) =            -1499.838038
G (1 atm) =               -1499.488484
qh-G (1 mol/L) =          -1499.481094
qh-G (24.56 mol/L) =      -1499.478072
```

H

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1500.406824
G (1 atm) =               -1500.045210
qh G-E (1 mol/L) =            0.371090
qh G-E (24.56 mol/L) =        0.374112
```

```
Lowest Frequency =           14.57

HF SCF energy (TZ) =      -1493.083621
HF SCF energy (QZ) =      -1493.145936
Correlation energy (DZ) =    -4.184253
Correlation energy (TZ) =    -5.123563
DLPNO-CCSD(T1)/CBS =      -1498.837148

PBE0+D3BJ (ATZ) =         -1499.697200
M06-2X (ATZ) =            -1500.380812
wB97M-V (ATZ) =           -1500.433171
B2GP-PLYP (ATZ) =         -1499.670991
B2K-PLYP (ATZ) =          -1499.502420
PWPB95 (ATZ) =            -1500.072746
PWPB95+D3BJ (ATZ) =       -1500.111499
PWPB95+D4 (ATZ) =         -1500.123645

*xyz 0 1
 Ru  -0.245939   -0.574727   -0.438572
 C   -1.699409    0.873211   -0.602769
 N    0.838211    1.214691   -0.110921
 C   -3.053952    0.713110   -0.924211
 C   -1.251194    2.205343   -0.404375
 Cl   0.118378   -0.201439   -2.846033
 C    0.154927    2.318722   -0.143603
 C    2.223231    1.246677    0.189792
 C   -3.913446    1.810703   -1.002538
 H   -3.459038   -0.285063   -1.126476
 C   -2.108896    3.312425   -0.490720
 H    0.649155    3.290732    0.002760
 C    3.118732    0.544564   -0.623907
 C    2.693275    1.943762    1.306995
 C   -3.450465    3.112821   -0.781846
 H   -4.968916    1.649292   -1.243242
 H   -1.712534    4.320783   -0.332895
 C    4.477944    0.565597   -0.331716
 H    2.729081    0.001267   -1.490211
 C    4.056511    1.952503    1.595718
 H    1.981923    2.458498    1.959908
 H   -4.136640    3.960380   -0.847996
 C    4.951847    1.267841    0.777761
 H    5.176087    0.027421   -0.977771
 H    4.417374    2.492687    2.474513
 H    6.019990    1.273861    1.007757
 C    0.411236   -1.400383    1.441366
 C   -1.010621   -1.404476    1.425947
 C    1.185876   -2.118394    0.475746
 H    0.939642   -0.830784    2.211445
 C   -1.851688   -0.750652    2.494131
 C   -1.636666   -2.065846    0.322801
 C    0.562302   -2.729794   -0.615222
 H    2.277279   -2.088286    0.530956
 C   -1.171881    0.428669    3.170955
 C   -2.262811   -1.806734    3.517337
 H   -2.764718   -0.380444    1.989467
 C   -0.872880   -2.661006   -0.700245
 H   -2.726255   -2.026518    0.227879
 C    1.342967   -3.356937   -1.720535
 H   -0.824079    1.176112    2.438783
 H   -0.306107    0.107013    3.775296
 H   -1.874444    0.925439    3.858051
 H   -2.796048   -2.646950    3.043918
 H   -1.372412   -2.214988    4.027037
 H   -2.922879   -1.371482    4.284395
 H   -1.374599   -3.066974   -1.582796
 H    1.227189   -4.452847   -1.699891
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Lowest Frequency =           10.21

HF SCF energy (TZ) =      -1493.086057
HF SCF energy (QZ) =      -1493.146921
Correlation energy (DZ) =    -4.184425
Correlation energy (TZ) =    -5.123820
DLPNO-CCSD(T1)/CBS =      -1498.838001

PBE0+D3BJ (ATZ) =         -1499.697172
M06-2X (ATZ) =            -1500.389210
wB97M-V (ATZ) =           -1500.438217
B2GP-PLYP (ATZ) =         -1499.680316
B2K-PLYP (ATZ) =          -1499.514170
PWPB95 (ATZ) =            -1500.078997
PWPB95+D3BJ (ATZ) =       -1500.117784
PWPB95+D4 (ATZ) =         -1500.129917

SMD (MeOH)
HF SCF energy (TZ) =      -1493.094018
HF SCF energy (QZ) =      -1493.154944
Correlation energy (DZ) =    -4.183900
Correlation energy (TZ) =    -5.123544
DLPNO-CCSD(T1)/CBS =      -1498.845913


* xyz 0 1
 Ru  -0.252039   -0.556386   -0.389695
 C   -1.686714    0.915877   -0.494541
 N    0.889452    1.205856   -0.164997
 C   -3.071831    0.794911   -0.694600
 C   -1.191864    2.239046   -0.368225
 C    0.241806    2.323156   -0.193850
 C    2.299261    1.208289    0.046453
 C   -3.903227    1.916831   -0.736852
 C   -2.015970    3.372487   -0.420189
 C    3.127216    0.530920   -0.854408
 C    2.845900    1.841140    1.164823
 C   -3.384202    3.210013   -0.599315
 C    4.502527    0.508379   -0.642940
 C    4.225922    1.809192    1.371428
 C    5.056728    1.146166    0.470040
 C    0.293928   -1.290880    1.558677
 C   -1.111645   -1.411051    1.416441
 C    1.202226   -1.939995    0.658461
 C   -2.096893   -0.836292    2.414106
 C   -1.593913   -2.141861    0.280967
 C    0.730556   -2.629189   -0.460116
 C   -1.594234    0.417025    3.127412
 C   -2.483073   -1.934399    3.413128
 C   -0.696281   -2.681057   -0.655850
 C    1.657259   -3.231552   -1.475329
 H   -3.523433   -0.193184   -0.821897
 H    0.768432    3.281934   -0.103999
 H   -4.978761    1.781932   -0.882304
 H   -1.579308    4.370226   -0.320643
 H    2.678206    0.032792   -1.716252
 H    2.187145    2.337769    1.880895
 H   -4.045282    4.078150   -0.637222
 H    5.147095   -0.015819   -1.351917
 H    4.649907    2.298597    2.250896
 H    6.135616    1.119290    0.636602
 H    0.707229   -0.684612    2.365565
 H    2.276494   -1.806596    0.798407
 H   -2.997367   -0.562945    1.839072
 H   -2.667480   -2.212499    0.098861
 H   -1.283236    1.189685    2.408009
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 H    0.978644   -2.999303   -2.696577
 H    2.414083   -3.120579   -1.639294
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 H   -0.742843    0.195543    3.790469
 H   -2.396357    0.835179    3.753257
 H   -2.888370   -2.820813    2.901568
 H   -1.606039   -2.251619    4.000608
 H   -3.247737   -1.566515    4.113829
 H   -1.090837   -3.137828   -1.565128
 H    1.617994   -4.330019   -1.417135
 H    1.359699   -2.934506   -2.491128
 H    2.693220   -2.910156   -1.303443
 Cl   0.012485   -0.241094   -2.821647
*
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H•S

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CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1616.119558
G (1 atm) =               -1615.709671
qh G-E (1 mol/L) =            0.422368
qh G-E (24.56 mol/L) =        0.425391
Lowest Frequency =            9.72

HF SCF energy (TZ) =      -1608.179726
HF SCF energy (QZ) =      -1608.248536
Correlation energy (DZ) =    -4.566970
Correlation energy (TZ) =    -5.597770
DLPNO-CCSD(T1)/CBS =      -1614.469373

SMD (MeOH)
HF SCF energy (TZ) =      -1608.189001
HF SCF energy (QZ) =      -1608.257849
Correlation energy (DZ) =    -4.565742
Correlation energy (TZ) =    -5.596791
DLPNO-CCSD(T1)/CBS =      -1614.477863

* xyz 0 1
 Ru   0.459924    0.282482   -0.407185
 C    1.704695    1.207045    0.945081
 C    2.985508    1.746321    0.740770
 C    1.199601    1.283745    2.266614
 C    3.697862    2.341353    1.784267
 C    1.911232    1.870221    3.323870
 C   -0.109357    0.693744    2.437709
 C    3.167663    2.409612    3.078857
 N   -0.673496    0.197184    1.385074
 C   -1.985719   -0.351793    1.485155
 C   -2.268834   -1.567766    0.855080
 C   -2.995976    0.332544    2.168539
 C   -3.550373   -2.105317    0.935541
 C   -4.278322   -0.212032    2.240098
 C   -4.559401   -1.432398    1.627912
 C    0.479657    2.021427   -1.665918
 C   -0.872431    1.693469   -1.393451
 C    1.368612    1.063926   -2.243776
 C   -1.858176    2.677294   -0.790666
 C   -1.327595    0.379704   -1.753298
 C    0.918522   -0.243974   -2.520678
 C   -1.215774    3.711695    0.131776
 C   -2.647392    3.347249   -1.922293
 C   -0.463299   -0.568733   -2.302803
 C    1.855013   -1.287865   -3.058198
 H    3.446656    1.706087   -0.250311
 H    4.688685    2.760649    1.587306
 H    1.476288    1.898812    4.326779
 H   -0.606171    0.651764    3.415250
 H    3.736592    2.877761    3.884580
 H   -1.487883   -2.082990    0.292852
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 H   -2.785367    1.304583    2.620350
 H   -3.762066   -3.058286    0.445567
 H   -5.064196    0.331044    2.769419
 H   -5.565273   -1.854155    1.679645
 H    0.869409    2.998428   -1.379559
 H    2.416234    1.320494   -2.404875
 H   -2.564407    2.078313   -0.190719
 H   -2.353346    0.092628   -1.510257
 H   -0.622522    3.232292    0.925037
 H   -0.557335    4.398698   -0.423458
 H   -1.997066    4.320976    0.609783
 H   -3.150995    2.602256   -2.557148
 H   -1.977858    3.944312   -2.562840
 H   -3.415796    4.019531   -1.511565
 H   -0.806034   -1.591568   -2.466087
 H    1.562908   -2.289052   -2.714931
 H    1.811830   -1.278777   -4.158616
 H    2.890538   -1.089929   -2.751453
 Cl   1.524231   -1.815618    0.379445
 O   -0.425367   -3.572996   -1.351839
 C   -0.666986   -4.819385   -0.728257
 H    0.222225   -3.086318   -0.805638
 H    0.239444   -5.449311   -0.688215
 H   -1.054788   -4.699756    0.299661
 H   -1.427319   -5.349969   -1.319324
*
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H•S_2

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1731.831192
G (1 atm) =               -1731.372638
qh G-E (1 mol/L) =            0.473261
qh G-E (24.56 mol/L) =        0.476284
Lowest Frequency =            8.04

SMD (MeOH)
HF SCF energy (TZ) =      -1723.282476
HF SCF energy (QZ) =      -1723.359407
Correlation energy (DZ) =    -4.947539
Correlation energy (TZ) =    -6.070233
DLPNO-CCSD(T1)/CBS =      -1730.108851

* xyz 0 1
 Ru  -0.655113   -0.385594    0.252352
 C   -0.929285    0.050105    2.337114
 C   -1.534850    1.416407   -0.229861
 C    0.462464   -0.094554    2.099345
 C   -1.852613   -0.980924    1.995485
 H   -1.316269    0.990446    2.731023
 O   -4.466971   -0.894883   -0.000452
 Cl  -1.769129   -1.229275   -1.805021
 C   -0.785224    2.228730   -1.114632
 C   -2.774509    1.929504    0.183331
 C    1.487436    0.966044    2.454206
 C    0.902872   -1.325503    1.511278
 C   -1.390807   -2.174012    1.389925
 H   -2.923377   -0.826175    2.128970
 C   -5.472789   -0.314823   -0.807338
 H   -3.645938   -0.913543   -0.523559
 H   -0.736481   -3.169432   -1.686284
 C   -1.226797    3.484796   -1.557229
 C    0.475598    1.653054   -1.527418
 C   -3.220148    3.181593   -0.245777
 H   -3.417237    1.336687    0.839025
 C    0.944854    2.392814    2.407725
```

```
 C    2.088519    0.639763    3.827160
 H    2.289748    0.881024    1.701090
 C    0.010718   -2.353737    1.175452
 H    1.959990   -1.434962    1.256944
 C   -2.356658   -3.252213    0.986559
 H   -5.240604    0.733584   -1.068579
 H   -5.636332   -0.878955   -1.742825
 H   -6.410555   -0.324429   -0.233017
 O   -0.233935   -3.999842   -1.585276
 C   -2.451361    3.967823   -1.113186
 H   -0.608299    4.073020   -2.240922
 N    0.780982    0.494053   -1.041179
 H    1.146859    2.164664   -2.228840
 H   -4.187169    3.554957    0.103310
 H    0.491036    2.620275    1.431474
 H    0.186121    2.565840    3.187695
 H    1.762286    3.107939    2.582855
 H    2.519876   -0.372655    3.847246
 H    1.315929    0.697040    4.611276
 H    2.885231    1.355723    4.079309
 H    0.367677   -3.246329    0.660136
 H   -1.963829   -3.833693    0.142785
 H   -2.494730   -3.935688    1.839208
 H   -3.332879   -2.829409    0.717728
 C   -0.086934   -4.571716   -2.871902
 H   -2.813948    4.944248   -1.440847
 C    2.041507   -0.090268   -1.362011
 H   -1.059888   -4.750427   -3.361982
 H    0.529052   -3.939413   -3.536626
 H    0.420964   -5.539349   -2.752777
 C    2.102792   -1.443888   -1.707415
 C    3.215246    0.666936   -1.292486
 C    3.330910   -2.024378   -2.011309
 H    1.191590   -2.044397   -1.720668
 C    4.441866    0.075308   -1.594812
 H    3.170780    1.712275   -0.978468
 C    4.504171   -1.268523   -1.959974
 H    3.369508   -3.081336   -2.284263
 H    5.355134    0.670972   -1.533018
 H    5.466074   -1.730853   -2.191104
*
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```

***cis*-INT(D⁺-E⁺)**

```
CPCM (MeOH)
M06 SCF (DZ) =            -1268.424835
G (1 atm) =               -1268.018408
qh-G (1 mol/L) =          -1268.009876
qh-G (24.56 mol/L) =      -1268.006854
Lowest Frequency =           11.97

HF SCF energy (TZ) =      -1261.299913
HF SCF energy (QZ) =      -1261.374581
Correlation energy (DZ) =    -4.696362
Correlation energy (TZ) =    -5.733180
DLPNO-CCSD(T1)/CBS =      -1267.736109

*xyz 1 1
 Ru  -0.203077    0.754768   -0.316793
 C   -1.284614   -1.245879   -1.394396
 N    0.772661   -0.994386    0.485683
 C   -2.467957   -1.246857   -2.130728
 C   -1.093629   -2.188881   -0.364979
 H   -0.379582   -0.735102   -1.817181
 O    1.561326    0.940218   -1.373311
 C    2.109218   -1.003129    0.974310
```

***cis*-INT(D⁺-E⁺)**

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1269.058726
G (1 atm) =               -1268.637891
qh G-E (1 mol/L) =            0.431817
qh G-E (24.56 mol/L) =        0.434840
Lowest Frequency =          10.94

HF SCF energy (TZ) =      -1261.308366
HF SCF energy (QZ) =      -1261.381991
Correlation energy (DZ) =    -4.690654
Correlation energy (TZ) =    -5.726608
DLPNO-CCSD(T1)/CBS =      -1267.736129

SMD (MeOH)
HF SCF energy (TZ) =      -1261.328371
HF SCF energy (QZ) =      -1261.401845
Correlation energy (DZ) =    -4.686534
Correlation energy (TZ) =    -5.723053
DLPNO-CCSD(T1)/CBS =      -1267.752712

* xyz 1 1
 Ru   0.003016    0.699255   -0.124212
```

C	0.144641	-2.121434	0.383991
C	-3.462847	-2.175292	-1.831250
H	-2.600396	-0.535562	-2.949925
C	-2.084232	-3.136772	-0.090201
O	1.543121	-1.028870	-2.454225
C	2.103425	0.008651	-2.107773
C	2.536101	-0.032024	1.882223
C	3.008734	-1.968511	0.508490
H	0.558386	-3.029920	0.845842
C	-3.270374	-3.117230	-0.816665
H	-4.390711	-2.180717	-2.407242
H	-1.928945	-3.869591	0.706028
C	3.529897	0.312633	-2.480175
C	3.848089	-0.043306	2.340956
H	1.832623	0.718222	2.246488
C	4.321496	-1.970957	0.970882
H	2.685943	-2.687538	-0.248982
H	-4.053087	-3.846168	-0.597230
H	3.621875	1.337082	-2.867876
H	4.146586	0.254094	-1.567613
H	3.903054	-0.409248	-3.217052
C	4.744401	-1.010979	1.886996
H	4.172387	0.711638	3.060506
H	5.021379	-2.722187	0.598005
H	5.777027	-1.010120	2.243063
C	0.085051	2.459828	0.950226
C	-0.776741	1.546714	1.623909
C	-0.242315	2.973251	-0.340345
H	1.035184	2.748524	1.406903
C	-1.972340	1.081223	1.026242
H	-0.460780	1.139779	2.588403
C	0.693335	3.883217	-1.053308
C	-1.408378	2.479310	-0.963545
C	-2.924945	0.120588	1.695067
C	-2.234262	1.537418	-0.292110
H	0.606218	3.770474	-2.142521
H	0.445983	4.925693	-0.795295
H	1.733527	3.696412	-0.754210
H	-1.631826	2.754938	-1.996399
C	-2.304215	-0.675720	2.830872
C	-4.138433	0.908383	2.187361
H	-3.267550	-0.583679	0.912543
H	-3.080206	1.103868	-0.833978
H	-1.383937	-1.202248	2.528609
H	-2.061057	-0.028094	3.690425
H	-3.019788	-1.431195	3.189471
H	-4.637686	1.448141	1.367438
H	-3.835183	1.647965	2.948000
H	-4.872905	0.229188	2.646898

*

O	-0.544102	2.097164	2.570281
O	-1.724301	1.107233	0.951183
C	-1.622375	1.785177	2.054692
C	-2.947635	2.181346	2.661456
C	-0.562878	1.370797	-2.065952
C	0.482924	0.414604	-2.220381
C	-0.374884	2.537687	-1.266534
C	1.715755	0.542364	-1.540754
C	-1.484819	3.524375	-1.079485
C	0.849386	2.673437	-0.571404
C	2.843277	-0.466355	-1.653077
C	1.849147	1.673848	-0.688662
C	2.385807	-1.850047	-2.109910
C	3.918492	0.098629	-2.590665
H	-3.620531	1.313914	2.701412
H	-3.419050	2.938138	2.016733
H	-2.803247	2.598090	3.664683
H	-1.529451	1.189904	-2.538321
H	0.284004	-0.480584	-2.809710
H	-2.464415	3.036259	-1.155299
H	-1.411576	4.281606	-1.875273
H	-1.402548	4.032441	-0.110218
H	0.989335	3.491744	0.134489
H	3.281755	-0.558984	-0.644528
H	2.733370	1.748962	-0.052157
H	1.559741	-2.237532	-1.495186
H	2.055280	-1.840598	-3.160761
H	3.223515	-2.558066	-2.033851
H	4.292796	1.071351	-2.237462
H	3.513941	0.233943	-3.606584
H	4.771010	-0.594033	-2.650025
C	1.391005	-0.336173	1.804451
C	2.611627	0.119669	2.298238
C	1.226158	-1.688213	1.462127
N	-0.721993	-1.290802	0.156624
C	3.672659	-0.773800	2.446099
C	2.283185	-2.585315	1.640936
C	-0.038627	-2.118391	0.863854
C	-2.023372	-1.694637	-0.292641
C	3.506239	-2.122249	2.122226
C	-2.275555	-1.851296	-1.655370
C	-3.031782	-1.907335	0.647986
C	-3.547873	-2.231749	-2.076134
C	-4.302717	-2.284391	0.216854
C	-4.563774	-2.445731	-1.143442
H	0.528250	0.366782	1.893367
H	2.725090	1.169287	2.575846
H	4.631137	-0.418945	2.829711
H	2.152547	-3.637504	1.379821
H	-0.395544	-3.145581	1.012553
H	4.336606	-2.819492	2.247638
H	-1.477382	-1.700578	-2.382488
H	-2.818492	-1.761279	1.708512
H	-3.742912	-2.365229	-3.141959
H	-5.092566	-2.449151	0.952477
H	-5.560246	-2.740347	-1.478535

*

***cis*-INT(D⁺-E⁺)•S^p**

CPCM (MeOH)

wB97X-D3 SCF (DZ) = -1384.774457

G (1 atm) = -1384.304988

qh G-E (1 mol/L) = 0.483226

qh G-E (24.56 mol/L) = 0.486248

Lowest Frequency = 10.90

SMD (MeOH)
HF SCF energy (TZ) =   -1376.423691
HF SCF energy (QZ) =   -1376.505218
Correlation energy (DZ) =   -5.067166
Correlation energy (TZ) =   -6.195660
DLPNO-CCSD(T1)/CBS =   -1383.384863

```
* xyz 1 1
Ru  -0.509134   -0.066613   -0.231657
 C   -1.467172    0.542759   -2.091295
 C    0.356799   -1.037958   -1.938839
 C   -2.332386   -0.380728   -1.420942
 C   -0.125213    0.233484   -2.388069
 H   -1.840392    1.544337   -2.313117
 C   -0.483632   -1.943425   -1.256190
 C   -1.014165    2.278557    0.574528
 N    1.367900    0.740679    0.377558
 H   -1.198582    1.301648    1.092152
 O   -0.474749   -0.988285    1.650270
 H    1.418661   -1.274307   -2.037113
 C   -1.866625   -1.640427   -1.007947
 H   -3.338290   -0.054164   -1.157846
 C    0.781989    1.219536   -3.063038
 H   -0.052910   -2.859358   -0.847377
 C   -2.154360    3.045432    0.355518
 C    0.263707    2.851205    0.464190
 C    2.565615   -0.048466    0.407185
 C    1.451064    2.007599    0.585704
 O   -2.249197    0.139815    2.391874
 C   -1.344190   -0.701035    2.555527
 C   -2.715465   -2.650028   -0.263690
 H    1.813987    1.116659   -2.701651
 H    0.780385    1.030742   -4.146956
 H    0.439948    2.248657   -2.890045
 C   -2.022172    4.393104    0.015899
 H   -3.140833    2.592563    0.471292
 C    0.388042    4.207426    0.151369
 C    2.567977   -1.266457    1.091597
 C    3.701437    0.381306   -0.284383
 H    2.417051    2.469230    0.825155
 H   -2.494062    1.109682    3.879079
 C   -1.224756   -1.454370    3.855179
 C   -3.986435   -2.066946    0.348298
 C   -3.035572   -3.805354   -1.223537
 H   -2.082261   -3.042959    0.549616
 C   -0.755635    4.971508   -0.078445
 H   -2.912840    4.999562   -0.159114
 H    1.379890    4.656518    0.067050
 C    3.725186   -2.040877    1.100684
 H    1.665689   -1.586948    1.613885
 C    4.852073   -0.406106   -0.272106
 H    3.679070    1.315766   -0.849585
 O   -2.316971    1.662293    4.665807
 H   -0.234251   -1.908244    3.973014
 H   -1.986726   -2.248703    3.862715
 H   -1.443077   -0.767847    4.683946
 H   -3.764989   -1.223296    1.017793
 H   -4.690371   -1.728152   -0.428685
 H   -4.496138   -2.843816    0.936511
 H   -2.122261   -4.264424   -1.630802
 H   -3.647375   -3.449384   -2.067768
 H   -3.601594   -4.585390   -0.693851
 H   -0.656920    6.028373   -0.332963
 C    4.868301   -1.615207    0.421352
 H    3.731561   -2.988311    1.643487
```

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 H    5.736554   -0.072149   -0.818235
 C   -1.197480    2.457176    4.338458
 H    5.769784   -2.231308    0.426104
 H   -1.412260    3.182354    3.530061
 H   -0.325000    1.852451    4.023776
 H   -0.906137    3.026332    5.234137
*
```

***cis*-INT(D⁺-E⁺)•S_2^{kp}**

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1500.489292
G (1 atm) =               -1499.970759
qh G-E (1 mol/L) =            0.534422
qh G-E (24.56 mol/L) =        0.537444
Lowest Frequency =           11.13

SMD (MeOH)
HF SCF energy (TZ) =      -1491.517803
HF SCF energy (QZ) =      -1491.607393
Correlation energy (DZ) =    -5.450420
Correlation energy (TZ) =    -6.670413
DLPNO-CCSD(T1)/CBS =      -1499.017685

* xyz 1 1
Ru  -0.500079   -0.105204   -0.242529
 C   -1.380834    0.496111   -2.143667
 C    0.404102   -1.123322   -1.906444
 C   -2.286061   -0.398220   -1.486415
 C   -0.036245    0.153984   -2.386682
 H   -1.724618    1.501164   -2.395046
 C   -0.479079   -2.002408   -1.247161
 C   -1.082789    2.213466    0.531431
 N    1.347653    0.753533    0.397271
 H   -1.247747    1.234063    1.055116
 O   -0.490534   -1.053534    1.644547
 H    1.463396   -1.383032   -1.964827
 C   -1.860148   -1.660582   -1.040168
 H   -3.291306   -0.044876   -1.256770
 C    0.912002    1.110995   -3.045988
 H   -0.086378   -2.911890   -0.784772
 C   -2.242451    2.944621    0.293680
 C    0.177623    2.829171    0.456322
 C    2.573469    0.008777    0.442209
 C    1.387644    2.023867    0.600509
 O   -2.189231    0.139770    2.455330
 C   -1.313915   -0.729766    2.590107
 H    0.007358   -2.837569    1.553953
 C   -2.746355   -2.632519   -0.289793
 H    1.936896    0.966871   -2.679580
 H    0.910482    0.928951   -4.131111
 H    0.606597    2.150960   -2.869175
 C   -2.146812    4.299056   -0.031304
 H   -3.216024    2.459218    0.384143
 C    0.264530    4.191303    0.157680
 C    2.620045   -1.198733    1.141175
 C    3.695510    0.470224   -0.252029
 H    2.335148    2.516438    0.851897
 H   -2.305045    1.168825    3.942553
 C   -1.162286   -1.479919    3.887506
 O    0.354475   -3.705052    1.274874
 C   -4.001363   -2.000426    0.304961
 C   -3.089034   -3.798294   -1.227544
 H   -2.130096   -3.029903    0.532674
 C   -0.898314    4.919585   -0.091729
 H   -3.052811    4.877789   -0.220839
```

H	1.242758	4.673237	0.100357
C	3.800499	-1.936309	1.155707
H	1.735527	-1.550757	1.669025
C	4.872244	-0.277407	-0.231106
H	3.642946	1.398363	-0.825629
O	-2.031402	1.722232	4.698592
H	-0.185941	-1.972869	3.962357
H	-1.955979	-2.240568	3.941966
H	-1.307609	-0.776293	4.717792
C	-0.249419	-4.711736	2.065803
H	-3.756913	-1.150946	0.959645
H	-4.692586	-1.654702	-0.480283
H	-4.535788	-2.749677	0.906830
H	-2.182958	-4.288097	-1.615131
H	-3.684008	-3.446264	-2.085323
H	-3.678350	-4.552851	-0.686326
H	-0.828823	5.981506	-0.334551
C	4.928758	-1.479841	0.472043
H	3.832748	-2.879860	1.704282
H	5.745368	0.081874	-0.779430
C	-0.933189	2.486051	4.246550
H	-1.349518	-4.722240	1.959250
H	-0.004881	-4.601779	3.136949
H	0.135811	-5.682540	1.723259
H	5.849833	-2.066170	0.480796
H	-0.528453	3.045323	5.103365
H	-0.118901	1.857333	3.837216
H	-1.217275	3.218043	3.466211

*

***trans*-INT(D⁺-E)**

CPCM (MeOH)

M06 SCF (DZ) = -1268.426133

G (1 atm) = -1268.017778

qh-G (1 mol/L) = -1268.009714

qh-G (24.56 mol/L) = -1268.006692

Lowest Frequency = 23.10

HF SCF energy (TZ) = -1261.305576

HF SCF energy (QZ) = -1261.380229

Correlation energy (DZ) = -4.693504

Correlation energy (TZ) = -5.729980

DLPNO-CCSD(T1)/CBS = -1267.738352

*xyz 1 1

Ru	-0.137637	0.562708	0.260742
C	-1.652222	-0.385645	-1.577943
N	0.601844	-1.365701	-0.211529
C	-1.427157	-1.759828	-1.378885
C	-2.916053	0.089222	-1.913353
H	-0.778655	0.290905	-1.694985
O	-1.442688	-0.590347	1.393924
C	1.891576	-1.799523	0.219537
C	-0.141922	-2.190771	-0.874218
C	-2.474488	-2.665294	-1.573134
C	-3.960542	-0.817519	-2.072685
H	-3.072439	1.159158	-2.067521
C	-2.681351	-0.216171	1.568515
C	2.162862	-1.868976	1.586927
C	2.873873	-2.107252	-0.721226
H	0.188288	-3.229103	-1.024204
C	-3.736046	-2.187550	-1.912492
H	-2.303011	-3.734279	-1.425503
H	-4.956140	-0.458551	-2.341657
C	-3.492054	-1.233042	2.332594

***trans*-INT(D⁺-E)**

CPCM (MeOH)

wB97X-D3 SCF (DZ) = -1269.060063

G (1 atm) = -1268.639973

qh G-E (1 mol/L) = 0.431359

qh G-E (24.56 mol/L) = 0.434381

Lowest Frequency = 10.89

HF SCF energy (TZ) = -1261.309644

HF SCF energy (QZ) = -1261.383111

Correlation energy (DZ) = -4.691716

Correlation energy (TZ) = -5.728006

DLPNO-CCSD(T1)/CBS = -1267.738795

SMD (MeOH)

HF SCF energy (TZ) = -1261.330695

HF SCF energy (QZ) = -1261.404013

Correlation energy (DZ) = -4.687388

Correlation energy (TZ) = -5.724390

DLPNO-CCSD(T1)/CBS = -1267.756452

*xyz 1 1

Ru	-0.146847	0.587120	0.268477
C	-1.723194	-0.400463	-1.590001
N	0.585027	-1.334289	-0.209590
C	-1.465856	-1.758522	-1.351792
C	-2.993191	0.032482	-1.959233
O	-1.422224	-0.556597	1.414583
C	1.886511	-1.771498	0.205498
C	-0.158027	-2.166879	-0.852984
C	-2.489705	-2.696326	-1.525565
C	-4.013628	-0.904860	-2.107962
C	-2.673586	-0.225314	1.578490
C	2.160924	-1.888712	1.569015
C	2.867541	-2.034256	-0.749452

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 O   -3.166075    0.834575    1.159606
 C    3.431312   -2.249601    2.011203
 H    1.369329   -1.636570    2.302880
 C    4.144733   -2.477221   -0.284423
 H    2.643381   -2.034184   -1.787933
 H   -4.560293   -2.890479   -2.050570
 H   -3.011439   -1.455558    3.296933
 H   -3.526797   -2.176374    1.765840
 H   -4.512549   -0.866906    2.500169
 C    4.425421   -2.546648    1.077775
 H    3.645324   -2.315057    3.080327
 H    4.919882   -2.709176   -1.018262
 H    5.423356   -2.834389    1.416123
 C    1.051469    1.486789    1.784368
 C    1.833885    1.396988    0.599001
 C   -0.195319    2.183984    1.789510
 H    1.399923    1.001132    2.699439
 C    1.387789    1.931592   -0.634062
 H    2.761225    0.814637    0.620209
 C   -1.004801    2.265455    3.035600
 C   -0.669921    2.682827    0.557776
 C    2.230459    1.821449   -1.882205
 C    0.096989    2.527025   -0.630041
 H   -2.070869    2.388750    2.809105
 H   -0.662413    3.130744    3.626167
 H   -0.866905    1.365984    3.653555
 H   -1.678081    3.094683    0.496774
 C    1.485318    1.253313   -3.081340
 C    2.813792    3.198160   -2.193938
 H    3.063936    1.136709   -1.639591
 H   -0.355582    2.837648   -1.577697
 H    1.136902    0.222963   -2.899139
 H    0.616153    1.872642   -3.361697
 H    2.152748    1.224974   -3.956030
 H    3.365956    3.609104   -1.334468
 H    2.012377    3.910201   -2.456493
 H    3.504003    3.136758   -3.049145
*
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```
 C   -3.759747   -2.263335   -1.896685
 C   -3.463336   -1.248519    2.364994
 O   -3.190992    0.798211    1.135356
 C    3.433529   -2.280376    1.975895
 C    4.141424   -2.419691   -0.330219
 C    4.426213   -2.542386    1.028796
 C    1.033855    1.506770    1.788496
 C    1.823754    1.405542    0.611586
 C   -0.209904    2.211796    1.778837
 C    1.386518    1.926604   -0.631271
 C   -1.031289    2.315229    3.026059
 C   -0.670204    2.708483    0.542858
 C    2.248736    1.794623   -1.872073
 C    0.103150    2.534408   -0.640157
 C    1.482499    1.320658   -3.106873
 C    2.955439    3.133824   -2.116806
 H   -0.877188    0.313754   -1.663742
 H   -3.175407    1.091903   -2.143599
 H    0.181187   -3.198797   -1.008190
 H   -2.293947   -3.755328   -1.345140
 H   -5.012561   -0.578185   -2.403044
 H    1.377137   -1.677445    2.299504
 H    2.635787   -1.919500   -1.810443
 H   -4.562891   -2.991773   -2.023370
 H   -2.968399   -1.450848    3.325208
 H   -3.491508   -2.192853    1.801301
 H   -4.485794   -0.892833    2.536787
 H    3.650585   -2.379978    3.041175
 H    4.914342   -2.620394   -1.074735
 H    5.424664   -2.842145    1.353184
 H    1.375386    1.024589    2.705226
 H    2.747058    0.823536    0.646470
 H   -2.097482    2.398005    2.788248
 H   -0.715930    3.214785    3.576733
 H   -0.867437    1.444635    3.674464
 H   -1.667779    3.139198    0.469548
 H    3.015382    1.038435   -1.636966
 H   -0.338770    2.843499   -1.590016
 H    1.040912    0.324913   -2.947904
 H    0.678676    2.018777   -3.389178
 H    2.168141    1.247819   -3.963316
 H    3.531703    3.447797   -1.233587
 H    2.223886    3.925155   -2.347194
 H    3.647514    3.048913   -2.967467
*
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INT(E$^+$-H)$^+$

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CPCM (MeOH)
M06 SCF (DZ) =            -1039.423559
G (1 atm) =               -1039,073257
qh-G (1 mol/L) =          -1039.065834
qh-G (24.56 mol/L) =      -1039.062812
Lowest Frequency =           22.89

HF SCF energy (TZ) =      -1033.381071
HF SCF energy (QZ) =      -1033.439695
Correlation energy (DZ) =    -3.995807
Correlation energy (TZ) =    -4.865051
DLPNO-CCSD(T1)/CBS =      -1038.830341

*xyz 1 1
 Ru  -0.301263   -0.567871   -0.635666
 C   -0.877037   -1.464626    1.208421
 N    0.823561    1.208209   -0.316426
 C   -1.551451   -0.835892    2.401142
```

```
 C    0.546525   -1.542617    1.071237
 C   -1.664541   -2.061460    0.173090
 C   -1.752953    0.907670   -0.709776
 C    0.146223    2.315585   -0.281421
 C    2.223979    1.217462   -0.077910
 C   -0.756273    0.289863    3.041723
 C   -1.849748   -1.940061    3.414829
 H   -2.512050   -0.424475    2.037953
 C    1.163914   -2.212421   -0.017843
 H    1.182807   -1.037223    1.803499
 C   -1.053318   -2.617793   -0.962635
 H   -2.754359   -1.978440    0.217944
 C   -3.111401    0.771042   -1.003407
 C   -1.274538    2.225714   -0.491870
 H    0.654163    3.278322   -0.123065
 C    2.751114    1.862275    1.044197
 C    3.070413    0.545207   -0.964069
 H   -0.491587    1.076221    2.316159
 H    0.172611   -0.080093    3.508450
 H   -1.351058    0.756753    3.841450
 H   -2.468792   -2.740209    2.978909
 H   -0.911344   -2.394400    3.777440
 H   -2.385148   -1.528187    4.284235
 C    0.376168   -2.701590   -1.071304
 H    2.252980   -2.217425   -0.103339
 H   -1.671010   -2.951596   -1.800343
 C   -3.954124    1.889778   -1.045832
 H   -3.542252   -0.215067   -1.207008
 C   -2.110655    3.345935   -0.529271
 C    4.126432    1.846258    1.265786
 H    2.078422    2.354856    1.752385
 C    4.442246    0.540563   -0.738088
 H    2.642937    0.041041   -1.836590
 C    0.988646   -3.231927   -2.323994
 C   -3.464253    3.172240   -0.800958
 H   -5.016452    1.751989   -1.266751
 H   -1.697186    4.343531   -0.353144
 C    4.973897    1.189500    0.376998
 H    4.534900    2.344938    2.147871
 H    5.102551    0.025762   -1.439901
 H    0.441421   -2.877281   -3.210583
 H    0.934194   -4.332984   -2.328867
 H    2.044128   -2.939966   -2.414329
 H   -4.136312    4.032623   -0.828212
 H    6.051466    1.175929    0.555831
*
```

INT(E-H)⁺S

```
CPCM (MeOH)
M06 SCF (DZ) =            -1155.116662
G (1 atm) =               -1154.714308
qh-G (1 mol/L) =          -1154.707077
qh-G (24.56 mol/L) =      -1154.704055
Lowest Frequency =           22.89

HF SCF energy (TZ) =      -1148.495249
HF SCF energy (QZ) =      -1148.562149
Correlation energy (DZ) =    -4.392199
Correlation energy (TZ) =    -5.351260
DLPNO-CCSD(T1)/CBS =      -1154.493980

*xyz 1 1
 Ru  -0.199110   -0.572104   -0.377054
 C   -1.691630    0.831683   -0.666527
 N    0.831159    1.264713   -0.124521
```

INT(E-H)⁺S

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1155.721179
G (1 atm) =               -1155.307423
qh G-E (1 mol/L) =            0.423922
qh G-E (24.56 mol/L) =        0.426944
Lowest Frequency =          13.73

HF SCF energy (TZ) =      -1148.497587
HF SCF energy (QZ) =      -1148.563088
Correlation energy (DZ) =    -4.392766
Correlation energy (TZ) =    -5.351862
DLPNO-CCSD(T1)/CBS =      -1154.495120

SMD (MeOH)
HF SCF energy (TZ) =      -1148.511656
HF SCF energy (QZ) =      -1148.577108
Correlation energy (DZ) =    -4.391094
```

```
 C   -3.022115    0.617856   -1.040237
 C   -1.273857    2.182032   -0.539074
 O    0.127768   -0.133420   -2.527954
 C    0.122763    2.344972   -0.234694
 C    2.204694    1.343082    0.222938
 C   -3.899617    1.692152   -1.225704
 H   -3.401056   -0.399020   -1.189454
 C   -2.147147    3.260631   -0.727486
 C    0.497588   -1.116129   -3.495847
 H   -0.640404    0.362688   -2.853356
 H    0.586390    3.335693   -0.120071
 C    2.611647    2.071512    1.343370
 C    3.145113    0.651519   -0.545717
 C   -3.472069    3.011262   -1.063264
 H   -4.939132    1.492716   -1.501969
 H   -1.779557    4.285275   -0.615654
 H    0.613563   -0.642609   -4.480803
 H   -0.250849   -1.922668   -3.557560
 H    1.465760   -1.528871   -3.184296
 C    3.962603    2.119729    1.681352
 H    1.861616    2.576802    1.959289
 C    4.491499    0.711039   -0.204978
 H    2.806592    0.080851   -1.415172
 H   -4.170519    3.838078   -1.209423
 C    4.903999    1.443887    0.909197
 H    4.277367    2.683864    2.562516
 H    5.226260    0.180131   -0.814885
 H    5.962021    1.480611    1.178820
 C    0.268188   -1.185244    1.627131
 C   -1.131187   -1.329724    1.428356
 C    1.222060   -1.896943    0.834320
 H    0.634538   -0.503917    2.399717
 C   -2.159116   -0.685813    2.325277
 C   -1.550740   -2.138677    0.325124
 C    0.807179   -2.676203   -0.248144
 H    2.289979   -1.755947    1.022754
 C   -1.674463    0.577294    3.017286
 C   -2.620814   -1.723253    3.347302
 H   -3.020190   -0.423194    1.682080
 C   -0.603291   -2.737513   -0.525202
 H   -2.615930   -2.224586    0.093193
 C    1.791531   -3.400831   -1.106273
 H   -1.291901    1.322774    2.300789
 H   -0.879230    0.358937    3.750409
 H   -2.504086    1.039304    3.574075
 H   -3.019428   -2.628416    2.861951
 H   -1.779384   -2.026747    3.994228
 H   -3.410203   -1.304970    3.991118
 H   -0.949078   -3.276513   -1.411740
 H    2.751749   -2.865722   -1.159604
 H    1.989794   -4.397157   -0.677860
 H    1.409005   -3.560349   -2.124471
*
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Correlation energy (TZ) =    -5.350415
DLPNO-CCSD(T1)/CBS =      -1154.507810

* xyz 1 1
 Ru  -0.214298   -0.550723   -0.333713
 C   -1.686474    0.875294   -0.593214
 N    0.870945    1.254252   -0.165179
 C   -3.042992    0.697830   -0.896858
 C   -1.226473    2.214696   -0.531276
 C    0.195682    2.348140   -0.281464
 C    2.266549    1.308491    0.125914
 C   -3.893740    1.793849   -1.081572
 C   -2.067393    3.317783   -0.719504
 C    2.722791    1.965943    1.269573
 C    3.166424    0.655840   -0.720801
 C   -3.415743    3.103575   -0.989099
 C    4.088608    1.981369    1.555999
 C    4.527415    0.681973   -0.431221
 C    4.992275    1.343460    0.708194
 C    0.168846   -1.125204    1.705810
 C   -1.202625   -1.349971    1.432843
 C    1.199181   -1.766216    0.945346
 C   -2.315248   -0.777064    2.287907
 C   -1.525274   -2.174860    0.306478
 C    0.889247   -2.573746   -0.152455
 C   -1.961197    0.542405    2.970479
 C   -2.737274   -1.843629    3.307184
 C   -0.501846   -2.719168   -0.490006
 C    1.963093   -3.259239   -0.948823
 H   -3.460870   -0.308493   -0.990750
 H    0.689888    3.325257   -0.208895
 H   -4.950335    1.620116   -1.302326
 H   -1.662924    4.331613   -0.658733
 H    2.006391    2.444345    1.941219
 H    2.793003    0.136243   -1.605027
 H   -4.091349    3.948271   -1.136758
 H    4.444042    2.490508    2.454285
 H    5.229653    0.179018   -1.099223
 H    6.059907    1.355830    0.936775
 H    0.457289   -0.443235    2.505589
 H    2.244058   -1.557168    1.182972
 H   -3.166335   -0.594928    1.611625
 H   -2.567666   -2.328931    0.024363
 H   -1.616919    1.292358    2.242297
 H   -1.177921    0.412354    3.733963
 H   -2.850090    0.944788    3.477975
 H   -3.038905   -2.778442    2.810636
 H   -1.908493   -2.074339    3.995979
 H   -3.589069   -1.485516    3.904256
 H   -0.773229   -3.270420   -1.392774
 H    2.888899   -2.667913   -0.957439
 H    2.185268   -4.234908   -0.489672
 H    1.643846   -3.444982   -1.982342
 O   -0.013427   -0.184825   -2.492987
 C    0.532887   -1.107157   -3.445646
 H   -0.855934    0.155156   -2.828680
 H    0.554289   -0.631720   -4.435282
 H   -0.058009   -2.034195   -3.484558
 H    1.557899   -1.329221   -3.127785
*
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INT(E-H)$^{+}$S•AcO^{-}

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1384.325990
G (1 atm) =               -1383.869000
```

```
qh G-E (1 mol/L) =            0.469330
qh G-E (24.56 mol/L) =        0.472353
Lowest Frequency =            5.78

HF SCF energy (TZ) =      -1375.932138
HF SCF energy (QZ) =      -1376.014485
Correlation energy (DZ) =    -5.097820
Correlation energy (TZ) =    -6.230096
DLPNO-CCSD(T1)/CBS =      -1382.931023

SMD (MeOH)
HF SCF energy (TZ) =      -1375.949709
HF SCF energy (QZ) =      -1376.031734
Correlation energy (DZ) =    -5.093271
Correlation energy (TZ) =    -6.226452
DLPNO-CCSD(T1)/CBS =      -1382.945060

* xyz 1 1
Ru   -0.060453    0.037421   -0.536202
 C    1.166746    0.704379    0.980860
 N   -1.272573   -0.231468    1.186093
 C    0.600778    0.644369    2.277660
 C    2.486312    1.172654    0.901054
 C   -2.612928   -0.716092    1.154503
 C   -0.748560    0.122158    2.314945
 C    1.295073    1.034051    3.432248
 C    3.186151    1.568071    2.043223
 C   -2.901716   -1.871166    0.421301
 C   -3.637976   -0.031213    1.813150
 C    2.597103    1.505262    3.311778
 C   -4.206060   -2.354649    0.376075
 C   -4.943737   -0.518656    1.756844
 C   -5.231513   -1.681027    1.042887
 C    0.354958    1.829928   -1.654057
 C    0.962930    0.739316   -2.338929
 C   -1.028574    1.828492   -1.336209
 C    0.184122   -0.386526   -2.719047
 C   -1.728121    2.973024   -0.626487
 C   -1.783343    0.680375   -1.733665
 C    0.837368   -1.562570   -3.386118
 C   -1.211427   -0.394707   -2.443165
 C   -0.845969    3.720257    0.372306
 C   -2.312839    3.924268   -1.678841
 H    2.992109    1.221912   -0.067646
 H   -1.303745    0.007317    3.254555
 H    0.813914    0.960710    4.411451
 H    4.213127    1.930594    1.944918
 H   -2.097757   -2.384508   -0.109896
 H   -3.415401    0.894416    2.348864
 H    3.157205    1.817170    4.195622
 H   -4.423305   -3.262889   -0.189875
 H   -5.742189    0.022549    2.268828
 H   -6.255205   -2.058081    0.996961
 H    0.987214    2.650815   -1.313402
 H    2.036696    0.743504   -2.526692
 H   -2.566237    2.521855   -0.067908
 H   -2.831017    0.613522   -1.428769
 H    1.845370   -1.726321   -2.983292
 H    0.915137   -1.363205   -4.466161
 H    0.241893   -2.474842   -3.248704
 H   -1.816420   -1.264544   -2.700824
 H   -0.413389    3.036789    1.117700
 H   -0.019123    4.249004   -0.128432
 H   -1.443237    4.475825    0.904050
 H   -2.977021    3.390608   -2.375678
 H   -1.506212    4.392308   -2.266856
```

```
 H   -2.893408    4.725620   -1.197554
 O    3.095263   -1.891741   -1.090239
 C    4.074184   -1.938485   -0.256492
 C    5.451676   -1.772049   -0.884288
 O    3.962934   -2.098502    0.966795
 H    5.534156   -0.766068   -1.324092
 H    5.584264   -2.495457   -1.702469
 H    6.244172   -1.906990   -0.137120
 O    0.802519   -1.907590   -0.182355
 C    0.742975   -2.614192    1.047068
 H    1.817601   -1.903429   -0.521749
 H   -0.304781   -2.846768    1.283666
 H    1.300287   -3.557862    0.947103
 H    1.183108   -2.038632    1.876528
*
```

INT(E-H)$^{+}$$S_2$•AcO^{-}

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1500.047477
G (1 atm) =               -1499.539171
qh G-E (1 mol/L) =            0.522798
qh G-E (24.56 mol/L) =        0.525821
Lowest Frequency =           14.84

SMD (MeOH)
HF SCF energy (TZ) =      -1491.047260
HF SCF energy (QZ) =      -1491.137490
Correlation energy (DZ) =    -5.473605
Correlation energy (TZ) =    -6.698064
DLPNO-CCSD(T1)/CBS =      -1498.578237

* xyz 1 1
Ru   0.043904    0.015449   -0.434335
 C    1.194027    0.806772    1.082062
 O   -0.522467   -3.891246   -0.506577
 C    2.527234    1.241558    1.038332
 C    0.562347    0.855419    2.349173
 O    0.886814   -1.907039    0.125524
 C   -0.992985   -4.358584   -1.611296
 H   -0.588452   -4.821790    0.917420
 C    3.176202    1.710506    2.183730
 H    3.084842    1.209658    0.098015
 C    1.204570    1.319403    3.505382
 C   -0.787860    0.332978    2.364001
 C    1.251149   -2.313586    1.442174
 H    0.317940   -2.659620   -0.261974
 C   -2.015520   -5.472521   -1.455002
 O   -0.693373   -3.940624   -2.738801
 O   -0.631516   -5.325439    1.763210
 C    2.521619    1.755683    3.420058
 H    4.215174    2.044409    2.113398
 H    0.672740    1.327091    4.460792
 N   -1.256062   -0.123691    1.248290
 H   -1.389714    0.300259    3.281463
 H    0.449802   -2.101820    2.167685
 H    1.442536   -3.396295    1.440826
 H    2.160460   -1.776489    1.741199
 H   -3.007456   -5.010061   -1.324567
 H   -1.807899   -6.076113   -0.561307
 H   -2.048981   -6.103514   -2.352331
 C   -1.655400   -4.736422    2.530393
 H    3.041545    2.123703    4.306753
 C   -2.599019   -0.603735    1.201679
 H   -1.439298   -3.682558    2.794358
 H   -1.757086   -5.302083    3.469751
```

```
 H   -2.636362   -4.754899    2.017822
 C   -3.648184    0.177381    1.694974
 C   -2.859706   -1.848945    0.624312
 C   -4.958442   -0.295442    1.618994
 H   -3.439675    1.163861    2.115710
 C   -4.170752   -2.314127    0.558811
 H   -2.035408   -2.457029    0.242824
 C   -5.223976   -1.540896    1.051743
 H   -5.775596    0.322206    1.997448
 H   -4.369101   -3.292242    0.114686
 H   -6.250630   -1.907359    0.987975
 C    0.201047    1.824541   -1.582216
 C    1.140369    0.888560   -2.114515
 C   -1.172157    1.495947   -1.465766
 H    0.564954    2.781235   -1.207185
 C    0.714364   -0.397550   -2.503292
 H    2.200710    1.141602   -2.149114
 C   -2.207089    2.464078   -0.924075
 C   -1.598037    0.208194   -1.943293
 C    1.697213   -1.434358   -2.967689
 C   -0.685539   -0.721167   -2.446204
 C   -1.671919    3.416871    0.143027
 C   -2.830304    3.227661   -2.099337
 H   -2.997331    1.847725   -0.463865
 H   -2.644747   -0.079969   -1.820400
 H    1.294772   -2.442132   -2.798389
 H    1.864693   -1.313099   -4.049428
 H    2.663070   -1.323897   -2.456716
 H   -0.999437   -1.734648   -2.708344
 H   -2.501053    4.002600    0.566725
 H   -0.943997    4.132413   -0.271301
 H   -1.184778    2.871600    0.965226
 H   -3.256048    2.538240   -2.844386
 H   -2.072198    3.848498   -2.604161
 H   -3.635539    3.889692   -1.747136
*
```

INT(E-H)⁺S•Cl⁻

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1616.120814
G (1 atm) =               -1615.625586
qh G-E (1 mol/L) =            0.423421
qh G-E (24.56 mol/L) =        0.426444
Lowest Frequency =           24.83

HF SCF energy (TZ) =      -1608.179957
HF SCF energy (QZ) =      -1608.249651
Correlation energy (DZ) =    -4.561596
Correlation energy (TZ) =    -5.594684
DLPNO-CCSD(T1)/CBS =      -1614.469005

SMD (MeOH)
HF SCF energy (TZ) =      -1608.187277
HF SCF energy (QZ) =      -1608.257154
Correlation energy (DZ) =    -4.560322
Correlation energy (TZ) =    -5.593704
DLPNO-CCSD(T1)/CBS =      -1614.475754

* xyz 1 1
 Ru  -0.593026   -0.373232    0.445289
 C   -0.660999    0.029958    2.552985
 C   -1.902343    1.169333    0.049244
 C    0.698033   -0.040580    2.160395
 C   -1.560085   -1.048580    2.284020
 N    0.554137    0.876712   -0.841448
```

C	-1.373969	2.202594	-0.764880
C	-3.238822	1.317781	0.447542
C	1.690328	1.076418	2.422768
C	1.159097	-1.252702	1.537345
C	-1.113892	-2.190836	1.590174
C	1.889362	0.603236	-1.263257
C	-0.020999	1.969989	-1.224647
C	-2.116238	3.328940	-1.145933
C	-3.986465	2.440048	0.078338
C	1.058443	2.465207	2.492380
C	2.473407	0.751441	3.700935
C	0.281147	-2.297821	1.251524
C	-2.065749	-3.285012	1.198724
C	2.194705	-0.661141	-1.774568
C	2.890135	1.571418	-1.138741
C	-3.431819	3.451642	-0.713507
C	3.497167	-0.945859	-2.175495
C	4.193474	1.274192	-1.536773
C	4.501136	0.017406	-2.055853
H	-1.050251	0.940521	3.007724
H	-2.615582	-0.952302	2.540940
H	-3.720603	0.546520	1.054906
H	2.400508	1.063912	1.579254
H	2.194659	-1.312503	1.194834
H	0.492409	2.668013	-1.898177
H	-1.662849	4.094876	-1.781157
H	-5.023543	2.527619	0.413959
H	0.454365	2.684002	1.598565
H	0.412426	2.574130	3.378032
H	1.847182	3.228273	2.566748
H	2.968433	-0.229096	3.630373
H	1.801960	0.732548	4.574787
H	3.248494	1.511603	3.880241
H	0.624977	-3.156402	0.672064
H	-1.801563	-3.695282	0.214224
H	-2.004054	-4.101883	1.934130
H	-3.100593	-2.918863	1.172105
H	1.413559	-1.420760	-1.861360
H	2.653805	2.546494	-0.706290
H	-4.028587	4.321676	-0.994543
H	3.727853	-1.933669	-2.580451
H	4.973782	2.030226	-1.426468
H	5.524110	-0.215499	-2.358607
O	-1.403673	-1.332023	-1.336945
C	-1.686437	-0.707088	-2.589870
H	-0.898541	-2.173581	-1.537338
H	-2.107549	-1.457253	-3.274395
H	-0.778087	-0.275162	-3.039458
H	-2.424555	0.085714	-2.419268
Cl	0.040702	-3.801761	-2.091638

*

INT(E-H)$^{+}$$S_2$•Cl^{-}

CPCM (MeOH)
wB97X-D3 SCF (DZ) = -1731.834033
G (1 atm) = -1731.373757
qh G-E (1 mol/L) = 0.473207
qh G-E (24.56 mol/L) = 0.476230
Lowest Frequency = 21.93

SMD (MeOH)
HF SCF energy (TZ) = -1723.285279
HF SCF energy (QZ) = -1723.363444
Correlation energy (DZ) = -4.939919
Correlation energy (TZ) = -6.065104

```
DLPNO-CCSD(T1)/CBS =      -1730.109586

* xyz 1 1
 Ru  -1.108969   -0.181478    0.422223
 C   -0.853739    0.100195    2.534195
 C   -2.003356    1.668994    0.261475
 C    0.398858   -0.270160    1.985621
 C   -2.011843   -0.713607    2.338447
 H   -0.958393    1.049501    3.059532
 O   -2.360668   -0.768017   -1.270580
 Cl  -1.745600   -3.388218   -2.557750
 C   -1.327669    2.586491   -0.580726
 C   -3.191898    2.127290    0.848618
 C    1.658480    0.552704    2.177446
 C    0.481539   -1.521184    1.282247
 C   -1.930208   -1.889116    1.565564
 H   -2.978433   -0.381613    2.718839
 C   -2.682320    0.024343   -2.416134
 H   -2.115835   -1.672407   -1.606790
 H   -0.663097   -4.641133   -1.213603
 C   -1.785559    3.890806   -0.812295
 C   -0.152507    2.045485   -1.230076
 C   -3.655503    3.427822    0.628365
 H   -3.780481    1.466477    1.490993
 C    1.413587    2.057071    2.275872
 C    2.405123    0.026129    3.409842
 H    2.289618    0.364808    1.292466
 C   -0.647412   -2.312711    1.071552
 H    1.432374   -1.813254    0.830058
 C   -3.155366   -2.700519    1.256417
 H   -1.777844    0.298328   -2.982040
 H   -3.357759   -0.551292   -3.064538
 H   -3.189948    0.932494   -2.070954
 O   -0.105924   -5.125685   -0.570059
 C   -2.956644    4.316688   -0.195800
 H   -1.225286    4.557507   -1.473473
 N    0.157795    0.818577   -0.963792
 H    0.440827    2.632771   -1.942519
 H   -4.581716    3.756129    1.108176
 H    0.848386    2.435126    1.411193
 H    0.859723    2.323297    3.190063
 H    2.376689    2.587319    2.310736
 H    2.623215   -1.048858    3.318462
 H    1.802919    0.175434    4.320848
 H    3.359372    0.558831    3.538095
 H   -0.566304   -3.228029    0.479540
 H   -3.079704   -3.159496    0.260961
 H   -3.254139   -3.509832    1.996167
 H   -4.061761   -2.081986    1.298167
 C    1.238393   -4.914631   -0.951091
 H   -3.331815    5.329314   -0.356492
 C    1.313184    0.245668   -1.573555
 H    1.429865   -5.215235   -1.997295
 H    1.549341   -3.858459   -0.838049
 H    1.878140   -5.527287   -0.298412
 C    1.210543   -1.008953   -2.179964
 C    2.539098    0.917302   -1.548334
 C    2.330127   -1.575010   -2.783992
 H    0.253471   -1.536502   -2.187264
 C    3.656803    0.337797   -2.148485
 H    2.620404    1.881563   -1.040994
 C    3.555677   -0.905915   -2.770586
 H    2.241905   -2.551211   -3.265810
 H    4.613947    0.862850   -2.120664
 H    4.432572   -1.358039   -3.238584
*
```

INT(F^C-F^S)

CPCM (MeOH)
M06 SCF (DZ) = -1612.648340
G (1 atm) = -1612.143949
qh-G (1 mol/L) = -1612.135022
qh-G (24.56 mol/L) = -1612.132
Lowest Frequency = 25.14

HF SCF energy (TZ) = -1603.882585
HF SCF energy (QZ) = -1603.980815
Correlation energy (DZ) = -5.732106
Correlation energy (TZ) = -7.031404
DLPNO-CCSD(T1)/CBS = -1611.801043

*xyz 0 1

Ru	-0.309845	0.004325	-0.303596
C	-1.466600	-1.637126	-1.474793
C	-2.425210	-0.660038	-1.152656
C	-1.443252	-2.884992	-0.778142
H	-0.890821	-1.553330	-2.400577
N	1.302409	1.044049	0.529592
O	-0.466934	1.277255	-2.031384
O	-1.560182	0.777659	1.258657
O	1.191152	-0.919978	-1.492212
O	-0.423944	-1.040882	1.565846
C	-3.411651	-0.913592	-0.149875
H	-2.588762	0.179677	-1.834767
C	-0.409327	-3.898643	-1.149497
C	-2.380083	-3.093307	0.206758
C	1.179635	2.477824	0.515785
C	2.465476	0.637106	0.937436
C	-1.136149	2.522906	-1.955169
H	0.487444	1.343845	-2.352449
C	-1.226468	-0.173761	2.030369
C	2.044469	-0.338021	-2.243901
C	-4.489715	0.122476	0.062539
C	-3.361632	-2.117385	0.515611
H	0.598333	-3.448923	-1.112883
H	-0.551407	-4.253653	-2.185306
H	-0.434871	-4.775079	-0.484535
H	-2.377793	-4.039377	0.758776
C	0.383696	3.129346	1.458345
C	1.888287	3.210736	-0.438790
C	3.058467	-0.692262	1.048459
H	3.165243	1.434344	1.238708
H	-0.674587	3.201161	-1.218721
H	-1.144530	3.007930	-2.944435
H	-2.177082	2.331829	-1.650631
C	-1.738819	-0.274855	3.425742
C	3.237970	-1.182106	-2.610897
O	1.975577	0.843047	-2.655398
C	-5.551655	-0.001500	-1.029853
C	-5.138265	0.071898	1.435688
H	-3.999572	1.109519	-0.049024
H	-4.099774	-2.346618	1.290747
C	0.292839	4.518487	1.435216
H	-0.158153	2.541715	2.200870
C	1.786705	4.600117	-0.455318
H	2.487630	2.671552	-1.177964
C	2.404933	-1.926498	0.884500
C	4.435441	-0.696024	1.340656
H	-2.338443	0.605574	3.690332
H	-0.897676	-0.378397	4.126741
H	-2.356884	-1.181545	3.520768

```
 H    2.949236   -2.234260   -2.746459
 H    3.955550   -1.146492   -1.772548
 H    3.734794   -0.797751   -3.511303
 H   -6.312877    0.790561   -0.934005
 H   -6.064006   -0.976979   -0.953223
 H   -5.113974    0.068310   -2.038953
 H   -5.847270    0.906561    1.556336
 H   -4.391140    0.138532    2.242567
 H   -5.711701   -0.860782    1.577845
 C    0.988003    5.257631    0.478207
 H   -0.325095    5.028701    2.178514
 H    2.337526    5.171764   -1.206686
 C    3.119292   -3.112131    0.996425
 H    1.338695   -1.951584    0.672263
 C    5.149027   -1.884377    1.437398
 H    4.953100    0.257641    1.482473
 H    0.909969    6.347488    0.463988
 C    4.489603   -3.098803    1.262519
 H    2.598469   -4.065143    0.870597
 H    6.219483   -1.861979    1.653845
 H    5.041838   -4.038890    1.339515
*
```

***cis*-INT(F^A-G^A)**

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CPCM (MeOH)
M06 SCF (DZ) =            -1664.123868
G (1 atm) =               -1663.681644
qh-G (1 mol/L) =          -1663.671473
qh-G (24.56 mol/L) =      -1663.674492
Lowest Frequency =           24.41

HF SCF energy (TZ) =      -1655.132652
HF SCF energy (QZ) =      -1655.233360
Correlation energy (DZ) =    -5.855073
Correlation energy (TZ) =    -7.168243
DLPNO-CCSD(T1)/CBS =      -1663.199280

*xyz 0 1
 Ru   0.879866   -0.193903    0.073848
 C    2.637884    1.020318   -0.610985
 N   -0.901343   -0.911920    0.916391
 C    3.908317    1.138536   -0.035562
 C    2.109694    2.110926   -1.344396
 H    2.387450   -0.082476   -0.897484
 O    2.881383   -2.096404   -1.410944
 N    0.006508    1.038548   -1.348278
 O    2.040135   -1.049999    1.702062
 O    0.669753   -1.723892   -1.313902
 O    1.226546    0.956450    1.892285
 C   -1.041715   -2.345158    0.842780
 C   -1.943768   -0.311770    1.405939
 C    4.626516    2.323882   -0.160669
 H    4.331881    0.285190    0.502666
 C    2.853974    3.288294   -1.488286
 C    0.757306    1.994137   -1.821530
 C    1.712660   -2.414173   -1.648691
 C   -1.351977    0.982920   -1.780956
 C    1.915036    0.011190    2.386543
 C   -0.095746   -3.184312    1.433800
 C   -2.128622   -2.896167    0.158876
 C   -2.285496    1.099807    1.534310
 H   -2.749641   -0.972425    1.763372
 C    4.105839    3.395025   -0.894640
 H    5.612833    2.412048    0.301929
 H    2.428885    4.127914   -2.046014
```

***cis*-INT(F^A-G^A)**

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1664.894786
G (1 atm) =               -1664.437372
qh G-E (1 mol/L) =            0.471867
qh G-E (24.56 mol/L) =        0.474890
Lowest Frequency =          15.2

HF SCF energy (TZ) =      -1655.145402
HF SCF energy (QZ) =      -1655.244498
Correlation energy (DZ) =    -5.845770
Correlation energy (TZ) =    -7.157849
DLPNO-CCSD(T1)/CBS =      -1663.198900

SMD (MeOH)
HF SCF energy (TZ) =      -1655.162717
HF SCF energy (QZ) =      -1655.261557
Correlation energy (DZ) =    -5.839507
Correlation energy (TZ) =    -7.153033
DLPNO-CCSD(T1)/CBS =      -1663.211912

*xyz 0 1
 Ru   0.869914   -0.209662    0.146406
 C    2.664302    1.009627   -0.647780
 N   -0.908215   -0.939893    1.018631
 C    3.962737    1.104594   -0.144200
 C    2.075283    2.125462   -1.272906
 O    2.786359   -1.985633   -1.663909
 N   -0.050607    1.077142   -1.224122
 O    0.599754   -1.736267   -1.237430
 C   -1.026403   -2.382185    0.994973
 C   -1.980013   -0.349278    1.430691
 C    4.661600    2.307044   -0.241423
 C    2.790785    3.322304   -1.387587
 C    0.689125    2.023754   -1.702438
 C    1.604494   -2.336389   -1.780908
 C   -1.409902    1.020503   -1.678324
 C   -0.137036   -3.176373    1.718107
 C   -2.035897   -2.976694    0.234345
 C   -2.320800    1.079630    1.489946
 C    4.079699    3.412033   -0.869005
 C    1.218965   -3.546759   -2.608127
```

```
 H    0.361382    2.706377   -2.557788
 C    1.368077   -3.695584   -2.367500
 C   -1.919390   -0.250414   -2.109160
 C   -2.127678    2.146204   -1.843973
 C    2.593379    0.165315    3.704569
 C   -0.249656   -4.564675    1.347103
 H    0.754709   -2.743714    1.955789
 C   -2.268704   -4.279032    0.067550
 H   -2.854303   -2.234420   -0.322267
 C   -1.434079    2.196875    1.320761
 C   -3.625579    1.350045    1.886099
 H    4.682435    4.316908   -0.998829
 H    0.690627   -3.494340   -3.210722
 H    0.827255   -4.358508   -1.671570
 H    2.272676   -4.202890   -2.726465
 C   -3.255149   -0.312036   -2.497347
 H   -1.293265   -1.144809   -2.058341
 C   -3.463636    2.073079   -2.226030
 H   -1.692687    3.106464   -1.554395
 H    2.696767   -0.805503    4.206087
 H    3.604344    0.568975    3.532703
 H    2.048812    0.873818    4.341702
 C   -1.331147   -5.119300    0.662341
 H    0.488033   -5.215956    1.823188
 H   -3.118021   -4.698743   -0.477481
 C   -1.916650    3.492387    1.454844
 H   -0.390621    2.031449    1.060228
 C   -4.109743    2.647029    1.997264
 H   -4.297808    0.504707    2.061781
 C   -4.033787    0.843391   -2.550365
 H   -3.692903   -1.279179   -2.760385
 H   -4.065612    2.984903   -2.255343
 H   -1.440907   -6.204295    0.592323
 C   -3.252633    3.724608    1.782351
 H   -1.240580    4.335594    1.291793
 H   -5.156539    2.817408    2.258744
 H   -5.084856    0.785465   -2.843472
 H   -3.624313    4.748082    1.875877
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 C   -1.943920   -0.210953   -2.061918
 C   -2.194591    2.175890   -1.731483
 C   -0.259429   -4.563948    1.672858
 C   -2.148227   -4.365189    0.188952
 C   -1.408051    2.138446    1.592804
 C   -3.695544    1.362795    1.439848
 C   -3.261126   -0.278948   -2.511343
 C   -3.512348    2.096961   -2.176208
 C   -1.259541   -5.164722    0.906635
 C   -1.869218    3.451308    1.617041
 C   -4.150449    2.677600    1.440878
 C   -4.049845    0.871325   -2.568871
 C   -3.235089    3.726167    1.527526
 H    2.345964   -0.073139   -0.889946
 H    4.425844    0.230582    0.318350
 H   -2.806769   -1.002274    1.742550
 H    5.673970    2.380520    0.161489
 H    2.324646    4.187544   -1.864876
 H    0.284431    2.747929   -2.419130
 H    0.654723   -2.702139    2.295978
 H   -2.720508   -2.350762   -0.341042
 H    4.634998    4.348396   -0.951131
 H    0.592994   -3.229434   -3.455417
 H    0.616509   -4.233820   -1.995954
 H    2.109959   -4.062711   -2.984917
 H   -1.308684   -1.096445   -2.003344
 H   -1.787814    3.128409   -1.386661
 H    0.436102   -5.181385    2.245702
 H   -2.934508   -4.821320   -0.416589
 H   -0.344486    1.930388    1.682483
 H   -4.411591    0.539254    1.376500
 H   -3.673596   -1.242439   -2.819416
 H   -4.125644    3.000276   -2.198792
 H   -1.345197   -6.252747    0.868167
 H   -1.152304    4.270336    1.705705
 H   -5.220856    2.883466    1.379788
 H   -5.084920    0.811565   -2.911982
 H   -3.587123    4.760174    1.536724
 O    2.079484   -1.113957    1.700953
 O    1.364537    0.923098    1.953066
 C    2.041434   -0.054671    2.399645
 C    2.801023    0.055517    3.685013
 H    2.946643   -0.934584    4.133067
 H    3.788479    0.490073    3.465757
 H    2.277903    0.722880    4.380727
*
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INT(F^A-G^A)
CPCM (MeOH)
M06 SCF (DZ) = -1664.124111
G (1 atm) = -1663.682060
qh-G (1 mol/L) = -1663.671801
qh-G (24.56 mol/L) = -1663.668778
Lowest Frequency = 18.33

HF SCF energy (TZ) = -1655.137733
HF SCF energy (QZ) = -1655.236656
Correlation energy (DZ) = -5.850985
Correlation energy (TZ) = -7.162890
DLPNO-CCSD(T1)/CBS = -1663.198312

```
*xyz 0 1
 Ru   0.020864   -0.363201   -0.055101
 C    1.658038   -1.518198    0.971207
 N    0.983625    1.458014   -0.600348
```

INT(F^A-G^A)
CPCM (MeOH)
wB97X-D3 SCF (DZ) = -1664.893235
G (1 atm) = -1664.436715
qh G-E (1 mol/L) = 0.472679
qh G-E (24.56 mol/L) = 0.475702
Lowest Frequency = 18.06

HF SCF energy (TZ) = -1655.144534
HF SCF energy (QZ) = -1655.243716
Correlation energy (DZ) = -5.845045
Correlation energy (TZ) = -7.156377
DLPNO-CCSD(T1)/CBS = -1663.196236

SMD (MeOH)
HF SCF energy (TZ) = -1655.162420
HF SCF energy (QZ) = -1655.261377
Correlation energy (DZ) = -5.838553

```
C    3.044272   -1.316213    1.023700
C    1.172251   -2.846292    1.127103
H    1.080755   -0.586042    1.385602
N   -0.956429   -2.084162    0.510140
O    1.007277    1.127865    2.604634
O   -1.296983   -0.116608   -1.729876
O   -0.881210    0.723735    1.458943
O    0.465470   -1.372018   -1.915682
C    2.401579    1.360875   -0.790465
C    0.546350    2.679511   -0.628510
C    3.916794   -2.389951    1.171092
H    3.439293   -0.299839    0.963961
C    2.059657   -3.915149    1.304491
C   -0.240592   -3.061569    0.979806
C   -2.347609   -2.267319    0.284751
C   -0.195809    1.304532    2.392060
C   -0.596005   -0.910871   -2.435589
C    3.264216    2.033351    0.079653
C    2.917999    0.591871   -1.834124
C   -0.778841    3.252553   -0.405132
H    1.304774    3.454234   -0.830396
C    3.430031   -3.692081    1.318512
H    4.994344   -2.205547    1.194003
H    1.658289   -4.927940    1.404554
H   -0.698030   -4.023882    1.249377
C   -3.233781   -1.258800    0.677770
C   -2.825309   -3.411934   -0.359257
C   -1.005832    2.280378    3.209806
C   -1.036272   -1.307594   -3.801021
C    4.642730    1.936497   -0.098162
H    2.841138    2.592033    0.919232
C    4.296085    0.506472   -2.007846
H    2.230326    0.058101   -2.492728
C   -0.790537    4.642986   -0.188760
C   -2.003139    2.563426   -0.396709
H    4.121603   -4.527814    1.445982
C   -4.596447   -1.419202    0.454592
H   -2.828987   -0.362856    1.157091
C   -4.192693   -3.557430   -0.585553
H   -2.121838   -4.174480   -0.705620
H   -0.485484    2.538508    4.141361
H   -1.143880    3.199602    2.614767
H   -2.007260    1.882616    3.428191
H   -0.187997   -1.669395   -4.395284
H   -1.531571   -0.467556   -4.305425
H   -1.771034   -2.123417   -3.709244
C    5.162876    1.174089   -1.142091
H    5.313273    2.455349    0.591565
H    4.697758   -0.090236   -2.830834
C   -1.975636    5.321627    0.069850
H    0.154139    5.194936   -0.213298
C   -3.187390    3.247784   -0.156898
H   -2.027457    1.496146   -0.597078
C   -5.081361   -2.566578   -0.175542
H   -5.289523   -0.635973    0.772890
H   -4.562051   -4.450517   -1.095715
H    6.244075    1.097668   -1.280745
C   -3.180180    4.621967    0.088440
H   -1.959147    6.399194    0.248526
H   -4.132632    2.698360   -0.160139
H   -6.152800   -2.682511   -0.356123
H   -4.117534    5.148920    0.284224
*
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```

```
Correlation energy (TZ) =    -7.151271
DLPNO-CCSD(T1)/CBS =      -1663.209533

*xyz 0 1
Ru  -0.307094   -0.045253   -0.059354
 C    0.935008   -1.293851    1.356966
 N    1.197896    1.401781   -0.662601
 C    0.205028   -2.492309    1.529721
 C    2.295505   -1.282620    1.680440
 H    0.447348   -0.239797    1.528013
 N   -1.685038   -1.446943    0.584634
 O   -1.412436    0.311691   -1.842609
 O   -0.059568   -1.385167   -1.778556
 O   -1.184706    1.440617    1.080574
 C    0.703462    2.757151   -0.582825
 C    2.459430    1.348849   -0.925902
 C    0.849569   -3.662436    1.946647
 C   -1.212107   -2.473086    1.210139
 C    2.934678   -2.453100    2.083040
 H    2.853401   -0.346751    1.624929
 C   -3.075003   -1.422461    0.254778
 C   -0.931414   -0.717142   -2.415221
 C   -0.765628    1.813052    2.242856
 C   -0.253709    3.200791   -1.494795
 C    1.181659    3.611971    0.411057
 C    3.350174    0.184282   -1.049440
 H    2.980507    2.309756   -1.047130
 C    2.216001   -3.645110    2.210828
 H    0.274937   -4.585583    2.053743
 H   -1.861814   -3.306044    1.505413
 H    4.002116   -2.432401    2.313648
 C   -3.662262   -2.493872   -0.421400
 C   -3.831448   -0.299806    0.600433
 C   -1.413160   -1.147641   -3.763746
 C   -1.574947    2.931248    2.865423
 O    0.198571    1.313366    2.838201
 C   -0.729780    4.507210   -1.408548
 H   -0.628964    2.511717   -2.251683
 C    0.693423    4.915620    0.495745
 H    1.912327    3.243561    1.134320
 C    2.952803   -1.086727   -1.480441
 C    4.697485    0.410319   -0.723611
 H    2.721137   -4.557907    2.532479
 C   -5.022298   -2.450198   -0.729700
 H   -3.051604   -3.349762   -0.717910
 C   -5.189213   -0.270268    0.295245
 H   -3.336115    0.535265    1.098466
 H   -2.244626   -1.854417   -3.618016
 H   -1.782623   -0.286527   -4.333057
 H   -0.612641   -1.661282   -4.309501
 H   -2.529808    2.521705    3.230344
 H   -1.803765    3.699340    2.114235
 H   -1.034554    3.375668    3.709914
 C   -0.262428    5.367830   -0.413194
 H   -1.475736    4.855062   -2.126596
 H    1.061398    5.578349    1.282130
 C    3.885760   -2.117252   -1.555453
 H    1.915724   -1.266068   -1.758416
 C    5.621629   -0.629056   -0.775384
 H    5.017235    1.408017   -0.411362
 C   -5.789075   -1.343654   -0.367826
 H   -5.481373   -3.287860   -1.258952
 H   -5.784905    0.601215    0.575655
 H   -0.646158    6.388039   -0.345704
 C    5.215018   -1.897433   -1.192301
 H    3.568823   -3.105669   -1.895009
```

INT(F^c-G^c)
CPCM (MeOH)
M06 SCF (DZ) = -1496.958421
G (1 atm) = -1496.506496
qh-G (1 mol/L) = -1496.497529
qh-G (24.56 mol/L) = -1496.494506
Lowest Frequency = 31.50

HF SCF energy (TZ) = -1488.759910
HF SCF energy (QZ) = -1488.850373
Correlation energy (DZ) = -5.365641
Correlation energy (TZ) = -6.572188
DLPNO-CCSD(T1)/CBS = -1496.154849

*xyz 0 1

Ru	0.122840	-0.268941	-0.266967
C	1.361550	-2.094826	-0.234639
C	-2.151897	-0.495174	-1.258643
C	1.134160	-3.392397	-0.723261
C	2.718081	-1.680253	-0.098469
H	0.588097	-1.763373	0.605667
C	-1.828581	-1.784204	-0.813544
N	1.919079	0.476296	0.348463
O	-0.707348	0.048103	1.585369
O	0.749838	0.087096	-2.299199
O	-0.244867	1.644688	-1.152305
C	-3.099579	0.301255	-0.567622
H	-1.826241	-0.178130	-2.253800
C	2.192092	-4.210638	-1.105769
H	0.117170	-3.784186	-0.781800
C	3.776524	-2.522319	-0.459575
C	2.942186	-0.326515	0.311454
O	0.157370	-1.770823	2.580072
C	-2.450608	-2.327378	0.341641
H	-1.254871	-2.438978	-1.474888
C	2.123980	1.852250	0.653800
C	-0.512268	-0.732089	2.598037
C	0.334159	1.286763	-2.227520
C	-3.466715	1.674279	-1.081637
C	-3.695338	-0.244140	0.554186
C	3.517247	-3.785335	-0.971826
H	1.979899	-5.210294	-1.493566
H	4.803723	-2.160871	-0.355442
H	3.945428	0.033181	0.576561
C	-2.102811	-3.699444	0.824735
C	-3.376093	-1.539211	0.999972
C	1.308748	2.478521	1.599831
C	3.112186	2.577807	-0.016632
C	-1.168409	-0.242599	3.865241
C	0.494726	2.243849	-3.355681
C	-4.898068	1.697545	-1.609733
C	-3.260500	2.750231	-0.021226
H	-2.782084	1.895209	-1.921192
H	-4.445793	0.331686	1.106536
H	4.339131	-4.442298	-1.263694
H	-2.865207	-4.086714	1.516964
H	-2.003477	-4.415727	-0.007710
H	-1.141821	-3.682695	1.369381
H	-3.882705	-1.939478	1.884961
C	1.512784	3.821399	1.896282
H	6.662912	-0.445569	-0.502965
H	-6.853621	-1.312575	-0.609266
H	5.939077	-2.713675	-1.245469

*

INT(F^c-G^c)
CPCM (MeOH)
wB97X-D3 SCF (DZ) = -1497.662320
G (1 atm) = -1497.198606
qh G-E (1 mol/L) = 0.479048
qh G-E (24.56 mol/L) = 0.482071
Lowest Frequency = 4.65

HF SCF energy (TZ) = -1488.773378
HF SCF energy (QZ) = -1488.862386
Correlation energy (DZ) = -5.354198
Correlation energy (TZ) = -6.560526
DLPNO-CCSD(T1)/CBS = -1496.154632

SMD (MeOH)
HF SCF energy (TZ) = -1488.791731
HF SCF energy (QZ) = -1488.880537
Correlation energy (DZ) = -5.347405
Correlation energy (TZ) = -6.555210
DLPNO-CCSD(T1)/CBS = -1496.168270

* xyz 0 1

Ru	0.181081	-0.244803	-0.279117
C	1.419321	-2.117341	-0.173804
C	1.192287	-3.406341	-0.669392
C	2.760612	-1.685227	-0.031544
N	1.968794	0.494934	0.324494
O	-0.648775	0.109234	1.567706
C	2.259322	-4.221035	-1.045397
C	3.828145	-2.516282	-0.386860
C	2.980518	-0.308129	0.358292
O	-0.031232	-1.822610	2.526060
C	2.177721	1.885656	0.595809
C	-0.599542	-0.722148	2.554315
C	3.578495	-3.785080	-0.898925
C	1.372770	2.534217	1.534364
C	3.155276	2.589340	-0.110169
C	-1.284662	-0.230032	3.811817
C	1.571811	3.889559	1.782364
C	3.342337	3.948491	0.141796
C	2.555303	4.600029	1.089785
H	0.594137	-1.740152	0.584582
H	0.176813	-3.791718	-0.749199
H	2.057328	-5.219186	-1.439974
H	4.852036	-2.149990	-0.280613
H	3.975247	0.051260	0.645539
H	4.407799	-4.434677	-1.184433
H	0.593854	1.966927	2.045395
H	3.749805	2.077980	-0.870331
H	-2.251556	0.229750	3.566958
H	-0.656307	0.543636	4.280059
H	-1.424083	-1.052523	4.523638
H	0.948302	4.397843	2.521029
H	4.104261	4.498821	-0.414167
H	2.701634	5.664592	1.284113
C	-2.223152	-0.484640	-1.242347
C	-1.911028	-1.795224	-0.865856
C	-3.116417	0.302784	-0.479428
C	-2.497403	-2.375931	0.284721

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 H    0.519396    1.896291    2.081028
 C    3.302322    3.925147    0.282605
 H    3.713942    2.088822   -0.788244
 H   -2.187943    0.116341    3.662578
 H   -0.595008    0.612332    4.259853
 H   -1.185296   -1.033336    4.626187
 H    1.138602    1.826068   -4.138868
 H    0.912929    3.189968   -2.982671
 H   -0.495996    2.468312   -3.781354
 H   -5.145850    2.685977   -2.030831
 H   -5.618693    1.490001   -0.799334
 H   -5.052754    0.941507   -2.396628
 H   -3.477052    3.749029   -0.435253
 H   -3.936341    2.598805    0.838408
 H   -2.224163    2.749340    0.352752
 C    2.508537    4.548343    1.242446
 H    0.883013    4.308280    2.645077
 H    4.072770    4.491150   -0.246675
 H    2.658261    5.605393    1.475092
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 C   -3.440105    1.725705   -0.898072
 C   -3.691250   -0.281968    0.638300
 C   -2.156952   -3.777618    0.712171
 C   -3.387531   -1.600558    1.012077
 C   -4.884022    1.846243   -1.397817
 C   -3.155042    2.723928    0.229801
 H   -1.880557   -0.111147   -2.209676
 H   -1.322456   -2.415356   -1.545478
 H   -2.765375    1.968976   -1.734343
 H   -4.398687    0.287006    1.247987
 H   -2.964193   -4.214814    1.316356
 H   -1.977772   -4.435078   -0.151346
 H   -1.245381   -3.766849    1.331130
 H   -3.868157   -2.027518    1.896990
 H   -5.090553    2.870735   -1.745612
 H   -5.602529    1.612444   -0.594926
 H   -5.076257    1.155994   -2.233693
 H   -3.328374    3.755474   -0.114830
 H   -3.813034    2.548258    1.096360
 H   -2.112428    2.645522    0.571589
 O    0.779769    0.058136   -2.323360
 O   -0.206312    1.638364   -1.205147
 C    0.358277    1.257810   -2.280308
 C    0.501466    2.189985   -3.440325
 H    1.157336    1.760928   -4.205922
 H    0.901697    3.150251   -3.088144
 H   -0.493739    2.375273   -3.870803
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INT(F^S-G^S)

```
CPCM (MeOH)
M06 SCF (DZ) =            -1223.433812
G (1 atm) =               -1223.134402
qh-G (1 mol/L) =          -1223.125622
qh-G (24.56 mol/L) =      -1223.1226
Lowest Frequency =           34.18

HF SCF energy (TZ) =      -1216.920976
HF SCF energy (QZ) =      -1216.997087
Correlation energy (DZ) =    -4.199038
Correlation energy (TZ) =    -5.202047
DLPNO-CCSD(T1)/CBS =      -1222.808160

*xyz 0 1
 Ru   0.392722    0.401068    0.359973
 C    1.880456   -0.906460   -0.429471
 O    1.774462    1.671640    1.491838
 C    3.252256   -0.981231   -0.127154
 C    1.239804   -2.072834   -0.942413
 H    1.595738    0.161166   -0.898515
 O    1.969953    1.818474   -2.029602
 N   -0.765838   -0.896328   -0.675632
 O    0.071396    2.029376   -0.849731
 O   -1.094295    0.845711    1.833055
 O    0.227666   -0.864686    2.089390
 C    1.324267    2.952416    1.945865
 H    2.118703    1.171048    2.247495
 C    3.944916   -2.174000   -0.292931
 H    3.771674   -0.086324    0.229152
 C    1.959127   -3.260591   -1.130687
 C   -0.176217   -1.970299   -1.131882
 C    0.937406    2.423444   -1.733061
 C   -2.178984   -0.773143   -0.767648
 C   -0.752352   -0.172256    2.515118
 H    2.158768    3.502462    2.404141
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```
 H    0.494324    2.850656    2.661678
 H    0.969280    3.490943    1.058183
 C    3.306527   -3.313284   -0.803835
 H    5.007514   -2.219360   -0.039193
 H    1.441848   -4.146826   -1.510551
 H   -0.752835   -2.755352   -1.638257
 C    0.572950    3.734058   -2.384099
 C   -2.727360    0.443089   -1.185075
 C   -3.013264   -1.836615   -0.411320
 C   -1.496912   -0.560668    3.743415
 H    3.868966   -4.239496   -0.940771
 H   -0.455660    3.697551   -2.772144
 H    0.602994    4.537260   -1.630903
 H    1.271562    3.973289   -3.195470
 C   -4.108078    0.575124   -1.280698
 H   -2.050897    1.267373   -1.426911
 C   -4.395648   -1.689847   -0.502535
 H   -2.577272   -2.768826   -0.041373
 H   -2.344320   -1.201147    3.450936
 H   -1.902355    0.326770    4.246128
 H   -0.853942   -1.132819    4.424088
 C   -4.946195   -0.488583   -0.942717
 H   -4.536323    1.521753   -1.619771
 H   -5.045489   -2.520994   -0.217710
 H   -6.030808   -0.375880   -1.012438
*
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INT(F^{2S}-G^{2S})

```
CPCM (MeOH)
M06 SCF (DZ) =            -1339.115506
G (1 atm) =               -1338.763323
qh-G (1 mol/L) =          -1338.754905
qh-G (24.56 mol/L) =      -1338.751882
Lowest Frequency =           31.25

HF SCF energy (TZ) =      -1332.020789
HF SCF energy (QZ) =      -1332.105141
Correlation energy (DZ) =    -4.582412
Correlation energy (TZ) =    -5.678758
DLPNO-CCSD(T1)/CBS =      -1338.449949

*xyz 0 1
 Ru  -0.361498    0.376705    0.066359
 C   -1.569016   -1.413823    0.390610
 O    0.713976    2.014667   -0.858741
 C   -0.926865   -2.520834   -0.226201
 C   -2.928961   -1.514267    0.709191
 H   -0.935413   -0.817487    1.198961
 O   -1.355846    0.481886   -1.907899
 O    0.540005   -1.237450    2.699618
 N    0.905392   -1.101055   -0.508863
 O    0.748464    0.779437    1.732941
 O   -1.781044    1.833084    0.749165
 C    1.749124    2.716598   -0.176745
 H   -0.029443    2.635677   -1.065524
 C   -1.649388   -3.674679   -0.543154
 C    0.456224   -2.319386   -0.576148
 C   -3.643694   -2.660588    0.372399
 H   -3.422954   -0.683394    1.221137
 C   -2.557353   -0.177308   -2.289316
 H   -1.548200    1.454787   -1.884739
 C    1.017252   -0.102086    2.643533
 C    2.283252   -0.843571   -0.752489
 C   -2.154837    2.802599    0.019334
 H    1.371628    3.202670    0.736781
```

```
 H    2.524401    1.990111    0.101886
 H    2.181533    3.470502   -0.852633
 C   -3.007478   -3.740858   -0.248348
 H   -1.144765   -4.510469   -1.036538
 H    1.108479   -3.144133   -0.892966
 H   -4.709214   -2.722745    0.608162
 H   -2.830242    0.118488   -3.314224
 H   -3.387665    0.066035   -1.603728
 H   -2.379903   -1.261139   -2.266363
 C    2.025261    0.381991    3.657360
 C    3.230367   -1.224846    0.199140
 C    2.668642   -0.164599   -1.908881
 C   -3.175428    3.745181    0.590333
 O   -1.729757    3.022178   -1.152639
 H   -3.577142   -4.638635   -0.498643
 H    3.013468    0.446838    3.172957
 H    1.772056    1.391993    4.010221
 H    2.087855   -0.310931    4.506006
 C    4.573530   -0.919628   -0.010644
 H    2.893778   -1.738811    1.105080
 C    4.014117    0.124786   -2.114551
 H    1.906103    0.128763   -2.634702
 H   -4.080857    3.713228   -0.034793
 H   -2.789639    4.773971    0.536714
 H   -3.434206    3.495132    1.626313
 C    4.967326   -0.245542   -1.165441
 H    5.316870   -1.212225    0.735192
 H    4.321269    0.647029   -3.024105
 H    6.021522   -0.008161   -1.327641
*
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MeOH (S)

```
CPCM (MeOH)
M06 SCF (DZ) =             -115.655157
G (1 atm) =                -115.627122
qh-G (1 mol/L) =           -115.624105
qh-G (24.56 mol/L) =       -115.621083
Lowest Frequency =          301.28

HF SCF energy (TZ) =       -115.095802
HF SCF energy (QZ) =       -115.105553
Correlation energy (DZ) =    -0.370631
Correlation energy (TZ) =    -0.461212
DLPNO-CCSD(T1)/CBS =       -115.622632

PBE0+D3BJ (ATZ) =          -115.645862
M06-2X (ATZ) =             -115.725166
wB97M-V (ATZ) =            -115.722702
B2GP-PLYP (ATZ) =          -115.670180
B2K-PLYP (ATZ) =           -115.656086
PWPB95 (ATZ) =             -115.696735
PWPB95+D3BJ (ATZ) =        -115.697228
PWPB95+D4 (ATZ) =          -115.698248

*xyz 0 1
 C    0.653221   -0.019191    0.000011
 O   -0.744466    0.122777   -0.000067
 H    1.036152   -0.547162    0.894098
 H   -1.126959   -0.763032    0.000413
 H    1.036192   -0.547725   -0.893982
 H    1.091015    0.990848   -0.000058
*
```

MeOH (S)

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =        -115.696843
G (1 atm) =                -115.668250
qh G-E (1 mol/L) =            0.031612
qh G-E (24.56 mol/L) =        0.034634
Lowest Frequency =         320.3

HF SCF energy (TZ) =       -115.096048
HF SCF energy (QZ) =       -115.105628
Correlation energy (DZ) =    -0.370772
Correlation energy (TZ) =    -0.461388
DLPNO-CCSD(T1)/CBS =       -115.622853

PBE0+D3BJ (ATZ) =          -115.646025
M06-2X (ATZ) =             -115.724815
wB97M-V (ATZ) =            -115.722228
B2GP-PLYP (ATZ) =          -115.669766
B2K-PLYP (ATZ) =           -115.655664
PWPB95 (ATZ) =             -115.696297
PWPB95+D3BJ (ATZ) =        -115.696790
PWPB95+D4 (ATZ) =          -115.697809

SMD (MeOH)
HF SCF energy (TZ) =       -115.097473
HF SCF energy (QZ) =       -115.107020
Correlation energy (DZ) =    -0.370203
Correlation energy (TZ) =    -0.460915
DLPNO-CCSD(T1)/CBS =       -115.623819

*xyz 0 1
 C    0.659651   -0.018475    0.000019
 O   -0.747546    0.123136   -0.000014
 H    1.033399   -0.547838    0.895482
```

MeOH•Cl⁻ (S•Cl⁻)
CPCM (MeOH)
M06 SCF (DZ) = -576.022543
G (1 atm) = -575.998889
qh-G (1 mol/L) = -575.995788
qh-G (24.56 mol/L) = -575.992766
Lowest Frequency = 123.41

HF SCF energy (TZ) = -574.773994
HF SCF energy (QZ) = -574.788872
Correlation energy (DZ) = -0.526507
Correlation energy (TZ) = -0.691785
DLPNO-CCSD(T1)/CBS = -575.581719

PBE0+D3BJ (ATZ) = -575.900652
M06-2X (ATZ) = -576.118390
wB97M-V (ATZ) = -576.106749
B2GP-PLYP (ATZ) = -575.904167
B2K-PLYP (ATZ) = -575.859279
PWPB95 (ATZ) = -576.052807
PWPB95+D3BJ (ATZ) = -576.053880
PWPB95+D4 (ATZ) = -576.055569

```
*xyz -1 1
 O    2.125189    0.647710   -0.398989
 C    2.514711   -0.468207    0.341299
 H    1.156441    0.789036   -0.208020
 H    2.742945   -0.236145    1.406519
 H    1.739404   -1.258628    0.336839
 H    3.439412   -0.896000   -0.089228
 Cl  -0.722888    1.062816    0.162644
*
```

MeOH•Cl⁻ (S•Cl⁻)
CPCM (MeOH)
wB97X-D3 SCF (DZ) = -576.076648
G (1 atm) = -576.054588
qh G-E (1 mol/L) = 0.027507
qh G-E (24.56 mol/L) = 0.030529
Lowest Frequency = 94.71

HF SCF energy (TZ) = -574.778760
HF SCF energy (QZ) = -574.793532
Correlation energy (DZ) = -0.524328
Correlation energy (TZ) = -0.689393
DLPNO-CCSD(T1)/CBS = -575.583830

PBE0+D3BJ (ATZ) = -575.902277
M06-2X (ATZ) = -576.118865
wB97M-V (ATZ) = -576.107789
B2GP-PLYP (ATZ) = -575.904875
B2K-PLYP (ATZ) = -575.859964
PWPB95 (ATZ) = -576.053633
PWPB95+D3BJ (ATZ) = -576.054692
PWPB95+D4 (ATZ) = -576.057363

SMD (MeOH)
HF SCF energy (TZ) = -574.773839
HF SCF energy (QZ) = -574.789009
Correlation energy (DZ) = -0.523968
Correlation energy (TZ) = -0.689157
DLPNO-CCSD(T1)/CBS = -575.579262

```
*xyz -1 1
 O    2.143961    0.543344   -0.561653
 C    2.499127   -0.494268    0.319755
 H    1.230999    0.807611   -0.314301
 H    2.462259   -0.186524    1.383017
 H    1.855363   -1.389313    0.211996
 H    3.533797   -0.798934    0.096287
 Cl  -0.730292    1.158666    0.415963
*
```

(MeOH)2•Cl⁻ (*S*₂•Cl⁻)
CPCM (MeOH)
wB97X-D3 SCF (DZ) = -691.789076
G (1 atm) = -691.718411
qh G-E (1 mol/L) = 0.076454
qh G-E (24.56 mol/L) = 0.079477
Lowest Frequency = 45.29

SMD (MeOH)
HF SCF energy (TZ) = -689.872486
HF SCF energy (QZ) = -689.895556
Correlation energy (DZ) = -0.902034
Correlation energy (TZ) = -1.159312
DLPNO-CCSD(T1)/CBS = -691.212156

```
*xyz -1 1
Cl  -3.498057    0.318846    0.065173
 H   -3.494261    0.879326    2.158486
 H   -2.864562    2.363582   -0.167700
 H    1.033400   -0.548219   -0.895220
 H    1.092185    0.992663   -0.000200
 H   -1.125934   -0.764751    0.000348
*
```

```
 O   -3.539663    1.289549    3.045528
 O   -2.727240    3.323774   -0.311309
 C   -4.049690    2.589566    2.842631
 C   -3.900703    3.795360   -0.936175
 H   -5.137591    2.591716    2.628987
 H   -3.543367    3.109239    2.009775
 H   -3.892005    3.172368    3.764039
 H   -4.789561    3.721401   -0.280444
 H   -4.126351    3.253969   -1.873950
 H   -3.753953    4.857529   -1.185362
*
```

(MeOH)3•Cl⁻ (***S*₃•Cl⁻**)

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =        -807.500180
G (1 atm) =                -807.381629
qh G-E (1 mol/L) =            0.125616
qh G-E (24.56 mol/L) =        0.128638
Lowest Frequency =           14.56

SMD (MeOH)
HF SCF energy (TZ) =       -804.970120
HF SCF energy (QZ) =       -805.001057
Correlation energy (DZ) =    -1.280854
Correlation energy (TZ) =    -1.629884
DLPNO-CCSD(T1)/CBS =       -806.844213

*xyz -1 1
Cl  -3.094132    1.535837    1.140596
 H   -2.786644    2.687689   -0.704062
 H   -4.980047    1.028716    0.147916
 H   -4.425003    0.771014    2.713814
 O   -2.825111    3.159084   -1.557654
 O   -5.899691    0.902880   -0.161021
 O   -5.028100    0.274222    3.299669
 C   -4.177175    3.521586   -1.740552
 C   -6.702003    1.729205    0.661323
 C   -5.212468   -0.988316    2.691031
 H   -4.499025    4.326080   -1.049888
 H   -4.862126    2.665775   -1.602737
 H   -4.295171    3.898345   -2.768520
 H   -7.757120    1.517287    0.431442
 H   -6.527835    1.530136    1.732931
 H   -6.522922    2.805083    0.473777
 H   -4.279806   -1.583446    2.666520
 H   -5.590346   -0.897365    1.656908
 H   -5.953801   -1.546420    3.282991
*
```

Ru(OAc)₂•S

```
CPCM (MeOH)
M06 SCF (DZ) =             -667.042706
G (1 atm) =                -666.930958
qh-G (1 mol/L) =           -666.924850
qh-G (24.56 mol/L) =       -666.921827
Lowest Frequency =           21.24

HF SCF energy (TZ) =       -663.619175
HF SCF energy (QZ) =       -663.662173
Correlation energy (DZ) =    -2.118291
Correlation energy (TZ) =    -2.720782
DLPNO-CCSD(T1)/CBS =       -666.747968

*xyz 0 1
```

```
 Ru   0.108393    0.223111   -0.420642
 O   -1.230598    1.910510   -0.374637
 O   -1.723715   -0.755015   -1.001329
 C   -1.378881    2.564403    0.888575
 H   -2.104532    1.624782   -0.689017
 O    1.995744    0.811607    0.368680
 O    1.666717   -1.221643   -0.316127
 O   -0.964112   -0.797369    1.023394
 C   -1.861462   -1.162045    0.192207
 H   -2.050942    3.429856    0.789174
 H   -1.763683    1.869850    1.651725
 H   -0.379528    2.909772    1.183775
 C    2.458417   -0.359666    0.175774
 C   -2.985033   -2.042875    0.605896
 C    3.874428   -0.688117    0.497873
 H   -3.897621   -1.778609    0.055612
 H   -2.730846   -3.084408    0.353639
 H   -3.153480   -1.979380    1.688066
 H    4.035002   -1.772961    0.495468
 H    4.532126   -0.227839   -0.255664
 H    4.147110   -0.262848    1.473669
*
```

Ru(OAc)₂•2S

```
CPCM (MeOH)
M06 SCF (DZ) =             -782.739087
G (1 atm) =                -782.576350
qh-G (1 mol/L) =           -782.570173
qh-G (24.56 mol/L) =       -782.567150
Lowest Frequency =           38.40

HF SCF energy (TZ) =       -778.745931
HF SCF energy (QZ) =       -778.797001
Correlation energy (DZ) =    -2.504126
Correlation energy (TZ) =    -3.197845
DLPNO-CCSD(T1)/CBS =       -782.415599

*xyz 0 1
 C    2.512883   -0.165780   -0.017741
 C    4.002058   -0.244416   -0.011470
 O    1.836249   -0.439263    1.024315
 H    4.334381   -1.115295    0.569682
 H    4.408752    0.655098    0.476674
 H    4.395145   -0.294341   -1.034582
 O    1.869169    0.196598   -1.048335
 O    0.177197    2.007655    0.725280
 C    0.365927    3.020945   -0.267699
 H    0.913125    2.045599    1.356734
 H    0.421888    4.010222    0.210591
 H    1.274288    2.829395   -0.859478
 H   -0.512687    2.979495   -0.923754
 O   -0.177198   -2.007615   -0.725281
 C   -0.366044   -3.020900    0.267686
 H   -0.913173   -2.045416   -1.356691
 H   -0.422317   -4.010143   -0.210637
 H   -1.274283   -2.829145    0.859586
 H    0.512669   -2.979696    0.923622
 C   -2.512864    0.165740    0.017725
 C   -4.002048    0.244272    0.011369
 O   -1.836206    0.439235   -1.024314
 O   -1.869176   -0.196579    1.048353
 H   -4.334371    1.115478   -0.569295
 H   -4.408637   -0.654958   -0.477382
 H   -4.395230    0.293564    1.034474
 Ru   0.000016    0.000016    0.000025
```

*

Ru(OAc)$_2$•3S^{fac}

CPCM (MeOH)
M06 SCF (DZ) = -898.417189
G (1 atm) = -898.205683
qh-G (1 mol/L) = -898.198914
qh-G (24.56 mol/L) = -898.195892
Lowest Frequency = 46.63

HF SCF energy (TZ) = -893.845678
HF SCF energy (QZ) = -893.905270
Correlation energy (DZ) = -2.886726
Correlation energy (TZ) = -3.672542
DLPNO-CCSD(T1)/CBS = -898.054948

*xyz 0 1
Ru 0.267344 -0.046203 0.136592
O -1.068062 0.079383 1.876086
O 0.044846 2.044330 -0.221893
C -1.843205 -1.070332 2.227006
H -0.559736 0.353910 2.652390
O 0.550786 -2.156859 0.495004
O -1.570697 -0.502615 -0.796368
O 2.315870 0.250207 0.753838
O 1.802281 -0.089017 -1.330502
C 0.126579 2.893681 0.909462
H -0.916880 2.017857 -0.548992
H -1.199165 -1.902403 2.551037
H -2.557904 -0.812228 3.022811
H -2.385626 -1.367322 1.320622
C 0.279825 -3.034566 -0.601580
H 1.468167 -2.288729 0.781257
C -2.479359 0.356688 -1.054347
C 2.692639 0.152359 -0.455857
H 0.033996 3.948824 0.602188
H -0.664694 2.666461 1.645412
H 1.109573 2.747060 1.380115
H 0.420426 -4.080598 -0.290571
H 0.929487 -2.802446 -1.460329
H -0.766659 -2.864200 -0.882439
C -3.802925 -0.220287 -1.487146
O -2.358230 1.599210 -0.956490
C 4.120901 0.342264 -0.839266
H -4.325020 -0.616327 -0.600471
H -3.655450 -1.061576 -2.178761
H -4.435721 0.547791 -1.949960
H 4.316956 1.418934 -0.963945
H 4.784326 -0.028918 -0.046801
H 4.339731 -0.159128 -1.790654
*

Ru(OAc)$_2$•3S^{mer}

CPCM (MeOH)
M06 SCF (DZ) = -898.422053
G (1 atm) = -898.211115
qh-G (1 mol/L) = -898.203784
qh-G (24.56 mol/L) = -898.200761
Lowest Frequency = 41.35

HF SCF energy (TZ) = -893.847853
HF SCF energy (QZ) = -893.907193
Correlation energy (DZ) = -2.886983
Correlation energy (TZ) = -3.673739

DLPNO-CCSD(T1)/CBS = -898.058541

*xyz 0 1
Ru -0.293835 -0.149872 -0.028292
O 0.905984 -1.297744 -1.431880
O 0.812250 -1.419271 1.344924
C 0.796755 -0.858324 -2.778356
H 1.808307 -1.083139 -1.086872
O -1.987304 -1.502976 -0.061237
O 1.258294 1.265821 0.042630
O -1.485592 1.275000 -1.085240
O -1.585331 1.132712 1.080665
C 0.599424 -1.107792 2.714110
H 1.733966 -1.165564 1.085994
H 1.026947 0.217574 -2.867883
H 1.470062 -1.437885 -3.429892
H -0.243260 -1.024975 -3.094595
C -1.712651 -2.903044 -0.103501
H -2.517925 -1.308002 0.727493
C 2.479479 0.916713 0.085069
C -1.966944 1.702841 0.007505
H 1.240519 -1.732140 3.356714
H 0.794739 -0.040313 2.917037
H -0.455195 -1.323793 2.941023
H -2.652858 -3.474040 -0.122688
H -1.095495 -3.214814 0.754310
H -1.154420 -3.085584 -1.031042
C 3.505190 2.012888 0.144458
O 2.883917 -0.281882 0.078487
C -2.924148 2.844819 0.044628
H 3.046808 3.009323 0.148554
H 4.183238 1.918990 -0.717333
H 4.121189 1.882217 1.047025
H -2.370381 3.769718 0.270060
H -3.422757 2.967360 -0.925137
H -3.665106 2.697537 0.841799
*

TS(B^0-B^{0+})
CPCM (MeOH)
M06 SCF (DZ) = -2808.599081
G (1 atm) = -2808.232037
qh-G (1 mol/L) = -2808.223390
qh-G (24.56 mol/L) = -2808.220368
Lowest Frequency = -106.34

HF SCF energy (TZ) = -2799.828397
HF SCF energy (QZ) = -2799.893416
Correlation energy (DZ) = -4.600539
Correlation energy (TZ) = -5.818928
DLPNO-CCSD(T1)/CBS = -2806.443883

*xyz 0 1
Ru -1.746702 0.560477 -0.002999
C -3.702033 0.659064 -0.900921
C -3.250324 1.977948 -0.604241
C -3.723866 -0.348071 0.094710
H -3.913894 0.399627 -1.940508
C -3.294118 0.013133 1.413651
C -2.855566 1.316638 1.713128
C -2.820681 2.327552 0.701093
Cl -0.526055 -1.616661 0.412452
Cl 0.465446 1.471802 0.807578
Cl -0.661782 0.503180 -2.182525
H -3.135972 2.701360 -1.415346

TS(B^0-B^{0+})
CPCM (MeOH)
wB97X-D3 SCF (DZ) = -2809.165497
G (1 atm) = -2808.786157
qh G-E (1 mol/L) = 0.391384
qh G-E (24.56 mol/L) = 0.394407
Lowest Frequency = -103.84

HF SCF energy (TZ) = -2567.575269
HF SCF energy (QZ) = -2567.651747
Correlation energy (DZ) = -5.142843
Correlation energy (TZ) = -6.460928
DLPNO-CCSD(T1)/CBS = -2574.905922

*xyz 0 1
Ru -1.740246 0.584335 -0.051503
Cl -0.641227 0.677263 -2.222693
C -3.284102 1.945948 -0.676061
C -2.818033 2.366267 0.590043
C -3.718701 0.604909 -0.898189
C -2.294217 3.755368 0.802916
C -2.804386 1.400132 1.649550
C -3.698127 -0.348804 0.144897
C -3.236409 0.079743 1.433526
C -4.108438 -1.793680 -0.053933
C -3.914536 -2.304941 -1.480012
C -5.565549 -1.939425 0.406807

C	-4.124462	-1.774006	-0.185968
H	-3.198868	-0.769917	2.172016
H	-2.429368	1.529675	2.696755
C	-2.265280	3.680390	0.990083
Ru	1.595639	-0.512986	-0.044044
C	-3.922456	-2.199206	-1.630275
C	-5.578443	-1.954914	0.248430
H	-3.488114	-2.408788	0.459217
H	-1.806211	4.122057	0.093997
H	-3.080991	4.345949	1.316397
H	-1.519023	3.644264	1.796325
C	2.844048	-0.022923	-1.716170
C	2.425211	-1.380515	-1.817101
C	3.659910	-0.445583	0.524959
C	3.243504	-1.802290	0.424570
C	2.643142	-2.303923	-0.761135
Cl	2.272582	-1.082976	3.489473
H	-4.618735	-1.677058	-2.308358
H	-2.892783	-2.009569	-1.974814
H	-4.123620	-3.276415	-1.731807
H	-5.725434	-1.696275	1.309056
H	-5.891238	-3.000670	0.104941
H	-6.243935	-1.313789	-0.354859
C	3.495683	0.465216	-0.552530
H	2.548571	0.668398	-2.508449
H	1.824522	-1.683640	-2.679178
H	3.985725	-0.084672	1.505300
H	3.265024	-2.409516	1.333645
C	2.115289	-3.696496	-0.829323
C	3.900724	1.906828	-0.372097
H	1.818833	-4.055855	0.166884
H	2.898843	-4.370068	-1.211851
H	1.251562	-3.763281	-1.506274
C	5.420940	1.995196	-0.501547
C	3.216382	2.869125	-1.327785
H	3.623506	2.177799	0.664821
H	5.757352	3.029743	-0.332908
H	5.934312	1.345454	0.224634
H	5.739826	1.694376	-1.514264
H	3.488259	3.903675	-1.069047
H	2.118433	2.786623	-1.285380
H	3.541351	2.701062	-2.368849
H	-3.215241	2.628468	-1.524214
H	-3.974844	0.300391	-1.912546
H	-1.914133	4.180821	-0.134862
H	-3.114830	4.393733	1.164193
H	-1.495039	3.767035	1.555335
H	-2.356517	1.664921	2.608903
H	-3.117941	-0.656906	2.230213
H	-3.474428	-2.394248	0.618934
H	-2.881126	-2.154608	-1.827604
H	-4.597041	-1.809260	-2.188210
H	-4.132554	-3.382097	-1.515813
H	-5.693991	-1.611340	1.449257
H	-6.235094	-1.337067	-0.227931
H	-5.879287	-2.991289	0.337742
Cl	0.468596	1.392266	0.832025
Ru	1.583090	-0.525649	-0.147346
Cl	-0.547702	-1.620166	0.203902
C	2.495895	-1.337555	-1.903364
C	2.646177	-2.295822	-0.870105
C	2.914506	0.012850	-1.730628
C	2.133192	-3.695871	-1.022346
C	3.182086	-1.838945	0.364018
C	3.501889	0.458130	-0.518409
C	3.601186	-0.490972	0.534654
C	3.912883	1.897230	-0.276371
C	3.234657	2.903741	-1.203281
C	5.441924	1.983527	-0.381745
H	1.950229	-1.606570	-2.809506
H	2.673052	0.729598	-2.515413
H	1.773167	-4.089146	-0.062649
H	2.954066	-4.340326	-1.371278
H	1.321242	-3.741215	-1.759530
H	3.160222	-2.486172	1.240902
H	3.892193	-0.164119	1.534110
H	3.625310	2.130640	0.762516
H	2.138592	2.811797	-1.175864
H	3.570004	2.785233	-2.245922
H	3.497462	3.923865	-0.887956
H	5.935585	1.302932	0.327952
H	5.775948	1.721940	-1.398624
H	5.775867	3.008368	-0.162862
Cl	1.849383	-1.318709	3.397936

*

TS(B^0-B^{0*})

CPCM (MeOH)

M06 SCF (DZ) = -2576.747206
G (1 atm) = -2576.337780
qh-G (1 mol/L) = -2576.327154
qh-G (24.56 mol/L) = -2576.324132
Lowest Frequency = -125.04

HF SCF energy (TZ) = -2567.574016
HF SCF energy (QZ) = -2567.652082
Correlation energy (DZ) = -5.139105
Correlation energy (TZ) = -6.456080
DLPNO-CCSD(T1)/CBS = -2574.901240

*xyz 0 1

Ru	-1.410521	0.116718	-0.590350
Cl	0.598042	1.534505	-0.534839
Cl	-0.346770	-0.979881	1.341313
Ru	1.874126	-0.459759	0.295634
O	-1.761066	2.001702	1.778180
Cl	0.876161	-1.538611	-1.661378

TS(B^0-B^{0*})

CPCM (MeOH)

wB97X-D3 SCF (DZ) = -2577.369277
G (1 atm) = -2576.941424
qh G-E (1 mol/L) = 0.439411
qh G-E (24.56 mol/L) = 0.442433
Lowest Frequency = -117.51

HF SCF energy (TZ) = -2799.832043
HF SCF energy (QZ) = -2799.896617
Correlation energy (DZ) = -4.599967
Correlation energy (TZ) = -5.818478
DLPNO-CCSD(T1)/CBS = -2806.446572

*xyz 0 1

Ru	-1.460432	0.259261	-0.752143
Cl	0.506070	1.674991	-0.621843
Cl	-0.447423	-0.909663	1.120328
C	-2.117397	-0.148347	-2.735575
C	-2.343339	1.232663	-2.489480
C	-2.627521	-1.154080	-1.865080

C	-2.785227	2.526666	2.295207
C	-2.572047	3.201809	3.651605
O	-3.946707	2.534879	1.816717
H	-2.353551	2.433500	4.412126
H	-1.694587	3.866821	3.616624
H	-3.456540	3.771629	3.972077
C	-2.571309	-1.198609	-1.822366
C	-3.254262	-1.059380	-0.585602
C	-2.176750	-0.060398	-2.583147
H	-2.230825	-2.183215	-2.150817
C	-3.636133	-2.230951	0.284106
C	-3.497286	0.264040	-0.123869
C	-2.450667	1.258052	-2.136075
H	-1.550428	-0.207901	-3.467421
C	-2.859286	-3.503309	-0.007752
C	-5.139551	-2.462980	0.139209
H	-3.431169	-1.921324	1.326715
C	-3.105090	1.398087	-0.880573
H	-3.886235	0.472123	0.879650
C	-1.941131	2.448098	-2.876710
H	-1.770159	-3.346469	0.050049
H	-3.103266	-3.904444	-1.006510
H	-3.128975	-4.279427	0.724645
H	-5.720673	-1.564256	0.399583
H	-5.388294	-2.740876	-0.899606
H	-5.464759	-3.283796	0.797086
H	-3.225236	2.367964	-0.389361
H	-1.678116	3.259793	-2.182754
H	-2.721458	2.825065	-3.557262
H	-1.057776	2.194888	-3.480750
C	3.880071	-0.895866	-0.363291
C	3.446866	-1.915778	0.533991
C	3.823360	0.471657	-0.000692
H	4.145599	-1.175889	-1.385176
C	2.951712	-1.595339	1.822320
H	3.398608	-2.950775	0.186283
C	4.215386	1.588319	-0.934304
C	3.323332	0.790272	1.304308
C	2.416103	-2.653680	2.725469
C	2.898867	-0.214279	2.195420
C	5.636867	2.025428	-0.582424
C	4.096038	1.233024	-2.406431
H	3.529866	2.429532	-0.719222
H	3.163797	1.840174	1.567872
H	1.617544	-2.262317	3.371562
H	3.225606	-3.023143	3.375764
H	2.026584	-3.506393	2.151001
H	2.420435	0.067300	3.136917
H	5.722996	2.332240	0.472127
H	6.348232	1.199866	-0.756690
H	5.941248	2.875867	-1.211823
H	3.091736	0.855515	-2.658550
H	4.838682	0.472290	-2.701782
H	4.289151	2.125316	-3.021067

*

TS(B^1-C^1)

CPCM (MeOH)

M06 SCF (DZ) = -1728.809388

G (1 atm) = -1728.405479

qh-G (1 mol/L) = -1728.396400

qh-G (24.56 mol/L) = -1728.393377

Lowest Frequency = -28.26

HF SCF energy (TZ) = -1720.995218

C	-1.739885	2.285731	-3.370807
C	-3.044833	1.572732	-1.302736
C	-3.361889	-0.812579	-0.703231
C	-3.534577	0.572973	-0.419608
C	-3.860043	-1.826912	0.308070
C	-3.196340	-3.197287	0.196754
C	-5.385241	-1.932840	0.172715
H	-1.458291	-0.444256	-3.553197
H	-2.339210	-2.189129	-2.049225
H	-1.500070	3.189293	-2.794993
H	-2.464767	2.556208	-4.153305
H	-0.827973	1.914902	-3.856889
H	-3.098786	2.616810	-0.991198
H	-3.903389	0.864141	0.575099
H	-3.639010	-1.393897	1.298472
H	-2.100046	-3.127435	0.252880
H	-3.465853	-3.702769	-0.744499
H	-3.534815	-3.838732	1.023258
H	-5.871565	-0.956858	0.320761
H	-5.665815	-2.308348	-0.824618
H	-5.782276	-2.629982	0.925329
Ru	1.821865	-0.244483	0.318436
Cl	1.150831	-1.379306	-1.728805
C	3.905658	-0.577337	-0.096234
C	3.729011	0.792100	0.205649
C	3.427758	-1.596757	0.781805
C	4.163473	1.908154	-0.723353
C	3.069055	1.116923	1.437556
C	2.770586	-1.268021	1.991050
C	4.143408	1.525428	-2.201604
C	5.549542	2.395551	-0.281647
C	2.601895	0.118245	2.310337
C	2.202876	-2.333013	2.881637
H	4.310551	-0.873052	-1.064006
H	3.490198	-2.640565	0.471649
H	3.446015	2.731491	-0.571536
H	2.828113	2.160266	1.650849
H	3.157188	1.144711	-2.508043
H	4.900199	0.760249	-2.435705
H	4.372856	2.410399	-2.812690
H	5.552378	2.698966	0.776191
H	6.301687	1.601225	-0.413502
H	5.855421	3.261721	-0.886839
H	2.013914	0.401949	3.184586
H	1.947933	-3.233898	2.308689
H	2.959850	-2.602049	3.634113
H	1.309265	-1.972849	3.407566
O	-2.027428	2.081891	1.733708
C	-2.604725	1.425299	2.642185
C	-1.818636	1.184662	3.934051
O	-3.759796	0.921820	2.568510
H	-1.173167	2.043016	4.169021
H	-1.164887	0.310186	3.779503
H	-2.486500	0.970286	4.779739

*

TS(B^1-C^1)

CPCM (MeOH)

wB97X-D3 SCF (DZ) = -1729.447832

G (1 atm) = -1729.031345

qh G-E (1 mol/L) = 0.431157

qh G-E (24.56 mol/L) = 0.434180

Lowest Frequency = -28.51

HF SCF energy (TZ) = -1721.000489

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HF SCF energy (QZ) =      -1721.073708
Correlation energy (DZ) =    -4.843012
Correlation energy (TZ) =    -5.950681
DLPNO-CCSD(T1)/CBS =      -1727.695290

*xyz 0 1
 Ru  -0.794608   -0.721767    0.041799
 C   -2.024073   -1.822992   -1.296239
 C   -2.856132   -0.917459   -0.564930
 C   -0.910604   -1.366784   -2.047576
 O    0.661078   -1.983819    0.680998
 Cl  -1.201275   -0.388446    2.386675
 C   -4.032730   -1.387880    0.251830
 C   -2.524609    0.461416   -0.603875
 C   -0.546274   -0.001806   -2.028901
 C    1.529131   -2.620168   -0.068648
 C   -3.860028   -2.774774    0.849800
 C   -5.276848   -1.320194   -0.632650
 C   -1.367134    0.897923   -1.279155
 C    0.702259    0.460459   -2.700963
 C    2.233752   -3.729736    0.671273
 O    1.759568   -2.384566   -1.248586
 H   -2.200621   -2.898499   -1.215064
 H   -0.237693   -2.089379   -2.509955
 H   -4.148081   -0.663114    1.078288
 H   -3.075380    1.163404    0.029038
 H   -2.932744   -2.852694    1.439627
 H   -3.848445   -3.556806    0.071708
 H   -4.707501   -2.999289    1.515557
 H   -5.441415   -0.306000   -1.029949
 H   -5.180637   -2.010609   -1.488769
 H   -6.169957   -1.614284   -0.059521
 H   -1.047802    1.939024   -1.170136
 H    1.518105   -0.252356   -2.506361
 H    0.540670    0.512954   -3.789992
 H    0.997214    1.461979   -2.354717
 H    2.465705   -3.434007    1.704046
 H    1.558846   -4.599881    0.724295
 H    3.149176   -4.027087    0.142469
 N    1.848326    1.247687    0.518086
 C    3.025061    0.495726    0.346705
 C    1.841737    2.476497    0.160698
 C    3.363416   -0.416479    1.353700
 C    3.843267    0.598087   -0.787383
 C    0.661237    3.332713    0.289732
 C    4.519460   -1.181400    1.248233
 C    4.987795   -0.187022   -0.896673
 C    0.564664    4.484804   -0.500631
 C   -0.385402    3.005262    1.164405
 C    5.334392   -1.074682    0.120630
 C   -0.579199    5.277314   -0.450834
 C   -1.517922    3.807435    1.223703
 C   -1.622268    4.938008    0.409079
 H    2.740855    2.959968   -0.273905
 H    2.704740   -0.501857    2.222518
 H    3.566553    1.277435   -1.599096
 H    4.781732   -1.878166    2.049212
 H    5.612563   -0.106891   -1.790233
 H    1.387971    4.746956   -1.172784
 H   -0.301181    2.108917    1.785387
 H    6.234321   -1.688314    0.031829
 H   -0.655846    6.165292   -1.082789
 H   -2.329767    3.549673    1.909667
 H   -2.518078    5.562615    0.453109
*
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HF SCF energy (QZ) =      -1721.077998
Correlation energy (DZ) =    -4.838739
Correlation energy (TZ) =    -5.944221
DLPNO-CCSD(T1)/CBS =      -1727.691546

SMD (MeOH)
HF SCF energy (TZ) =      -1721.013430
HF SCF energy (QZ) =      -1721.090882
Correlation energy (DZ) =    -4.835733
Correlation energy (TZ) =    -5.941728
DLPNO-CCSD(T1)/CBS =      -1727.702220

*xyz 0 1
  Ru     0.799158    0.163250   -0.185152
  N     -2.589139    1.221908    0.247282
  O      0.334773   -0.335838    1.722559
  C     -3.680539    0.558797    0.192992
  C     -2.691687    2.634506    0.222901
  Cl     1.144962    2.334791    0.719632
  C      0.645376   -1.412173    2.401519
  C     -3.736458   -0.912592    0.264348
  H     -4.652614    1.067413    0.063765
  C     -1.901497    3.357921   -0.678547
  C     -3.530591    3.324067    1.107909
  C     -0.176083   -1.581847    3.660829
  O      1.518726   -2.213906    2.084312
  C     -2.631624   -1.669101    0.676611
  C     -4.922585   -1.565113   -0.092468
  C     -1.979646    4.746928   -0.719519
  H     -1.227746    2.820165   -1.347202
  C     -3.592368    4.717398    1.072824
  H     -4.117582    2.764050    1.839908
  H     -0.138230   -0.663749    4.263288
  H     -1.228854   -1.753745    3.389658
  H      0.192198   -2.432681    4.245508
  C     -2.707546   -3.057535    0.714681
  H     -1.717936   -1.152241    0.972846
  C     -4.996924   -2.957109   -0.058525
  H     -5.789636   -0.976665   -0.404639
  C     -2.823860    5.433702    0.156336
  H     -1.367046    5.299722   -1.435475
  H     -4.245427    5.245104    1.771795
  C     -3.889443   -3.704583    0.342344
  H     -1.840555   -3.638550    1.038375
  H     -5.922503   -3.460181   -0.345953
  H     -2.874018    6.524313    0.129992
  H     -3.948188   -4.794927    0.371392
  C      1.511218   -1.760013   -0.881618
  C      2.536501   -0.770176   -0.977699
  C      0.237712   -1.537603   -1.433434
  H      1.672482   -2.624391   -0.239617
  C      3.861800   -1.008592   -0.282223
  C      2.256942    0.407131   -1.736663
  C     -0.051709   -0.331228   -2.138548
  H     -0.565163   -2.250452   -1.239752
  C      4.566020    0.269267    0.169782
  C      4.753858   -1.843837   -1.209948
  H      3.624817   -1.607950    0.611285
  C      0.988511    0.619149   -2.314472
  H      2.987999    1.215133   -1.771183
  C     -1.424970   -0.089064   -2.689573
  H      5.453824    0.008511    0.764259
  H      4.909398    0.873265   -0.685152
  H      3.909482    0.894526    0.793677
  H      4.270916   -2.792263   -1.489481
  H      4.982310   -1.289042   -2.134340
```

TS(B^2-C^2)
CPCM (MeOH)
M06 SCF (DZ) = -1496.970516
G (1 atm) = -1496.518831
qh-G (1 mol/L) = -1496.509602
qh-G (24.56 mol/L) = -1496.506580
Lowest Frequency = -20.61

HF SCF energy (TZ) = -1488.759523
HF SCF energy (QZ) = -1488.850472
Correlation energy (DZ) = -5.373709
Correlation energy (TZ) = -6.580833
DLPNO-CCSD(T1)/CBS = -1496.164075

*xyz 0 1

Ru	-0.618451	-0.749879	-0.164348
C	-1.594789	-2.085852	-1.497461
N	1.865006	1.304376	0.392472
C	-2.575930	-1.205080	-0.943290
C	-0.461454	-1.591620	-2.187350
H	-1.678822	-3.161838	-1.322083
O	0.768412	-1.931449	0.758309
O	-0.930414	-0.273884	1.811685
C	3.095196	0.622024	0.355396
C	1.822328	2.521780	-0.002519
C	-3.781489	-1.738587	-0.211874
C	-2.376867	0.193849	-1.099190
C	-0.225482	-0.202961	-2.263422
H	0.323495	-2.280110	-2.499768
C	1.729728	-2.605402	0.181668
C	-1.949796	0.335363	2.355469
C	3.397956	-0.236092	1.419487
C	4.001479	0.740195	-0.707786
C	0.586110	3.305136	-0.007480
H	2.730001	3.047645	-0.363276
C	-3.456129	-2.875658	0.745778
C	-4.819003	-2.165184	-1.248391
H	-4.180943	-0.898367	0.378854
C	-1.200377	0.679159	-1.699710
H	-3.051203	0.884248	-0.591069
C	1.037154	0.317524	-2.862666
C	2.382754	-3.601531	1.109904
O	2.089213	-2.489621	-0.985347
C	-1.713826	0.685764	3.804933
O	-2.994469	0.641562	1.787958
C	4.600830	-0.933546	1.437643
H	2.671121	-0.336530	2.230219
C	5.192958	0.020163	-0.694879
H	3.756696	1.376752	-1.563157
C	0.490788	4.449251	-0.808602
C	-0.516358	2.908293	0.761009
H	-4.360014	-3.160726	1.306550
H	-3.110642	-3.779374	0.215060
H	-2.680014	-2.583734	1.471759
H	-5.740522	-2.504821	-0.749848
H	-5.081854	-1.337587	-1.926547
H	-4.440429	-3.000890	-1.862852
H	-0.990295	1.753391	-1.671919
H	5.704485	-2.078462	-0.708472
H	0.767693	1.574404	-2.792483
H	-1.648097	0.982144	-2.765949
H	-1.467455	-0.522382	-3.701207
H	-2.191788	-0.578408	-2.076376

*

TS(B^2-C^2)
CPCM (MeOH)
wB97X-D3 SCF (DZ) = -1497.667583
G (1 atm) = -1497.202629
qh G-E (1 mol/L) = 0.477454
qh G-E (24.56 mol/L) = 0.480476
Lowest Frequency = -37.11

HF SCF energy (TZ) = -1488.764135
HF SCF energy (QZ) = -1488.853700
Correlation energy (DZ) = -5.372576
Correlation energy (TZ) = -6.579057
DLPNO-CCSD(T1)/CBS = -1496.164734

SMD (MeOH)
HF SCF energy (TZ) = -1488.784109
HF SCF energy (QZ) = -1488.873416
Correlation energy (DZ) = -5.366058
Correlation energy (TZ) = -6.573832
DLPNO-CCSD(T1)/CBS = -1496.179902

*xyz 0 1

Ru	-0.589714	-0.831628	-0.193686
O	-0.889026	-0.396662	1.774617
O	0.854883	-1.960216	0.686766
C	-1.873784	0.226514	2.368686
C	1.824754	-2.634969	0.124794
C	-1.632403	0.434549	3.849031
O	-2.892608	0.639967	1.821285
C	2.459423	-3.646019	1.056474
O	2.206744	-2.501204	-1.034675
C	-1.646943	-2.123690	-1.490973
C	-0.480248	-1.709615	-2.184256
C	-2.575002	-1.177071	-0.957355
C	-0.155749	-0.340955	-2.283044
C	-3.824314	-1.618948	-0.222263
C	-2.280860	0.201703	-1.120260
C	1.136856	0.100912	-2.902306
C	-1.070956	0.604651	-1.721499
C	-3.580183	-2.761064	0.764484
C	-4.895925	-1.978879	-1.258264
H	-1.291506	-0.499412	4.316050
H	-0.831534	1.179252	3.977326
H	-2.542708	0.798007	4.340153
H	2.626546	-3.203909	2.047545
H	1.764634	-4.491111	1.182754
H	3.404041	-4.016461	0.640328
H	-1.798304	-3.188431	-1.308891
H	0.251086	-2.454830	-2.492129
H	-4.161197	-0.746302	0.354212
H	-2.908195	0.941844	-0.626769
H	1.945532	-0.582607	-2.613867
H	1.035134	0.085915	-3.998173
H	1.392009	1.123848	-2.596963
H	-0.795499	1.660599	-1.704193
H	-2.812442	-2.489897	1.504533
H	-3.263373	-3.688051	0.260798
H	-4.511312	-2.984453	1.305909

```
 H    0.929663    0.377250   -3.958290
 H    1.269689    1.327747   -2.494153
 H    1.875162   -0.358624   -2.636381
 H    2.493784   -3.188337    2.122465
 H    1.733760   -4.489225    1.188792
 H    3.358926   -3.914491    0.715689
 H   -1.288848   -0.168236    4.351411
 H   -0.974436    1.502051    3.860076
 H   -2.645107    1.018264    4.281062
 C    5.500812   -0.814426    0.378180
 H    4.833746   -1.587820    2.282333
 H    5.885846    0.109949   -1.535723
 C   -0.703646    5.163157   -0.868423
 H    1.355143    4.768049   -1.399684
 C   -1.703686    3.626032    0.709766
 H   -0.414016    2.019575    1.386930
 H    6.437722   -1.376889    0.386201
 C   -1.800994    4.751340   -0.113007
 H   -0.778820    6.047057   -1.506363
 H   -2.557135    3.293410    1.307421
 H   -2.736391    5.314866   -0.159661
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TS(B⁺-D⁺)

```
CPCM (MeOH)
M06 SCF (DZ) =            -1268.413729
G (1 atm) =               -1268.006359
qh-G (1 mol/L) =          -1267.998203
qh-G (24.56 mol/L) =      -1267.995180
Lowest Frequency =          -80.41

HF SCF energy (TZ) =      -1261.305051
HF SCF energy (QZ) =      -1261.379549
Correlation energy (DZ) =    -4.667257
Correlation energy (TZ) =    -5.701238
DLPNO-CCSD(T1)/CBS =      -1267.707426

*xyz 1 1
 Ru   1.002769   -1.010779    0.035814
 C    2.297732   -2.110016    1.311956
 C    2.928188   -1.905412    0.044685
 C    1.798937   -1.026604    2.076791
 H    2.091337   -3.133318    1.637545
 C    3.052852   -0.556803   -0.415972
 C    2.548786    0.520263    0.340176
 C    1.884090    0.297391    1.579879
 N   -1.981241    0.689966   -0.595266
 O    0.334067   -1.441315   -1.944847
 O   -0.423618   -2.554051   -0.249969
 C    3.337461   -3.056976   -0.807371
 H    1.228486   -1.235951    2.984143
 H    3.424113   -0.373692   -1.428625
 H    2.545861    1.524919   -0.093894
 C    1.225850    1.454498    2.287011
 C   -3.208900    0.255968   -0.059785
 C   -1.663370    1.923780   -0.454770
 C   -0.506656   -2.284926   -1.495888
 H    2.700291   -3.933353   -0.618753
 H   -5.089162   -1.139419   -1.943295
 H   -4.589283   -2.848825   -1.861956
 H   -5.839921   -2.232168   -0.752902
 N    1.841072    1.388003    0.421920
 C    1.785827    2.591002   -0.004627
 C    3.086373    0.715659    0.397022
 C    0.526227    3.357076   -0.016047
 C    3.414155   -0.085269    1.497480
 C    3.966373    0.785457   -0.690720
 C    0.404511    4.479014   -0.843961
 C   -0.560514    2.960723    0.773829
 C    4.616889   -0.785764    1.521059
 C    5.162398    0.068546   -0.667867
 C   -0.801636    5.177277   -0.902180
 C   -1.760847    3.659640    0.720522
 C    5.494227   -0.715858    0.436479
 C   -1.884361    4.767604   -0.122905
 H    2.680103    3.113701   -0.387937
 H    2.712246   -0.148857    2.331283
 H    3.702937    1.380450   -1.567928
 H    1.253588    4.795452   -1.455700
 H   -0.443799    2.092615    1.421641
 H    4.866948   -1.402295    2.387607
 H    5.835536    0.120348   -1.526690
 H   -0.896253    6.045691   -1.557517
 H   -2.601156    3.327492    1.333406
 H    6.430224   -1.278345    0.449687
 H   -2.827733    5.316537   -0.167919*
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 H    3.286530   -2.796997   -1.874209
 H    4.377343   -3.338892   -0.575888
 C    2.175621    1.959492    3.371303
 C   -0.146882    1.120678    2.853349
 H    1.104019    2.251461    1.529976
 C   -3.259050   -0.992532    0.575605
 C   -4.386033    1.009209   -0.181256
 C   -0.458397    2.522146   -1.030877
 H   -2.291774    2.612468    0.146832
 C   -1.559707   -2.880095   -2.348054
 H    1.745546    2.841866    3.869612
 H    2.339681    1.182346    4.137342
 H    3.155277    2.242851    2.955529
 H   -0.083499    0.425805    3.707627
 H   -0.628751    2.039943    3.221556
 H   -0.807982    0.672227    2.092134
 C   -4.453810   -1.454683    1.117853
 H   -2.344297   -1.589418    0.639796
 C   -5.580644    0.531823    0.350448
 H   -4.366914    1.958192   -0.724950
 C   -0.014510    3.751427   -0.525918
 C    0.259477    1.904479   -2.065946
 H   -1.253953   -2.885395   -3.401207
 H   -2.462390   -2.254309   -2.249325
 H   -1.808907   -3.891878   -2.004244
 C   -5.619073   -0.695864    1.009399
 H   -4.476454   -2.423349    1.623822
 H   -6.493041    1.123875    0.240735
 C    1.148832    4.337510   -1.016481
 H   -0.584538    4.240980    0.270711
 C    1.414703    2.496921   -2.562499
 H   -0.096837    0.951470   -2.467008
 H   -6.559014   -1.067843    1.424290
 C    1.865303    3.709672   -2.034685
 H    1.494848    5.290119   -0.608816
 H    1.969021    2.013567   -3.371312
 H    2.774427    4.171663   -2.427578
*
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TS(B^{+S}-D^{+S})

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CPCM (MeOH)
M06 SCF (DZ) =            -1384.087819
G (1 atm) =               -1383.633874
qh-G (1 mol/L) =          -1383.624097
qh-G (24.56 mol/L) =      -1383.621074
Lowest Frequency =          -93.20

HF SCF energy (TZ) =      -1376.382060
HF SCF energy (QZ) =      -1376.464894
Correlation energy (DZ) =    -5.076140
Correlation energy (TZ) =    -6.201937
DLPNO-CCSD(T1)/CBS =      -1383.349633

*xyz 1 1
 Ru   0.030003   -1.110431    0.221251
 O   -2.021533   -0.609531    1.117520
 N   -0.636725    1.344408   -0.607313
 C   -2.370133   -0.259255    2.446005
 H   -2.581127   -1.325441    0.773085
 O   -0.480969   -1.134864   -2.023138
 O   -1.637837   -2.394914   -0.679634
 C   -2.003322    1.692510   -0.401599
 C    0.124628    2.320324   -0.942261
 H   -1.795151    0.641510    2.707864
 H   -3.442143   -0.014648    2.506014
```

H	-2.141424	-1.065055	3.164442
C	-1.416837	-1.962707	-1.855338
C	-2.387530	2.584847	0.599840
C	-2.969621	1.109654	-1.225609
C	1.530007	2.200164	-1.339152
H	-0.289317	3.347625	-0.969043
C	-2.261681	-2.432074	-2.993099
C	-3.738276	2.874705	0.789702
H	-1.627011	3.039934	1.242285
C	-4.313370	1.408042	-1.034481
H	-2.644337	0.433183	-2.020466
C	2.443611	3.175749	-0.919114
C	1.952759	1.167532	-2.184799
H	-1.971967	-1.947601	-3.933131
H	-3.319072	-2.220972	-2.773378
H	-2.164402	-3.523343	-3.093133
C	-4.704724	2.284169	-0.019900
H	-4.033627	3.568519	1.580926
H	-5.064623	0.954164	-1.686020
C	3.783113	3.077760	-1.280212
H	2.099791	4.001887	-0.288772
C	3.287814	1.094609	-2.571678
H	1.219119	0.437496	-2.539926
H	-5.762697	2.510247	0.132839
C	4.205914	2.035829	-2.105785
H	4.498901	3.824292	-0.928737
H	3.616566	0.296704	-3.242931
H	5.255244	1.967557	-2.402846
C	2.096130	-1.425035	-0.223602
C	2.005491	-0.388314	0.748410
C	1.483416	-2.688473	-0.019540
H	2.563161	-1.213147	-1.188091
C	1.309593	-0.587915	1.966871
H	2.424924	0.592307	0.511815
C	1.493174	-3.733669	-1.081307
C	0.730699	-2.864034	1.177936
C	1.223963	0.461628	3.045170
C	0.658085	-1.834579	2.153929
H	1.603383	-3.287071	-2.079491
H	2.346989	-4.410277	-0.915685
H	0.575267	-4.338046	-1.053727
H	0.121372	-3.763176	1.298782
C	2.378344	0.207209	4.016068
C	1.242487	1.893699	2.541322
H	0.277008	0.287843	3.588766
H	0.012804	-1.972891	3.025945
H	2.331576	0.919414	4.854052
H	2.349022	-0.813219	4.429059
H	3.347295	0.342910	3.505741
H	2.203687	2.146301	2.061190
H	1.113804	2.586484	3.386562
H	0.434240	2.084831	1.817505

*

TS(C^1-D^+)

CPCM (MeOH)

M06 SCF (DZ) =	-1728.791257
G (1 atm) =	-1728.384749
qh-G (1 mol/L) =	-1728.376250
qh-G (24.56 mol/L) =	-1728.373228
Lowest Frequency =	-53.99
HF SCF energy (TZ) =	-1720.985382
HF SCF energy (QZ) =	-1721.063285
Correlation energy (DZ) =	-4.839064

TS(C^1-D^+)

CPCM (MeOH)

wB97X-D3 SCF (DZ) =	-1729.435313
G (1 atm) =	-1729.016145
qh G-E (1 mol/L) =	0.431412
qh G-E (24.56 mol/L) =	0.434435
Lowest Frequency =	-49.36
HF SCF energy (TZ) =	-1720.986830
HF SCF energy (QZ) =	-1721.064945
Correlation energy (DZ) =	-4.841266

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Correlation energy (TZ) =    -5.948528
DLPNO-CCSD(T1)/CBS =      -1727.683587

PBE0+D3BJ (ATZ) =         -1728.602705
M06-2X (ATZ) =            -1729.457027
wB97M-V (ATZ) =           -1729.513309
B2GP-PLYP (ATZ) =         -1728.615278
B2K-PLYP (ATZ) =          -1728.416973
PWPB95 (ATZ) =            -1729.076343
PWPB95+D3BJ (ATZ) =       -1729.119392
PWPB95+D4 (ATZ) =         -1729.134026

*xyz 0 1
 Ru  -0.061199    0.622097    0.563147
 N   -0.294987   -1.055884   -0.821685
 O   -1.592258   -0.267432    1.571626
 C    0.591801   -1.836487   -1.347190
 C   -1.645771   -1.320428   -1.236225
 Cl  -2.741549    2.980094   -0.496186
 C   -1.536093   -1.440195    2.134909
 C    1.967193   -2.004569   -0.893283
 H    0.277186   -2.467191   -2.196101
 C   -2.457406   -0.305605   -1.741590
 C   -2.149212   -2.616829   -1.088048
 C   -2.884822   -1.936450    2.586941
 O   -0.506995   -2.093256    2.292067
 C    2.235018   -2.203066    0.468185
 C    3.005252   -2.059421   -1.833247
 C   -3.768214   -0.595539   -2.107980
 H   -2.085175    0.719952   -1.822363
 C   -3.460085   -2.898150   -1.462743
 H   -1.516325   -3.392049   -0.645286
 H   -3.336980   -1.216834    3.285710
 H   -3.556594   -2.003786    1.716032
 H   -2.798450   -2.918533    3.068173
 H    1.401343   -2.207882    1.179956
 C    3.546715   -2.411531    0.883584
 C    4.316243   -2.230662   -1.404102
 H    2.780995   -1.941239   -2.897404
 C   -4.272546   -1.888172   -1.974543
 H   -4.400678    0.207279   -2.495743
 H   -3.849975   -3.911608   -1.341852
 C    4.586701   -2.406032   -0.045885
 H    3.760580   -2.579197    1.942241
 H    5.130869   -2.242253   -2.131510
 H   -5.303869   -2.106994   -2.261365
 H    5.616276   -2.557242    0.287507
 C    0.420353    2.699100    0.205984
 C    0.075451    2.538509    1.577949
 C    1.464671    1.953791   -0.400045
 H   -0.234754    3.336733   -0.396132
 C    0.706077    1.562289    2.377357
 H   -0.797157    3.074889    1.959023
 C    1.851219    2.141873   -1.846782
 C    2.093417    0.976534    0.400517
 C    0.254425    1.263452    3.765317
 C    1.696459    0.745135    1.747426
 C    0.664189    2.105822   -2.798273
 C    2.629300    3.448799   -1.979290
 H    2.527955    1.305625   -2.105098
 H    2.834597    0.314614   -0.054598
 H   -0.773807    1.612583    3.933005
 H    0.913107    1.771054    4.488074
 H    0.303186    0.182136    3.962137
 H    2.130197   -0.091201    2.301996
 H    0.138705    1.138083   -2.753088

Correlation energy (TZ) =    -5.950231
DLPNO-CCSD(T1)/CBS =      -1496.164734

PBE0+D3BJ (ATZ) =         -1728.604633
M06-2X (ATZ) =            -1729.472449
wB97M-V (ATZ) =           -1729.522748
B2GP-PLYP (ATZ) =         -1728.632448
B2K-PLYP (ATZ) =          -1728.438218
PWPB95 (ATZ) =            -1729.088152
PWPB95+D3BJ (ATZ) =       -1729.131463
PWPB95+D4 (ATZ) =         -1729.145983

SMD (MeOH)
HF SCF energy (TZ) =      -1720.997958
HF SCF energy (QZ) =      -1721.076199
Correlation energy (DZ) =    -4.836265
Correlation energy (TZ) =    -5.945954
DLPNO-CCSD(T1)/CBS =      -1727.694158

*xyz 0 1
 Ru  -0.055944    0.536305    0.620310
 O   -0.598822   -2.332992    2.046306
 O   -1.542186   -0.333872    1.687603
 C   -1.568997   -1.578416    2.078319
 C   -2.921108   -2.030106    2.577574
 C    1.704216    0.780180    1.776033
 C    2.077662    0.958949    0.416541
 C    0.695828    1.596177    2.378059
 C    1.404529    1.867471   -0.427986
 C    0.288358    1.381057    3.803720
 C    0.016989    2.498920    1.538914
 C    1.809917    2.012781   -1.881597
 C    0.332804    2.592831    0.151491
 C    0.633233    2.001815   -2.855478
 C    2.651647    3.287611   -2.021403
 H   -3.317890   -1.310568    3.306650
 H   -3.616885   -2.060674    1.725186
 H   -2.849255   -3.027271    3.026346
 H    2.180571   -0.008417    2.360067
 H    2.842596    0.309844   -0.008858
 H    0.420626    0.329675    4.091860
 H    0.925726    1.999332    4.453863
 H   -0.757583    1.671156    3.963243
 H   -0.864375    3.027078    1.902659
 H    2.453486    1.148601   -2.114128
 H   -0.333273    3.192098   -0.469816
 H    0.095648    1.043515   -2.819592
 H   -0.085244    2.809934   -2.646628
 H    1.001992    2.141851   -3.882080
 H    3.512582    3.275941   -1.336044
 H    2.046902    4.181494   -1.798262
 H    3.032661    3.379714   -3.049264
 C    2.281440   -2.253137    0.483097
 N   -0.269688   -1.093985   -0.789678
 C    1.996004   -2.014741   -0.866900
 C    3.608087   -2.377393    0.891063
 C   -1.627892   -1.296980   -1.226852
 C    0.600994   -1.885194   -1.311182
 C    3.028913   -1.943227   -1.809508
 C    4.642120   -2.251176   -0.037962
 C   -2.361927   -0.227551   -1.734165
 C   -2.210561   -2.560129   -1.088718
 C    4.352804   -2.036499   -1.387569
 C   -3.683224   -0.429506   -2.127795
 C   -3.532487   -2.752159   -1.484485
 C   -4.269535   -1.688986   -2.008211
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 H   -0.067273    2.900650   -2.573267
 H    1.008718    2.257510   -3.833005
 H    3.496900    3.476657   -1.301226
 H    1.982458    4.310836   -1.740269
 H    2.993975    3.577254   -3.010243
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 H    1.454829   -2.336547    1.194149
 H    3.835868   -2.565150    1.942358
 H    0.278570   -2.533351   -2.138577
 H    2.795276   -1.783239   -2.864793
 H    5.681119   -2.330608    0.289143
 H   -1.918697    0.766724   -1.804397
 H   -1.637437   -3.375396   -0.642252
 H    5.162324   -1.946737   -2.114503
 H   -4.256358    0.412238   -2.520825
 H   -3.990011   -3.737149   -1.372367
 H   -5.307070   -1.841191   -2.312689
 Cl  -2.960518    2.756684   -0.086775
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TS(C^1-D^+)•*S*

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CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1845.155432
G (1 atm) =               -1844.688351
qh G-E (1 mol/L) =            0.482557
qh G-E (24.56 mol/L) =        0.485580
Lowest Frequency =          -57.75

SMD (MeOH)
HF SCF energy (TZ) =      -1836.091319
HF SCF energy (QZ) =      -1836.176766
Correlation energy (DZ) =    -5.222554
Correlation energy (TZ) =    -6.423768
DLPNO-CCSD(T1)/CBS =      -1843.328193

*xyz 0 1
 Ru  -0.373339    0.364424    0.598364
 C    1.249886    0.981405    1.841887
 C    1.647027    1.092726    0.484407
 C    0.094896    1.659803    2.326007
 H    1.793826    0.306767    2.502487
 C   -0.667812    2.368142    1.372822
 C   -0.277409    2.472065    0.004162
 C    0.908924    1.867669   -0.455144
 Cl  -3.788095    1.256846    0.723854
 C    2.090909   -2.103646    0.346862
 N   -0.468245   -1.056953   -1.025201
 O    0.231422   -1.624570    3.245194
 O   -1.194261   -1.187154    1.572845
 H    2.517146    0.532386    0.141388
 C   -0.353809    1.547660    3.753569
 H   -1.640877    2.765361    1.664258
 H   -0.959488    2.964671   -0.693033
 C    1.425935    2.011318   -1.873423
 H   -3.129250    2.487800   -0.939586
 H   -5.418999    1.145664   -0.777367
 H   -3.560292    0.624817    2.782361
 C    1.840306   -1.877321   -1.012298
 C    3.404453   -2.185395    0.802826
 H    1.263105   -2.207911    1.050831
 C   -1.788634   -1.274574   -1.559930
 C    0.464528   -1.786016   -1.526952
 C   -0.878985   -1.716185    2.730558
 H   -1.435510    1.356153    3.810169
 H   -0.136816    2.493265    4.272966
 H    0.174373    0.733483    4.263274
 C    0.355533    1.948423   -2.959980
 C    2.217607    3.325653   -1.938435
 H    2.131982    1.180689   -2.037425
 O   -2.844226    3.017553   -1.711740
 O   -6.216934    1.267844   -1.326077
```

```
 O   -3.554388    0.471724    3.748426
 C    2.906512   -1.771695   -1.914259
 C    4.466946   -2.031006   -0.089215
 H    3.596999   -2.363619    1.862740
 C   -2.517652   -0.211777   -2.090051
 C   -2.339841   -2.558666   -1.510670
 H    0.223007   -2.397920   -2.408143
 C   -2.020435   -2.464024    3.374768
 H    0.815683    2.148030   -3.938810
 H   -0.442930    2.690284   -2.804999
 H   -0.107060    0.952896   -3.006536
 H    2.999522    3.363356   -1.164800
 H    1.548514    4.189073   -1.792259
 H    2.700979    3.427737   -2.921285
 C   -3.959083    3.789070   -2.124588
 C   -7.138547    1.986942   -0.532756
 C   -4.577542    1.280494    4.294451
 C    4.217676   -1.825100   -1.447530
 H    2.706211   -1.620819   -2.977861
 H    5.495818   -2.082357    0.273704
 C   -3.790793   -0.444699   -2.604746
 H   -2.114181    0.800574   -2.094280
 C   -3.619417   -2.778904   -2.016000
 H   -1.771656   -3.373893   -1.057189
 H   -2.495500   -3.134856    2.645690
 H   -2.770120   -1.721785    3.690949
 H   -1.666954   -3.032733    4.242874
 H   -4.161535    4.625821   -1.431547
 H   -4.866642    3.167695   -2.199922
 H   -3.732634    4.210366   -3.114644
 H   -8.057719    2.124409   -1.121536
 H   -7.403782    1.447468    0.395232
 H   -6.760842    2.987434   -0.250088
 H   -5.573190    1.019002    3.892471
 H   -4.402475    2.355758    4.109356
 H   -4.593128    1.117628    5.381887
 H    5.048199   -1.713898   -2.147381
 C   -4.345522   -1.723068   -2.568400
 H   -4.363644    0.389867   -3.012491
 H   -4.050949   -3.780931   -1.970564
 H   -5.351062   -1.893863   -2.958451
*
```

TS(C^1-D^+)•S_2

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CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1960.872280
G (1 atm) =               -1960.356847
qh G-E (1 mol/L) =            0.533445
qh G-E (24.56 mol/L) =        0.536468
Lowest Frequency =           -44.4

SMD (MeOH)
HF SCF energy (TZ) =      -1951.192335
HF SCF energy (QZ) =      -1951.285792
Correlation energy (DZ) =    -5.602529
Correlation energy (TZ) =    -6.895177
DLPNO-CCSD(T1)/CBS =      -1958.964469

*xyz 0 1
  Ru    -0.275672    0.577613    0.713987
  C      2.093838   -2.208877    0.344657
  O     -0.646630   -2.645265    1.837940
  C      1.699190   -1.941101   -0.971902
  C      3.446417   -2.369993    0.637202
  H      1.326391   -2.302844    1.116641
```

```
  N     -0.551819   -0.974922   -0.753183
  Cl    -3.424686    2.105226    0.850733
  O     -1.410214   -0.549273    1.964176
  C     -1.520041   -1.824088    2.146323
  H     -1.046451   -4.220765    1.175002
  C      2.653069   -1.874444   -1.995113
  C      0.277548   -1.778839   -1.318740
  C      4.402695   -2.249729   -0.372518
  H      3.754977   -2.584500    1.662420
  C     -1.927153   -1.119243   -1.167685
  H     -2.725561    2.934547   -0.929762
  C     -2.825602   -2.252015    2.769772
  O     -1.199518   -5.029568    0.644157
  C      4.005630   -2.003844   -1.688488
  H      2.336625   -1.694181   -3.025535
  H     -0.101355   -2.403089   -2.140953
  H      5.463258   -2.360792   -0.136414
  C     -2.605353   -0.030460   -1.712008
  C     -2.568081   -2.350412   -0.996077
  O     -2.363683    3.330275   -1.756198
  H     -3.066333   -1.608625    3.626449
  H     -3.623323   -2.122859    2.022117
  H     -2.783944   -3.302300    3.080732
  C      0.041397   -5.379312    0.069006
  H      4.752327   -1.919872   -2.480483
  C     -3.931989   -0.184087   -2.110839
  H     -2.116542    0.938025   -1.826316
  C     -3.897917   -2.486458   -1.388793
  H     -2.038511   -3.189102   -0.535819
  C     -3.376376    4.139095   -2.319056
  H     -0.536046    3.191441   -0.596875
  H     -0.286077    2.538651   -2.746640
  H     -0.069655   -6.357575   -0.422450
  H      0.845243   -5.465822    0.822774
  H      0.373519   -4.653293   -0.696899
  C     -4.581104   -1.406897   -1.950769
  H     -4.459177    0.669382   -2.541601
  H     -4.401617   -3.445608   -1.251614
  H     -3.672124    4.963839   -1.645937
  H     -4.281157    3.556826   -2.569969
  H     -2.984360    4.578054   -3.247948
  C      0.104476    2.621925    0.081925
  C      0.490700    1.772406   -2.890977
  H     -5.623197   -1.518577   -2.257412
  C      1.170940    1.850093   -0.424503
  C     -0.214562    2.618651    1.475760
  C      1.621012    1.900400   -1.872132
  H      0.009433    0.786265   -2.828212
  H      0.898901    1.881633   -3.906528
  C      1.832769    0.991811    0.494333
  C      0.461353    1.793906    2.392338
  H     -1.097405    3.167200    1.803023
  C      2.417623    3.196167   -2.073976
  H      2.310522    1.052457   -2.013638
  C      1.470224    0.930485    1.864164
  H      2.598611    0.311739    0.124290
  C      0.050852    1.710331    3.831308
  H      3.232226    3.287176   -1.339474
  H      1.762686    4.076575   -1.971207
  H      2.859937    3.214137   -3.080962
  H      1.946615    0.187495    2.506448
  H      0.128055    0.679122    4.200405
  H      0.718064    2.342913    4.435972
  H     -0.979501    2.063150    3.966570
*
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```

TS(C^1-D^+)•S_3

CPCM (MeOH)
wB97X-D3 SCF (DZ) = -2076.583094
G (1 atm) = -2076.020169
qh G-E (1 mol/L) = 0.583911
qh G-E (24.56 mol/L) = 0.586934
Lowest Frequency = -37.83

SMD (MeOH)
HF SCF energy (TZ) = -2066.289473
HF SCF energy (QZ) = -2066.390462
Correlation energy (DZ) = -5.982357
Correlation energy (TZ) = -7.367186
DLPNO-CCSD(T1)/CBS = -2074.597283

*xyz 0 1

Ru	-0.373339	0.364424	0.598364
C	1.249886	0.981405	1.841887
C	1.647027	1.092726	0.484407
C	0.094896	1.659803	2.326007
H	1.793826	0.306767	2.502487
C	-0.667812	2.368142	1.372822
C	-0.277409	2.472065	0.004162
C	0.908924	1.867669	-0.455144
Cl	-3.788095	1.256846	0.723854
C	2.090909	-2.103646	0.346862
N	-0.468245	-1.056953	-1.025201
O	0.231422	-1.624570	3.245194
O	-1.194261	-1.187154	1.572845
H	2.517146	0.532386	0.141388
C	-0.353809	1.547660	3.753569
H	-1.640877	2.765361	1.664258
H	-0.959488	2.964671	-0.693033
C	1.425935	2.011318	-1.873423
H	-3.129250	2.487800	-0.939586
H	-5.418999	1.145664	-0.777367
H	-3.560292	0.624817	2.782361
C	1.840306	-1.877321	-1.012298
C	3.404453	-2.185395	0.802826
H	1.263105	-2.207911	1.050831
C	-1.788634	-1.274574	-1.559930
C	0.464528	-1.786016	-1.526952
C	-0.878985	-1.716185	2.730558
H	-1.435510	1.356153	3.810169
H	-0.136816	2.493265	4.272966
H	0.174373	0.733483	4.263274
C	0.355533	1.948423	-2.959980
C	2.217607	3.325653	-1.938435
H	2.131982	1.180689	-2.037425
O	-2.844226	3.017553	-1.711740
O	-6.216934	1.267844	-1.326077
O	-3.554388	0.471724	3.748426
C	2.906512	-1.771695	-1.914259
C	4.466946	-2.031006	-0.089215
H	3.596999	-2.363619	1.862740
C	-2.517652	-0.211777	-2.090051
C	-2.339841	-2.558666	-1.510670
H	0.223007	-2.397920	-2.408143
C	-2.020435	-2.464024	3.374768
H	0.815683	2.148030	-3.938810
H	-0.442930	2.690284	-2.804999
H	-0.107060	0.952896	-3.006536
H	2.999522	3.363356	-1.164800
H	1.548514	4.189073	-1.792259
H	2.700979	3.427737	-2.921285

```
 C   -3.959083    3.789070   -2.124588
 C   -7.138547    1.986942   -0.532756
 C   -4.577542    1.280494    4.294451
 C    4.217676   -1.825100   -1.447530
 H    2.706211   -1.620819   -2.977861
 H    5.495818   -2.082357    0.273704
 C   -3.790793   -0.444699   -2.604746
 H   -2.114181    0.800574   -2.094280
 C   -3.619417   -2.778904   -2.016000
 H   -1.771656   -3.373893   -1.057189
 H   -2.495500   -3.134856    2.645690
 H   -2.770120   -1.721785    3.690949
 H   -1.666954   -3.032733    4.242874
 H   -4.161535    4.625821   -1.431547
 H   -4.866642    3.167695   -2.199922
 H   -3.732634    4.210366   -3.114644
 H   -8.057719    2.124409   -1.121536
 H   -7.403782    1.447468    0.395232
 H   -6.760842    2.987434   -0.250088
 H   -5.573190    1.019002    3.892471
 H   -4.402475    2.355758    4.109356
 H   -4.593128    1.117628    5.381887
 H    5.048199   -1.713898   -2.147381
 C   -4.345522   -1.723068   -2.568400
 H   -4.363644    0.389867   -3.012491
 H   -4.050949   -3.780931   -1.970564
 H   -5.351062   -1.893863   -2.958451
*
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TS(C^1-D^+)•S_3^P

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -2076.586048
G (1 atm) =               -2076.022145
qh G-E (1 mol/L) =            0.583555
qh G-E (24.56 mol/L) =        0.586578
Lowest Frequency =           -28.6

SMD (MeOH)
HF SCF energy (TZ) =      -2066.290084
HF SCF energy (QZ) =      -2066.391786
Correlation energy (DZ) =    -5.980447
Correlation energy (TZ) =    -7.365565
DLPNO-CCSD(T1)/CBS =      -2074.597370

*xyz 0 1
Ru  -0.383218    0.497381    0.622392
 O    0.033877   -1.436349    3.281777
 C    1.929700   -2.155384    0.493373
 C   -1.075084   -1.533158    2.744141
 H    1.074599   -2.196467    1.169827
 H    1.200865   -2.677620    3.732106
 N   -0.511948   -0.961580   -0.955273
 Cl  -3.788342    1.769063    0.757777
 O   -1.373989   -0.955313    1.619270
 C    1.743358   -1.913867   -0.873075
 C    3.213948   -2.342930    0.998379
 C   -2.198716   -2.336045    3.344367
 O    1.848914   -3.404803    3.806073
 C   -1.830418   -1.112069   -1.514948
 C    0.393988   -1.740957   -1.431513
 H   -3.039793    2.782699   -0.975482
 H   -3.534205    0.908062    2.721294
 C    2.846289   -1.890143   -1.736318
 C    4.315445   -2.268543    0.144544
 H    3.329226   -2.558471    2.062708
```

H	-2.638309	-2.998735	2.586493
H	-2.972288	-1.622152	3.666453
H	-1.842690	-2.918453	4.202004
C	1.205760	-4.563891	3.320674
C	-2.510277	-0.004137	-2.017371
C	-2.432147	-2.374922	-1.517713
H	0.143244	-2.341140	-2.318039
O	-2.651059	3.238725	-1.752780
O	-3.514311	0.661066	3.669135
C	4.131601	-2.040564	-1.221254
H	2.696253	-1.728496	-2.806551
H	5.323976	-2.403116	0.541890
H	1.932012	-5.390404	3.333422
H	0.342896	-4.859882	3.946456
H	0.847060	-4.445270	2.280571
C	-3.782919	-0.170298	-2.560687
H	-2.066623	0.991386	-1.989529
C	-3.707519	-2.528888	-2.055493
H	-1.905967	-3.226411	-1.080491
C	-3.636115	4.100484	-2.287345
C	-4.330137	1.593414	4.349502
H	4.992982	-1.992564	-1.890435
C	-4.382970	-1.428036	-2.585162
H	-4.308630	0.700813	-2.956897
H	-4.176671	-3.514832	-2.054030
H	-3.960401	4.864154	-1.558214
H	-4.528291	3.547173	-2.630768
H	-3.198679	4.616677	-3.153939
H	-5.370559	1.585597	3.977130
H	-3.942757	2.625637	4.267360
H	-4.345108	1.317359	5.414054
H	-5.383104	-1.550528	-3.006080
C	1.264370	1.017632	1.877830
C	1.682386	1.089595	0.524273
C	0.155512	1.781067	2.345780
H	1.756769	0.316155	2.550706
C	1.004310	1.898456	-0.430945
H	2.515733	0.467489	0.196560
C	-0.313411	1.715389	3.769928
C	-0.551826	2.525627	1.380037
C	1.540366	1.989622	-1.846482
C	-0.146804	2.580243	0.011886
H	-1.389262	1.488966	3.813063
H	-0.138829	2.689065	4.251420
H	0.229187	0.940388	4.323066
H	-1.501500	2.985995	1.655409
C	0.476030	1.980399	-2.940819
C	2.416038	3.248964	-1.922014
H	2.192453	1.112944	-1.993750
H	-0.796676	3.098779	-0.697900
H	0.954955	2.138881	-3.918161
H	-0.275899	2.772024	-2.800609
H	-0.047885	1.015184	-2.979697
H	3.193015	3.246179	-1.142494
H	1.803488	4.155876	-1.792400
H	2.912259	3.306292	-2.902070

*

TS(C^2-D^+)

CPCM (MeOH)

M06 SCF (DZ) = -1496.944213

G (1 atm) = -1496.491936

qh-G (1 mol/L) = -1496.482980

qh-G (24.56 mol/L) = -1496.479958

Lowest Frequency = -62.48

TS(C^2-D^+)

CPCM (MeOH)

wB97X-D3 SCF (DZ) = -1497.641295

G (1 atm) = -1497.175965

qh G-E (1 mol/L) = 0.478458

qh G-E (24.56 mol/L) = 0.481481

Lowest Frequency = -65.97

```
HF SCF energy (TZ) =      -1488.731473
HF SCF energy (QZ) =      -1488.823135
Correlation energy (DZ) =    -5.380160
Correlation energy (TZ) =    -6.588799
DLPNO-CCSD(T1)/CBS =      -1496.145804

*xyz 0 1
 Ru  -0.324584   -0.629373   -0.026229
 N   -0.389555    1.512132    0.435690
 O    0.108804   -0.742701    1.919602
 C   -1.464891    2.227350    0.419776
 C    0.852169    2.186005    0.647889
 O    2.781985   -1.533367    0.629104
 C    0.486130   -1.835875    2.559736
 C   -2.817703    1.681957    0.447718
 H   -1.372817    3.325614    0.392936
 C    2.004138    1.717399    0.012781
 C    0.937276    3.287148    1.509863
 C    3.710968   -1.055055   -0.071289
 C    1.497072   -1.548745    3.631839
 O    0.088454   -2.962414    2.309014
 C   -3.808689    2.261933   -0.355805
 C   -3.148109    0.622005    1.305624
 C    3.216244    2.375383    0.190668
 H    1.980020    0.823794   -0.618184
 C    2.154182    3.938758    1.684672
 H    0.058929    3.615124    2.071815
 C    5.056234   -0.860875    0.626698
 O    3.628948   -0.697281   -1.277255
 H    1.236793   -0.644073    4.198735
 H    2.445609   -1.361066    3.102755
 H    1.612650   -2.408771    4.303905
 C   -5.098876    1.744047   -0.352039
 H   -3.553684    3.108266   -1.000295
 C   -4.450179    0.133754    1.333349
 H   -2.386282    0.208309    1.972879
 C    3.295279    3.493512    1.018638
 H    4.099223    1.987851   -0.324617
 H    2.211808    4.793628    2.362672
 H    5.299599   -1.728870    1.259116
 H    4.982171    0.012277    1.298283
 H    5.870605   -0.677611   -0.089913
 C   -5.419911    0.680786    0.492655
 H   -5.862647    2.179521   -0.999956
 H   -4.712237   -0.676413    2.018213
 H    4.248943    4.006956    1.162716
 H   -6.439245    0.287684    0.509095
 C   -2.041364   -1.248005   -1.151556
 C   -1.480205   -2.422062   -0.558096
 C   -1.284034   -0.406082   -2.003320
 H   -3.075105   -0.979621   -0.915733
 C   -2.315536   -3.285608    0.322625
 C   -0.102093   -2.665284   -0.765120
 C    0.084724   -0.654576   -2.221847
 H   -1.745419    0.511357   -2.378059
 H   -1.698512   -3.767230    1.090639
 H   -3.109152   -2.699528    0.810683
 H   -2.805686   -4.058383   -0.292721
 C    0.670177   -1.771076   -1.549822
 H    0.391373   -3.460640   -0.203836
 C    0.960706    0.214569   -3.088727
 H    1.765520   -1.838363   -1.554844
 C    0.450169    1.633648   -3.270452
 C    1.110606   -0.485255   -4.440457
 H    1.956569    0.226874   -2.608282
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HF SCF energy (TZ) =      -1488.734493
HF SCF energy (QZ) =      -1488.825018
Correlation energy (DZ) =    -5.380533
Correlation energy (TZ) =    -6.588670
DLPNO-CCSD(T1)/CBS =      -1496.146922

SMD (MeOH)
HF SCF energy (TZ) =      -1488.758242
HF SCF energy (QZ) =      -1488.848357
Correlation energy (DZ) =    -5.374209
Correlation energy (TZ) =    -6.583285
DLPNO-CCSD(T1)/CBS =      -1496.165302

*xyz 0 1
 Ru   0.306372   -0.612800    0.037293
 O   -0.119972   -0.728573   -1.908329
 C   -0.502765   -1.804407   -2.570321
 C   -1.535785   -1.502536   -3.626854
 O   -0.095599   -2.936847   -2.352687
 C    2.059684   -1.180624    1.119988
 C    1.288790   -0.366070    1.986575
 C    1.522740   -2.362385    0.524791
 C   -0.067787   -0.655464    2.227111
 C    2.376618   -3.208403   -0.369396
 C    0.157446   -2.654847    0.758903
 C   -0.957086    0.187183    3.119240
 C   -0.626356   -1.788021    1.560350
 C   -0.488474    1.631671    3.278637
 C   -1.064709   -0.515056    4.480430
 H   -1.276108   -0.593167   -4.184867
 H   -2.476657   -1.319547   -3.085587
 H   -1.656900   -2.353493   -4.307662
 H    3.081560   -0.885868    0.879326
 H    1.728899    0.558052    2.362749
 H    3.159619   -2.604714   -0.847580
 H    2.867944   -3.978959    0.244749
 H    1.765723   -3.687579   -1.141144
 H   -0.321563   -3.468951    0.216384
 H   -1.956604    0.167794    2.655529
 H   -1.712055   -1.903841    1.590450
 H   -0.340886    2.128479    2.307631
 H    0.456421    1.693131    3.841749
 H   -1.242340    2.204868    3.837778
 H   -1.460710   -1.536659    4.375814
 H   -0.079356   -0.576899    4.970489
 H   -1.741339    0.046966    5.141426
 N    0.394924    1.503776   -0.449264
 C    1.461207    2.222788   -0.461812
 C   -0.854299    2.170216   -0.687209
 C    2.821252    1.660762   -0.449143
 C   -1.993302    1.746404   -0.002470
 C   -0.946461    3.208519   -1.621008
 C    3.765692    2.148140    0.461888
 C    3.181816    0.670216   -1.372622
 C   -3.206460    2.400113   -0.200495
 C   -2.165368    3.853621   -1.818965
 C    5.048377    1.605841    0.485702
 C    4.476533    0.157034   -1.366841
 C   -3.295916    3.460726   -1.101396
 C    5.404638    0.612844   -0.429167
 H    1.366837    3.316745   -0.504843
 H   -1.958720    0.893900    0.678232
 H   -0.074463    3.495341   -2.212455
 H    3.485662    2.933835    1.167479
 H    2.447825    0.311614   -2.098061
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 H    0.274182    2.143710   -2.308711
 H   -0.489677    1.657258   -3.849031
 H    1.187393    2.227028   -3.833117
 H    0.132189   -0.579698   -4.943319
 H    1.776063    0.095452   -5.098406
 H    1.536973   -1.495374   -4.330895
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 H   -4.082708    2.059065    0.354160
 H   -2.232267    4.661375   -2.550507
 H    5.776316    1.965497    1.215501
 H    4.759115   -0.607317   -2.093291
 H   -4.249651    3.968491   -1.258865
 H    6.414623    0.197608   -0.417053
 O   -2.792465   -1.431806   -0.582711
 C   -3.741612   -1.006487    0.128508
 C   -5.093727   -0.827105   -0.570399
 O   -3.669785   -0.693000    1.347653
 H   -5.316377   -1.691930   -1.212605
 H   -5.037634    0.059047   -1.223776
 H   -5.907053   -0.676493    0.152420
*
---------------------------------------
```

***cis*-TS(D⁺-E⁺)1**

```
CPCM (MeOH)
M06 SCF (DZ) =             -1268.423417
G (1 atm) =                -1268.015545
qh-G (1 mol/L) =           -1268.007284
qh-G (24.56 mol/L) =       -1268.004262
Lowest Frequency =           -83.52

HF SCF energy (TZ) =       -1261.304965
HF SCF energy (QZ) =       -1261.379607
Correlation energy (DZ) =     -4.690606
Correlation energy (TZ) =     -5.726332
DLPNO-CCSD(T1)/CBS =       -1267.733641

PBE0+D3BJ (ATZ) =          -1268.358470
M06-2X (ATZ) =             -1269.066768
wB97M-V (ATZ) =            -1269.137265
B2GP-PLYP (ATZ) =          -1268.390678
B2K-PLYP (ATZ) =           -1268.223812
PWPB95 (ATZ) =             -1268.728763
PWPB95+D3BJ (ATZ) =        -1268.770053
PWPB95+D4 (ATZ) =          -1268.784186

*xyz 0 1
 Ru   0.012285   -0.754495    0.118315
 C   -0.524890   -1.586517    1.995378
 C    1.505992    0.443484   -1.823074
 C   -0.212192   -2.694798    1.146381
 C    0.418009   -0.542837    2.223423
 H   -1.524677   -1.514575    2.432317
 O   -0.515410   -1.944139   -2.441606
 H    0.646370   -0.248817   -1.947161
 N   -0.680175    1.267260   -0.161439
 O   -1.815634   -1.124736   -0.837433
 C    2.736887    0.042794   -2.333538
 C    1.322221    1.760966   -1.373165
 C   -1.230552   -3.743348    0.863621
 C    1.028030   -2.666221    0.477643
 C    1.685465   -0.530234    1.583851
 H    0.122109    0.304815    2.845927
 C   -1.639425   -1.718625   -1.973735
 C   -2.000196    1.660468    0.215628
 C    0.049240    2.133466   -0.784410
 C    3.786367    0.958749   -2.399210
 H    2.866717   -0.979405   -2.698408
 C    2.368699    2.684557   -1.475438
 H   -1.044962   -4.230981   -0.103835
 H   -1.184991   -4.515022    1.648787
 H   -2.244544   -3.318558    0.866407
 C    1.938191   -1.590068    0.679535
```

***cis*-TS(D⁺-E⁺)1**

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =        -1269.057300
G (1 atm) =                -1268.636115
qh G-E (1 mol/L) =             0.432212
qh G-E (24.56 mol/L) =         0.435234
Lowest Frequency =           -64.30

HF SCF energy (TZ) =       -1261.309240
HF SCF energy (QZ) =       -1261.382685
Correlation energy (DZ) =     -4.689597
Correlation energy (TZ) =     -5.724750
DLPNO-CCSD(T1)/CBS =       -1267.734441

PBE0+D3BJ (ATZ) =          -1268.358835
M06-2X (ATZ) =             -1269.082173
wB97M-V (ATZ) =            -1269.144367
B2GP-PLYP (ATZ) =          -1268.407975
B2K-PLYP (ATZ) =           -1268.244041
PWPB95 (ATZ) =             -1268.740983
PWPB95+D3BJ (ATZ) =        -1268.781821
PWPB95+D4 (ATZ) =          -1268.796103

SMD (MeOH)
HF SCF energy (TZ) =       -1261.327972
HF SCF energy (QZ) =       -1261.401370
Correlation energy (DZ) =     -4.684747
Correlation energy (TZ) =     -5.721239
DLPNO-CCSD(T1)/CBS =       -1267.750385

*xyz 0 1
 Ru  -0.007006    0.769426   -0.147251
 O   -0.714402    1.874600    2.512830
 O   -1.842437    1.143806    0.741326
 C   -1.784522    1.644123    1.933268
 C   -3.122130    1.942759    2.561932
 C    1.911617    1.630130   -0.682140
 C    0.963559    2.691064   -0.592922
 C    1.726931    0.507516   -1.521852
 C   -0.244335    2.632764   -1.314447
 C    2.748554   -0.586890   -1.620694
 C    0.487313    0.433020   -2.209169
 C   -1.318253    3.693650   -1.226565
 C   -0.493633    1.455858   -2.090938
 C   -1.174010    4.627741   -0.028632
 C   -1.320419    4.474479   -2.549768
 H   -3.775668    1.062246    2.489643
 H   -3.603304    2.761134    2.006014
 H   -2.997494    2.238147    3.609813
 H    2.787527    1.662049   -0.031602
```

H	1.244541	-3.413319	-0.288943
C	2.707219	0.563814	1.777075
C	-2.902053	-2.137727	-2.669684
C	-2.426558	1.524945	1.536884
C	-2.868255	2.164800	-0.755305
H	-0.298266	3.174612	-0.867187
C	3.600512	2.276657	-1.976169
H	4.753081	0.648994	-2.802332
H	2.217641	3.713434	-1.137606
H	2.838975	-1.546283	0.059343
C	2.131538	1.853436	2.339409
C	3.822252	0.032650	2.676826
H	3.137830	0.772695	0.778533
H	-3.632587	-1.316173	-2.668611
H	-3.353624	-2.974290	-2.113214
H	-2.692820	-2.460674	-3.696675
C	-3.714441	1.915409	1.888234
H	-1.740792	1.144708	2.296001
C	-4.158263	2.545340	-0.397068
H	-2.534025	2.228754	-1.794491
H	4.423631	2.991079	-2.041399
H	1.272603	2.226883	1.757633
H	1.805795	1.725446	3.385942
H	2.904083	2.637312	2.336519
H	4.293112	-0.870402	2.257759
H	3.424463	-0.221332	3.674218
H	4.603514	0.797166	2.807047
C	-4.583891	2.423274	0.923707
H	-4.039194	1.823021	2.926978
H	-4.836992	2.932233	-1.160575
H	-5.597398	2.720047	1.202743

*

H	1.152312	3.500160	0.110987
H	3.373551	-0.624294	-0.718294
H	3.402034	-0.393571	-2.484496
H	2.267188	-1.563565	-1.765282
H	0.252903	-0.467260	-2.780075
H	-2.276506	3.155853	-1.140097
H	-1.465196	1.325139	-2.571001
H	-1.103493	4.075697	0.920007
H	-0.282174	5.267525	-0.121407
H	-2.050858	5.288562	0.026292
H	-1.479443	3.811582	-3.413392
H	-0.363140	5.000562	-2.691633
H	-2.126387	5.222398	-2.540809
C	1.471148	-0.347119	1.857553
C	2.687603	0.091424	2.375548
C	1.329088	-1.670749	1.414086
N	-0.667738	-1.245935	0.169934
C	3.762109	-0.794774	2.456207
C	2.398177	-2.565548	1.530396
C	0.061065	-2.086688	0.816784
C	-1.989340	-1.664211	-0.205456
C	3.615129	-2.120791	2.040701
C	-2.382620	-1.653000	-1.543341
C	-2.885195	-2.055892	0.791222
C	-3.673760	-2.050278	-1.883086
C	-4.176661	-2.447858	0.443089
C	-4.574302	-2.445887	-0.893212
H	0.596477	0.330327	1.950732
H	2.788606	1.120072	2.726696
H	4.716902	-0.453119	2.860843
H	2.280519	-3.598965	1.197499
H	-0.275353	-3.125019	0.933260
H	4.456179	-2.812282	2.117069
H	-1.679773	-1.357861	-2.321664
H	-2.573498	-2.031343	1.837527
H	-3.975444	-2.051301	-2.932343
H	-4.876393	-2.748751	1.225305
H	-5.587420	-2.749309	-1.164509

*

TS(D^+-E^+)1•S^p

CPCM (MeOH)
wB97X-D3 SCF (DZ) = -1384.773345
G (1 atm) = -1384.302956
qh G-E (1 mol/L) = 0.483321
qh G-E (24.56 mol/L) = 0.486344
Lowest Frequency = -66.67

SMD (MeOH)
HF SCF energy (TZ) = -1376.424166
HF SCF energy (QZ) = -1376.505864
Correlation energy (DZ) = -5.064472
Correlation energy (TZ) = -6.192576
DLPNO-CCSD(T1)/CBS = -1383.382248

*xyz 0 1

Ru	-0.144996	0.945499	0.071897
C	1.451035	0.162659	2.136904
O	-0.858109	2.198040	2.685635
C	2.647729	0.731298	2.564806
C	1.379382	-1.210993	1.861564
H	0.538498	0.793067	2.178642
N	-0.664736	-1.051509	0.634897
O	-1.980740	1.392721	0.948911
C	-1.936038	1.925745	2.116811

H	-0.963319	1.738769	4.433297
C	3.777110	-0.074549	2.716238
H	2.691620	1.798428	2.790651
C	2.504067	-2.020865	2.048318
C	0.134881	-1.772710	1.336271
C	-1.901403	-1.649523	0.204371
C	-3.254180	2.226969	2.777636
O	-1.177356	1.246525	5.249569
C	3.703518	-1.446364	2.463166
H	4.718446	0.366642	3.049996
H	2.442532	-3.092087	1.844387
H	-0.113526	-2.822495	1.539349
C	-1.936526	-2.378659	-0.983928
C	-3.049184	-1.489767	0.980620
H	-3.179020	1.977866	3.844454
H	-3.443172	3.307940	2.693611
H	-4.077965	1.680699	2.304327
C	-1.022597	-0.121791	4.938868
H	4.587709	-2.073054	2.593376
C	-3.139884	-2.944584	-1.403830
H	-1.023556	-2.512425	-1.567746
C	-4.246047	-2.060879	0.552362
H	-2.997420	-0.924433	1.911405
H	0.034043	-0.400592	4.763417
H	-1.603072	-0.422037	4.044945
H	-1.390452	-0.711905	5.791606
C	-4.296027	-2.783113	-0.640684
H	-3.168445	-3.519110	-2.331860
H	-5.145389	-1.940776	1.159920
H	-5.237047	-3.226343	-0.972874
C	-0.806800	1.681667	-1.803092
C	-0.045672	0.505601	-2.013129
C	-0.263300	2.810791	-1.103558
H	-1.852452	1.696015	-2.115859
C	1.293411	0.385970	-1.524650
H	-0.524544	-0.350763	-2.490857
C	-1.134965	4.028519	-0.879248
C	1.033792	2.671737	-0.580857
C	2.084352	-0.874607	-1.712840
C	1.793213	1.475393	-0.787193
C	-0.702663	4.893229	0.302475
C	-1.175823	4.837312	-2.183495
H	-2.148974	3.645074	-0.677673
H	1.449080	3.441646	0.069396
H	1.437687	-1.760400	-1.648000
H	2.546485	-0.864221	-2.711267
H	2.881722	-0.953795	-0.962275
H	2.759470	1.378727	-0.289165
H	-0.632717	4.309695	1.232507
H	0.271171	5.374131	0.117700
H	-1.440313	5.693906	0.457076
H	-1.534093	4.229993	-3.028350
H	-0.173466	5.219177	-2.434911
H	-1.852714	5.696645	-2.070039

*

TS(D^+-E^+)1•S_2^{kp}

CPCM (MeOH)
wB97X-D3 SCF (DZ) = -1500.489575
G (1 atm) = -1499.970338
qh G-E (1 mol/L) = 0.534052
qh G-E (24.56 mol/L) = 0.537075
Lowest Frequency = -59.53

SMD (MeOH)

```
HF SCF energy (TZ) =      -1491.519672
HF SCF energy (QZ) =      -1491.609319
Correlation energy (DZ) =    -5.447107
Correlation energy (TZ) =    -6.667124
DLPNO-CCSD(T1)/CBS =      -1499.016354

*xyz 0 1
 Ru  -0.088462    0.962792    0.072379
 C   -0.703142    1.583167   -1.861204
 C    0.182776    0.483257   -1.993827
 C   -0.306894    2.776585   -1.170095
 H   -1.732830    1.490867   -2.214203
 C    1.832139    1.650920   -0.679490
 C    0.963019    2.780208   -0.566102
 C    1.486957    0.498728   -1.417390
 C    1.522419    0.043935    2.152241
 H    0.646395    0.720238    2.195074
 O   -1.922575    1.413722    0.963164
 N   -0.654613   -1.028732    0.604014
 H   -0.178340   -0.425984   -2.476143
 C   -1.307962    3.902868   -1.030456
 H    2.764867    1.654371   -0.112228
 H    1.265422    3.605405    0.078098
 C    2.402116   -0.686017   -1.516315
 C    2.746355    0.532945    2.600421
 C    1.376634   -1.315045    1.838372
 O   -0.777120    2.145855    2.707317
 C   -1.866181    1.911318    2.151617
 H   -3.246097    1.365504   -0.266701
 C   -1.933118   -1.547246    0.191892
 C    0.105686   -1.797738    1.298449
 C   -1.038452    4.833762    0.148649
 C   -1.348006    4.672687   -2.358407
 H   -2.286822    3.417453   -0.887661
 H    1.831564   -1.624962   -1.512128
 H    2.962955   -0.631471   -2.461284
 H    3.121975   -0.697052   -0.687080
 C    3.827915   -0.338568    2.737096
 H    2.848443    1.589413    2.855601
 C    2.452824   -2.191706    2.012053
 H   -0.871730    1.727903    4.478785
 C   -3.177315    2.210596    2.822480
 O   -3.730695    1.389475   -1.113539
 C   -2.069307   -2.140687   -1.061991
 C   -3.025598   -1.432780    1.051452
 H   -0.199998   -2.835007    1.487808
 H   -0.944199    4.283072    1.096419
 H   -0.118598    5.421578   -0.000140
 H   -1.870827    5.544838    0.250637
 H   -1.594879    4.012103   -3.203213
 H   -0.375287    5.147028   -2.564737
 H   -2.112085    5.462197   -2.308915
 C    3.679329   -1.697397    2.449339
 H    4.789829    0.040731    3.087904
 H    2.332791   -3.252272    1.780464
 O   -1.092897    1.246273    5.298364
 H   -3.992837    1.622976    2.384613
 H   -3.396713    3.280468    2.685377
 H   -3.081821    2.012000    3.897608
 C   -5.109928    1.511727   -0.830333
 C   -3.319497   -2.609106   -1.464282
 H   -1.199206   -2.249970   -1.711724
 C   -4.269749   -1.907129    0.641374
 H   -2.896051   -0.973535    2.032210
 H    4.525572   -2.376239    2.569703
 C   -0.932734   -0.125667    5.005417
```

***trans*-TS(D^+-E^+)1**
CPCM (MeOH)
M06 SCF (DZ) = -1268.423984
G (1 atm) = -1268,018208
qh-G (1 mol/L) = -1268.008804
qh-G (24.56 mol/L) = -1268.005781
Lowest Frequency = -94.81

HF SCF energy (TZ) = -1261.306201
HF SCF energy (QZ) = -1261.380774
Correlation energy (DZ) = -4.690084
Correlation energy (TZ) = -5.725573
DLPNO-CCSD(T1)/CBS = -1267.733889

*xyz 1 1

Ru	-0.168044	-0.692074	-0.182576
C	0.882952	-2.055540	-1.422859
C	1.774813	-1.549469	-0.438696
C	-0.325613	-2.726792	-1.052304
H	1.094050	-1.876109	-2.480943
C	0.256859	-2.237695	1.304968
C	-0.629837	-2.774184	0.320554
C	1.492330	-1.654644	0.955557
C	-1.775077	0.752558	1.654388
N	0.508519	1.329147	-0.045838
H	-0.920091	0.104510	1.893621
O	-2.940116	-0.785872	-0.721666
O	-1.236263	0.175499	-1.770930
H	2.662837	-0.995715	-0.760065
C	-1.274660	-3.214525	-2.091616
H	-0.075301	-2.224803	2.346729
H	-1.614933	-3.127812	0.634189
C	2.466437	-1.094270	1.960594
C	-1.560284	1.967287	0.985423
C	-3.033724	0.433598	2.154270
C	1.788709	1.711152	-0.552327
C	-0.269596	2.262068	0.394725
C	-2.498456	-0.099731	-1.648498
H	-2.304362	-3.232369	-1.711390
H	-1.233707	-2.579462	-2.989088
H	-0.993451	-4.236203	-2.393315
C	1.815390	-0.492519	3.194578
C	3.445115	-2.206018	2.337480
H	3.031993	-0.298085	1.439768
C	-2.617086	2.879080	0.850343
C	-4.083880	1.329465	1.987233
H	-3.186218	-0.511524	2.679560
C	2.708876	2.353049	0.277031
C	2.111241	1.414189	-1.878270
H	0.038510	3.313912	0.291698
C	-3.378377	0.479650	-2.719440
H	2.588031	-0.055886	3.845384
H	1.104089	0.311542	2.941358
H	-5.342382	2.440799	-0.279184
H	-5.651016	1.537975	-1.787289
H	-5.490878	0.655764	-0.244679
C	-4.421648	-2.487794	-0.618320
H	-3.427405	-3.077043	-2.444851
H	-5.125711	-1.819820	1.313718
H	-1.311210	-0.705952	5.860157
H	-1.500697	-0.436233	4.107261
H	0.126485	-0.404567	4.846928
H	-5.399702	-2.852798	-0.938270

*

***trans*-TS(D^+-E^+)1**
CPCM (MeOH)
wB97X-D3 SCF (DZ) = -1269.057905
G (1 atm) = -1268.637701
qh G-E (1 mol/L) = 0.432175
qh G-E (24.56 mol/L) = 0.435198
Lowest Frequency = -98.64

HF SCF energy (TZ) = -1261.309813
HF SCF energy (QZ) = -1261.383199
Correlation energy (DZ) = -4.689597
Correlation energy (TZ) = -5.724750
DLPNO-CCSD(T1)/CBS = -1267.734937

SMD (MeOH)
HF SCF energy (TZ) = -1261.331451
HF SCF energy (QZ) = -1261.404674
Correlation energy (DZ) = -4.684880
Correlation energy (TZ) = -5.720875
DLPNO-CCSD(T1)/CBS = -1267.752980

*xyz 1 1

Ru	-0.185278	-0.683953	-0.205516
C	0.767322	-2.122151	-1.434096
C	1.712579	-1.598378	-0.515787
C	-0.443546	-2.736063	-0.981379
C	0.265946	-2.176050	1.327988
C	-0.684477	-2.715568	0.403691
C	1.496663	-1.647001	0.896418
C	-1.452006	-3.258128	-1.959208
C	2.553092	-1.108195	1.839951
C	1.995512	-0.358119	3.047712
C	3.445448	-2.283438	2.263773
H	0.938232	-1.989670	-2.503713
H	2.597802	-1.090148	-0.902429
H	-0.011315	-2.126836	2.382222
H	-1.657625	-3.033613	0.780396
H	-2.456831	-3.264755	-1.521425
H	-1.460457	-2.647363	-2.871953
H	-1.178658	-4.286684	-2.239208
H	3.169670	-0.407540	1.253444
H	2.827334	0.018437	3.660213
H	1.385868	0.506324	2.743778
H	1.381629	-1.007508	3.691103
H	2.868624	-3.018877	2.847102
H	3.873762	-2.797163	1.389952
H	4.274035	-1.921711	2.889986
C	-1.724346	0.766017	1.778550
N	0.513235	1.322939	-0.032606
C	-1.593233	1.889163	0.949503
C	-2.978061	0.400121	2.270730
C	1.812234	1.724030	-0.489234
C	-0.284493	2.238391	0.391967

```
 H    1.284226   -1.251803    3.792983
 H    2.916048   -3.028576    2.848665
 H    3.948596   -2.623426    1.451258
 H    4.216762   -1.819682    3.020731
 C   -3.874807    2.549792    1.336838
 H   -2.448529    3.831027    0.340307
 H   -5.074307    1.086914    2.378765
 C    3.965384    2.688798   -0.224584
 H    2.444695    2.566777    1.316878
 C    3.363784    1.763227   -2.371102
 H    1.368068    0.924449   -2.513899
 H   -3.096425    0.059658   -3.697099
 H   -3.227352    1.567724   -2.780516
 H   -4.433700    0.260205   -2.516379
 H   -4.703550    3.250615    1.215981
 C    4.294940    2.394034   -1.544708
 H    4.690652    3.181586    0.426810
 H    3.614777    1.541011   -3.410706
 H    5.281312    2.656380   -1.933765
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 C   -2.719900    2.664100    0.638833
 C   -4.097300    1.152679    1.932751
 C    2.697811    2.349533    0.387703
 C    2.179190    1.461872   -1.810736
 C   -3.966929    2.283698    1.118868
 C    3.966201    2.713921   -0.065481
 C    3.443472    1.838208   -2.255264
 C    4.340599    2.459658   -1.383493
 H   -0.832453    0.239548    2.127374
 H   -3.068907   -0.468523    2.925123
 H    0.006773    3.294561    0.319138
 H   -2.615017    3.547209    0.004922
 H   -5.080531    0.868431    2.313083
 H    2.400184    2.532753    1.422463
 H    1.469514    0.973959   -2.482469
 H   -4.847985    2.875447    0.863234
 H    4.664037    3.196230    0.621706
 H    3.729400    1.641953   -3.290395
 H    5.334021    2.746316   -1.734082
 O   -2.999719   -0.647428   -0.766131
 O   -1.213089    0.179916   -1.795670
 C   -2.496262    0.004485   -1.685468
 C   -3.325156    0.670392   -2.756290
 H   -3.016396    0.306783   -3.746618
 H   -3.147660    1.755272   -2.730993
 H   -4.390313    0.466632   -2.597949
*
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***cis*-TS(D^+-E^+)2**

```
CPCM (MeOH)
M06 SCF (DZ) =            -1268.417869
G (1 atm) =               -1268.012919
qh-G (1 mol/L) =          -1268.005188
qh-G (24.56 mol/L) =      -1268.002165
Lowest Frequency =        -1224.78

HF SCF energy (TZ) =      -1261.272053
HF SCF energy (QZ) =      -1261.346291
Correlation energy (DZ) =    -4.714451
Correlation energy (TZ) =    -5.751333
DLPNO-CCSD(T1)/CBS =      -1267.725880

PBE0+D3BJ (ATZ) =         -1268.356554
M06-2X (ATZ) =            -1269.053588
wB97M-V (ATZ) =           -1269.129404
B2GP-PLYP (ATZ) =         -1268.389963
B2K-PLYP (ATZ) =          -1268.224294
PWPB95 (ATZ) =            -1268.724225
PWPB95+D3BJ (ATZ) =       -1268.766020
PWPB95+D4 (ATZ) =         -1268.780050

*xyz 0 1
 Ru  -0.072231    0.550217    0.504588
 C    0.641460    1.038844    2.560473
 C   -0.664513    1.582115    2.352756
 C    0.843247   -0.332777    2.292149
 C    1.780525    1.922218    2.934209
 C   -1.718744    0.754580    1.917444
 C   -0.234354   -1.157762    1.850771
 C   -1.539318   -0.645865    1.677765
 C   -1.528477    0.635435   -1.199163
 N    0.816377   -0.677145   -0.996124
 H   -0.647249    1.565262   -1.320690
 O    1.284604    2.051101   -0.117052
 H   -0.827004    2.656107    2.465318
```

***cis*-TS(D^+-E^+)2**

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1269.049411
G (1 atm) =               -1268.632403
qh G-E (1 mol/L) =            0.427438
qh G-E (24.56 mol/L) =        0.430461
Lowest Frequency =        -1123.81

HF SCF energy (TZ) =      -1261.275612
HF SCF energy (QZ) =      -1261.348299
Correlation energy (DZ) =    -4.714641
Correlation energy (TZ) =    -5.751095
DLPNO-CCSD(T1)/CBS =      -1267.726932

PBE0+D3BJ (ATZ) =         -1268.356979
M06-2X (ATZ) =            -1269.064659
wB97M-V (ATZ) =           -1269.135493
B2GP-PLYP (ATZ) =         -1268.402852
B2K-PLYP (ATZ) =          -1268.239081
PWPB95 (ATZ) =            -1268.733062
PWPB95+D3BJ (ATZ) =       -1268.774368
PWPB95+D4 (ATZ) =         -1268.788632

SMD (MeOH)
HF SCF energy (TZ) =      -1261.291123
HF SCF energy (QZ) =      -1261.363790
Correlation energy (DZ) =    -4.711281
Correlation energy (TZ) =    -5.748204
DLPNO-CCSD(T1)/CBS =      -1267.739801

*xyz 0 1
 Ru  -0.346987   -0.102092   -0.279959
 C   -1.277513    0.594517   -2.126542
 C    0.018998    0.140979   -2.437612
 C   -2.213301   -0.228478   -1.423722
 C    1.015757    1.025059   -3.127977
 C    0.364721   -1.195728   -2.037002
```

H	1.851916	-0.750551	2.350061
H	1.833583	2.002470	4.032115
H	1.648237	2.933991	2.526895
H	2.736468	1.514155	2.575694
H	-2.690797	1.206353	1.698414
H	-0.017899	-2.193583	1.575576
C	-2.713410	-1.493122	1.254269
C	-2.815952	1.187287	-1.219248
C	-1.278012	-0.476514	-2.047836
C	2.095797	-1.278972	-0.832903
C	0.050751	-1.037522	-1.976718
O	0.115907	2.545243	-1.944549
C	1.108155	2.709271	-1.195009
C	-3.598239	-1.736889	2.476583
C	-2.323813	-2.811813	0.606946
H	-3.291375	-0.895182	0.524242
C	-3.822112	0.630565	-2.009838
H	-3.028892	2.086067	-0.631773
C	-2.276273	-1.021160	-2.857217
C	3.203928	-0.478416	-0.539402
C	2.230193	-2.668109	-0.916337
H	0.404217	-1.757907	-2.728314
C	2.168891	3.700612	-1.556201
H	-4.487369	-2.321074	2.193175
H	-3.046237	-2.306635	3.243672
H	-3.941115	-0.795284	2.933579
H	-3.222524	-3.316768	0.221106
H	-1.627319	-2.680039	-0.237281
H	-1.856033	-3.495621	1.335900
C	-3.555669	-0.471843	-2.823544
H	-4.821828	1.071642	-2.004931
H	-2.055277	-1.881992	-3.494422
C	4.448580	-1.073054	-0.363815
H	3.074472	0.603635	-0.459268
C	3.480712	-3.251957	-0.731074
H	1.348344	-3.289942	-1.096940
H	2.410805	4.327290	-0.687108
H	3.083570	3.150569	-1.827088
H	1.855392	4.321436	-2.403009
H	-4.347635	-0.896461	-3.443982
C	4.591876	-2.457667	-0.459687
H	5.317182	-0.446621	-0.147745
H	3.581088	-4.338196	-0.789381
H	5.571354	-2.918310	-0.312238

*

C	-1.863116	-1.527660	-1.012043
C	-0.551380	-2.007234	-1.353776
C	-2.783696	-2.412539	-0.195808
C	-3.822908	-1.639615	0.614070
C	-3.443852	-3.432344	-1.132971
H	-1.546626	1.627044	-2.353964
H	-3.176331	0.194267	-1.139508
H	2.040630	0.779822	-2.819152
H	0.944434	0.874733	-4.215701
H	0.818312	2.083350	-2.911423
H	1.384033	-1.555703	-2.192110
H	-0.223222	-2.979149	-0.980411
H	-2.136391	-2.961486	0.507834
H	-3.359344	-0.866624	1.246229
H	-4.565299	-1.150427	-0.036208
H	-4.369167	-2.332954	1.269910
H	-2.694511	-4.022156	-1.682141
H	-4.086682	-2.923691	-1.868934
H	-4.068699	-4.127358	-0.553051
C	-0.748680	1.951408	0.495488
C	-1.923190	2.710429	0.406107
C	0.481815	2.652461	0.523572
N	1.584908	0.588182	0.266121
C	-1.874769	4.102691	0.317039
C	0.535411	4.046648	0.457183
C	1.690728	1.843599	0.541362
C	2.761565	-0.225182	0.221751
C	-0.649452	4.771482	0.345031
C	2.763299	-1.458747	0.878281
C	3.881817	0.195348	-0.500274
C	3.901461	-2.258791	0.828265
C	5.013941	-0.617747	-0.548638
C	5.028270	-1.843056	0.115908
H	-2.893198	2.206572	0.428877
H	-2.803280	4.672716	0.240226
H	1.500455	4.558238	0.474067
H	2.666276	2.287699	0.773872
H	-0.618415	5.860933	0.282925
H	1.875794	-1.771382	1.429519
H	3.861582	1.146220	-1.037636
H	3.906435	-3.217357	1.351211
H	5.886095	-0.289684	-1.117748
H	5.916106	-2.477345	0.076017
H	-0.978076	1.010371	1.402593
O	-0.302687	-1.185137	1.536085
O	-1.270152	0.494717	2.611827
C	-0.828142	-0.685203	2.581524
C	-0.953082	-1.558373	3.793652
H	-0.129366	-2.280426	3.834770
H	-1.898545	-2.115977	3.708161
H	-0.988080	-0.950127	4.704465

*

TS(D^+-E^+)2•S^p

CPCM (MeOH)

wB97X-D3 SCF (DZ) =	-1384.762812
G (1 atm) =	-1384.297313
qh G-E (1 mol/L) =	0.478354
qh G-E (24.56 mol/L) =	0.481377
Lowest Frequency =	-1193.32

SMD (MeOH)

HF SCF energy (TZ) =	-1376.385505
HF SCF energy (QZ) =	-1376.466790
Correlation energy (DZ) =	-5.092514

```
Correlation energy (TZ) =    -6.221497
DLPNO-CCSD(T1)/CBS =      -1383.372484

*xyz 0 1
 Ru  -0.617299   -0.089665   -0.313486
 C   -1.259723    0.445724   -2.331159
 C    0.416923   -1.255237   -1.857910
 C   -2.262874   -0.379208   -1.729272
 C    0.086568    0.036697   -2.397709
 H   -1.530261    1.446240   -2.671767
 C   -0.567443   -2.065797   -1.277272
 C   -1.323077    1.930714    0.283109
 N    1.144121    0.830758    0.445531
 H   -1.539176    1.031846    1.255929
 O   -0.729648   -1.101721    1.547661
 H    1.460671   -1.574701   -1.827587
 C   -1.934993   -1.632086   -1.178853
 H   -3.275155    0.012584   -1.633610
 C    1.147198    0.923226   -2.981049
 H   -0.268511   -2.996056   -0.790180
 C   -2.553896    2.546935    0.019994
 C   -0.190826    2.770626    0.426002
 C    2.394895    0.154757    0.609690
 C    1.082180    2.103599    0.647371
 O   -1.853535    0.575476    2.454081
 C   -1.333506   -0.582162    2.528808
 C   -2.939759   -2.512168   -0.462887
 H    2.120324    0.739493   -2.506678
 H    1.248631    0.706983   -4.055326
 H    0.882801    1.982832   -2.865442
 C   -2.647372    3.932507   -0.125695
 H   -3.459697    1.938619   -0.048475
 C   -0.280939    4.158665    0.301628
 C    2.429422   -1.061799    1.296730
 C    3.563559    0.689296    0.059780
 H    1.965873    2.665311    0.974347
 H   -1.333658    1.571364    4.022708
 C   -1.446537   -1.344536    3.811203
 C   -4.092930   -1.738329    0.173881
 C   -3.446829   -3.579284   -1.441479
 H   -2.381686   -3.018782    0.341720
 C   -1.515899    4.738269    0.015768
 H   -3.616377    4.389971   -0.337421
 H    0.612711    4.777372    0.411907
 C    3.642255   -1.728437    1.449824
 H    1.506880   -1.468814    1.712034
 C    4.771431    0.009888    0.214020
 H    3.525598    1.623383   -0.505165
 O   -0.734548    1.794636    4.753671
 H   -0.810878   -2.235726    3.795079
 H   -2.497543   -1.639386    3.946459
 H   -1.173361   -0.676937    4.639494
 H   -3.731838   -0.936372    0.836338
 H   -4.752143   -1.287622   -0.584820
 H   -4.707435   -2.423592    0.775503
 H   -2.617082   -4.165057   -1.865367
 H   -3.997133   -3.112118   -2.273958
 H   -4.126885   -4.273899   -0.926584
 H   -1.598397    5.821520   -0.091528
 C    4.815195   -1.197015    0.910249
 H    3.669162   -2.673823    1.995640
 H    5.681085    0.427156   -0.222619
 C    0.547322    1.968187    4.184333
 H    5.762076   -1.728170    1.026864
 H    0.584905    2.828140    3.489774
 H    0.896068    1.069917    3.638973
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 H    1.257026    2.161258    5.001630
*
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TS(D^+-E^+)2•*S*^{r}

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1384.747642
G (1 atm) =               -1384.281202
qh G-E (1 mol/L) =            0.477161
qh G-E (24.56 mol/L) =        0.480184
Lowest Frequency =        -1297.25

SMD (MeOH)
HF SCF energy (TZ) =      -1376.359408
HF SCF energy (QZ) =      -1376.440157
Correlation energy (DZ) =    -5.098837
Correlation energy (TZ) =    -6.227880
DLPNO-CCSD(T1)/CBS =      -1383.352107

*xyz 0 1
 Ru  -0.491555   -0.230169   -0.212095
 C   -1.054499    0.299451   -2.249813
 C    0.458344   -1.535706   -1.700775
 C   -2.130578   -0.422766   -1.652957
 C    0.248660   -0.241158   -2.282958
 H   -1.229020    1.307232   -2.628452
 C   -0.610284   -2.229620   -1.111850
 C   -1.939011   -1.691648   -1.072787
 C   -1.289827    1.771819    0.394128
 H   -1.629530    0.890230    1.362646
 N    1.273007    0.803929    0.434251
 O   -0.148128   -1.208080    1.658563
 H    1.466142   -1.950817   -1.650721
 H   -3.108456    0.053946   -1.592855
 C    1.386583    0.529049   -2.883242
 H   -0.404709   -3.165319   -0.586677
 C   -3.066585   -2.495591   -0.457606
 C   -2.516962    2.366412    0.057433
 C   -0.190991    2.648929    0.578209
 O   -2.168931    0.560530    2.502589
 C    2.595513    0.249917    0.452452
 C    1.120429    2.045235    0.746886
 C   -0.824134   -2.046739    2.352846
 H    2.347124    0.231573   -2.443896
 H    1.425430    0.315306   -3.962265
 H    1.244855    1.610204   -2.752272
 C   -4.212156   -1.634178    0.066807
 C   -3.555411   -3.520645   -1.489365
 H   -2.635860   -3.040511    0.396244
 C   -2.645860    3.748732   -0.093600
 H   -3.405953    1.740398   -0.055605
 C   -0.317126    4.034834    0.458330
 C   -3.351827    1.242508    2.914220
 H   -2.270274   -0.456608    2.520380
 C    2.807911   -1.038682    0.950265
 C    3.667029    0.985246   -0.067446
 H    1.971736    2.648511    1.085660
 C   -0.038641   -3.201530    2.923716
 O   -2.049160   -1.948026    2.582845
 H   -3.844015   -0.863708    0.759164
 H   -4.762398   -1.139738   -0.749553
 H   -4.929451   -2.264023    0.612626
 H   -2.735889   -4.170749   -1.831951
 H   -3.982108   -3.014639   -2.370453
 H   -4.335510   -4.159344   -1.048983
 C   -1.551135    4.586388    0.117528
```

```
 H   -3.615676    4.174585   -0.360168
 H    0.555948    4.675803    0.602885
 H   -4.225850    0.931207    2.321851
 H   -3.185240    2.319357    2.779318
 H   -3.533181    1.037714    3.978747
 C    4.093860   -1.573285    0.950597
 H    1.958995   -1.595878    1.345167
 C    4.949602    0.439545   -0.064434
 H    3.495383    1.972377   -0.502081
 H   -0.648643   -3.784342    3.623000
 H    0.292259   -3.846213    2.095359
 H    0.862362   -2.824540    3.427187
 H   -1.657148    5.667817    0.012821
 C    5.168494   -0.838691    0.447087
 H    4.255274   -2.576670    1.350456
 H    5.778883    1.017746   -0.477122
 H    6.173569   -1.265554    0.445521
*
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TS(D^+-E^+)2•S_2^{kp}

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1500.476528
G (1 atm) =               -1499.961655
qh G-E (1 mol/L) =            0.529629
qh G-E (24.56 mol/L) =        0.532652
Lowest Frequency =        -1226.26

SMD (MeOH)
HF SCF energy (TZ) =      -1491.480146
HF SCF energy (QZ) =      -1491.569592
Correlation energy (DZ) =    -5.474460
Correlation energy (TZ) =    -6.694312
DLPNO-CCSD(T1)/CBS =      -1499.003659

*xyz 0 1
 Ru  -0.599916   -0.083853   -0.319226
 C   -1.283568    0.425085   -2.325453
 C    0.470142   -1.201592   -1.875826
 C   -2.246797   -0.444433   -1.721853
 C    0.080235    0.077670   -2.404591
 H   -1.598977    1.415132   -2.658198
 C   -0.470537   -2.059797   -1.292708
 C   -1.304484    1.938579    0.249990
 N    1.158459    0.840811    0.444897
 H   -1.515308    1.063232    1.255826
 O   -0.741960   -1.073388    1.569494
 H    1.527964   -1.471996   -1.850600
 C   -1.854175   -1.682712   -1.180935
 H   -3.275145   -0.099551   -1.617460
 C    1.095129    1.015515   -2.989692
 H   -0.130416   -2.968594   -0.789728
 C   -2.534253    2.551474   -0.025621
 C   -0.175234    2.781379    0.400947
 C    2.410089    0.165814    0.608996
 C    1.095893    2.115581    0.636270
 O   -1.795701    0.649754    2.462201
 C   -1.305135   -0.515186    2.559517
 H   -0.225317   -2.876498    1.566846
 C   -2.806173   -2.611372   -0.454552
 H    2.075127    0.884760   -2.511557
 H    1.211164    0.801405   -4.062860
 H    0.775855    2.060395   -2.878333
 C   -2.628766    3.936552   -0.176203
 H   -3.437823    1.940761   -0.102259
 C   -0.266353    4.168846    0.271995
```

```
 C    2.442777   -1.066579    1.266595
 C    3.582732    0.712188    0.078709
 H    1.977796    2.680225    0.962718
 H   -1.273419    1.698615    4.016973
 C   -1.403102   -1.241180    3.862578
 O    0.187198   -3.723161    1.320693
 C   -4.002505   -1.902198    0.175721
 C   -3.246153   -3.719821   -1.419358
 H   -2.216626   -3.077435    0.350917
 C   -1.500075    4.744840   -0.026713
 H   -3.596495    4.391810   -0.398292
 H    0.624877    4.789800    0.388820
 C    3.653640   -1.737987    1.410386
 H    1.523060   -1.494844    1.662219
 C    4.790052    0.030470    0.226594
 H    3.549081    1.656657   -0.468912
 O   -0.670276    1.909748    4.747193
 H   -0.713150   -2.091093    3.892079
 H   -2.435786   -1.602973    3.976819
 H   -1.193004   -0.534558    4.675843
 C   -0.425846   -4.760421    2.064311
 H   -3.689633   -1.070213    0.825475
 H   -4.689856   -1.502717   -0.586721
 H   -4.571534   -2.615478    0.789340
 H   -2.381206   -4.259058   -1.834550
 H   -3.824069   -3.299817   -2.258182
 H   -3.881663   -4.448069   -0.894130
 H   -1.583888    5.827600   -0.137810
 C    4.830408   -1.193040    0.893740
 H    3.672260   -2.699402    1.927832
 H    5.702072    0.458127   -0.194803
 C    0.619243    2.035893    4.181872
 H   -1.508645   -4.837396    1.857388
 H   -0.288354   -4.629932    3.152127
 H    0.047344   -5.707506    1.769203
 H    5.776650   -1.726962    1.002703
 H    1.330300    2.216032    5.000643
 H    0.942066    1.120954    3.648663
 H    0.686601    2.886143    3.477860
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TS(D^+-E^+)2•S_2^r

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1500.458310
G (1 atm) =               -1499.944212
qh G-E (1 mol/L) =            0.527485
qh G-E (24.56 mol/L) =        0.530508
Lowest Frequency =        -1256.33

SMD (MeOH)
HF SCF energy (TZ) =      -1491.451114
HF SCF energy (QZ) =      -1491.540059
Correlation energy (DZ) =    -5.485464
Correlation energy (TZ) =    -6.706328
DLPNO-CCSD(T1)/CBS =      -1498.986582

*xyz 0 1
Ru  -0.619365   -0.153497   -0.134521
 C   -1.180211    0.375855   -2.163770
 C    0.490602   -1.316614   -1.627933
 C   -2.201706   -0.467049   -1.625220
 C    0.172393   -0.023565   -2.168813
 H   -1.442794    1.374717   -2.513970
 C   -0.515043   -2.132115   -1.094334
 C   -1.892787   -1.722899   -1.072981
```

C	-1.423574	1.845319	0.410620
H	-1.854155	0.975102	1.370156
N	1.099340	0.837890	0.662765
O	-0.428960	-1.183069	1.736351
H	1.533463	-1.630540	-1.557097
H	-3.223728	-0.092111	-1.584004
C	1.248016	0.882180	-2.691290
H	-0.231477	-3.059494	-0.591912
C	-2.938790	-2.653243	-0.491351
C	-2.607197	2.462018	-0.028031
C	-0.340156	2.702476	0.726769
O	-2.430235	0.690243	2.489013
C	2.406645	0.259571	0.766229
C	0.936984	2.067937	1.012410
C	-1.148142	-1.954195	2.455159
H	2.202118	0.702331	-2.178685
H	1.396261	0.683894	-3.763514
H	0.967179	1.936829	-2.570461
C	-4.209069	-1.941175	-0.036444
C	-3.244507	-3.747720	-1.522920
H	-2.481589	-3.133091	0.388683
C	-2.706658	3.849286	-0.151827
H	-3.484956	1.849038	-0.250354
C	-0.438390	4.091249	0.631372
C	-3.664086	1.359232	2.767026
H	-2.521018	-0.350405	2.546787
H	-0.835594	1.298436	3.420482
C	2.560723	-1.056495	1.212464
C	3.527759	0.998375	0.371995
H	1.760661	2.641169	1.452884
C	-0.438483	-3.136291	3.064117
O	-2.365717	-1.767667	2.693594
H	-3.980757	-1.123107	0.661410
H	-4.774119	-1.532458	-0.888822
H	-4.865032	-2.653936	0.483720
H	-2.336075	-4.296934	-1.813454
H	-3.687932	-3.311731	-2.432557
H	-3.960453	-4.471006	-1.105233
C	-1.628580	4.666345	0.187497
H	-3.640531	4.294357	-0.501844
H	0.422161	4.717602	0.878132
H	-4.456487	1.021311	2.083164
H	-3.502551	2.437691	2.642685
H	-3.951161	1.151494	3.806665
O	-0.011417	1.702754	3.738241
C	3.834175	-1.613683	1.290909
H	1.675584	-1.619061	1.507323
C	4.798576	0.430393	0.452471
H	3.406563	2.008634	-0.024575
H	-1.100528	-3.690137	3.738852
H	-0.089808	-3.798117	2.257641
H	0.449185	-2.784558	3.608920
H	-1.712935	5.751383	0.101952
C	0.788814	0.671452	4.284132
C	4.957356	-0.874505	0.915686
H	3.947336	-2.638137	1.651984
H	5.666846	1.012976	0.137849
H	1.062169	-0.083786	3.527641
H	0.289579	0.155999	5.124984
H	1.712247	1.130642	4.666221
H	5.952858	-1.319061	0.975677

*

***trans*-TS(D^+-E)2**
CPCM (MeOH)

***trans*-TS(D^+-E)2**
CPCM (MeOH)

M06 SCF (DZ) = -1496.947906
G (1 atm) = -1496.501420
qh-G (1 mol/L) = -1496.492080
qh-G (24.56 mol/L) = -1496.489058
Lowest Frequency = -1519.6507

HF SCF energy (TZ) = -1488.697333
HF SCF energy (QZ) = -1488.788123
Correlation energy (DZ) = -5.416970
Correlation energy (TZ) = -6.626930
DLPNO-CCSD(T1)/CBS = -1496.149432

*xyz 0 1

Ru	0.512068	-0.214553	-0.374000
C	0.313716	1.968200	0.165029
N	-1.169233	-0.136446	0.915511
C	1.338215	2.903144	-0.054602
C	-0.330533	1.992233	1.426813
H	-0.537290	1.849279	-0.777179
O	1.635044	-0.079061	1.410124
C	-2.184843	-1.130829	0.998395
C	-1.293763	0.935956	1.631777
C	1.698487	3.815771	0.932961
H	1.846811	2.933882	-1.024218
C	-0.000525	2.922294	2.410881
O	-1.533301	2.144954	-1.722899
C	1.823273	-1.086442	2.201375
C	-3.513499	-0.777125	0.744812
C	-1.839091	-2.450576	1.298356
H	-2.088306	1.017070	2.386363
C	1.026383	3.828344	2.159958
H	2.495711	4.540001	0.746229
H	-0.518934	2.917396	3.373951
C	-2.697462	2.383803	-1.228602
C	2.766151	-0.757875	3.338125
O	1.333459	-2.211360	2.083396
C	-4.498855	-1.762323	0.782141
H	-3.744189	0.263398	0.491931
C	-2.835706	-3.421218	1.337196
H	-0.790312	-2.678010	1.518147
H	1.310217	4.554507	2.925810
C	-3.768699	2.685941	-2.255930
O	-2.993508	2.348703	-0.025148
H	3.764960	-0.535913	2.928131
H	2.428744	0.148225	3.863789
H	2.840981	-1.595309	4.043698
C	-4.164041	-3.083117	1.072894
H	-5.537736	-1.493034	0.574717
H	-2.573318	-4.454072	1.580599
H	-3.358469	3.220948	-3.123990
H	-4.181119	1.729798	-2.621632
H	-4.593263	3.256100	-1.806309
H	-4.939782	-3.852556	1.096726
C	0.386990	-0.011707	-2.537932
C	-0.475464	-1.070147	-2.166453
C	1.764866	-0.007493	-2.162229
H	-0.037130	0.856680	-3.046462
C	-1.918279	-1.075191	-2.549778
C	0.080088	-2.123710	-1.377830
C	2.301577	-1.040134	-1.368219
H	2.378750	0.859832	-2.414683
H	-2.527264	-1.618716	-1.810088
H	-2.292934	-0.045870	-2.643529
H	-2.046217	-1.579124	-3.521804
C	1.429053	-2.108675	-0.979824
H	-0.580196	-2.910804	-1.003065

wB97X-D3 SCF (DZ) = -1497.642667
G (1 atm) = -1497.181307
qh G-E (1 mol/L) = 0.475418
qh G-E (24.56 mol/L) = 0.478441
Lowest Frequency = -1065.42

HF SCF energy (TZ) = -1488.702380
HF SCF energy (QZ) = -1488.791984
Correlation energy (DZ) = -5.415147
Correlation energy (TZ) = -6.625039
DLPNO-CCSD(T1)/CBS = -1496.151005

SMD (MeOH)
HF SCF energy (TZ) = -1488.721048
HF SCF energy (QZ) = -1488.810353
Correlation energy (DZ) = -5.409308
Correlation energy (TZ) = -6.619722
DLPNO-CCSD(T1)/CBS = -1496.164272

*xyz 0 1

Ru	0.491874	-0.183049	-0.410317
C	0.298204	1.988399	0.199053
N	-1.156300	-0.165739	0.905498
C	1.291105	2.957730	-0.012455
C	-0.339554	1.968357	1.459051
C	-2.135673	-1.201554	1.030829
C	-1.278964	0.875926	1.657303
C	1.630534	3.861724	0.992483
C	-0.030009	2.886006	2.463535
C	-1.734239	-2.489065	1.392297
C	-3.477435	-0.911057	0.774631
C	0.966669	3.830006	2.224662
C	-2.693753	-3.492963	1.503097
C	-4.427098	-1.927827	0.884918
C	-4.039221	-3.217197	1.247571
C	0.392028	0.083102	-2.568776
C	-0.502671	-0.956472	-2.233197
C	1.767203	0.047714	-2.180054
C	-1.941597	-0.926060	-2.659092
C	0.016621	-2.041858	-1.460515
C	2.269177	-1.020360	-1.415765
C	1.363125	-2.073968	-1.058416
C	3.695765	-1.077860	-0.907464
C	4.330293	0.293201	-0.685562
C	4.527900	-1.939135	-1.866555
H	1.791662	3.018891	-0.982562
H	-2.050132	0.917130	2.435083
H	2.405847	4.610798	0.815466
H	-0.540258	2.846027	3.428795
H	-0.675316	-2.673913	1.593796
H	-3.750996	0.103946	0.474710
H	1.231873	4.549417	3.002506
H	-2.387581	-4.500482	1.793347
H	-5.477414	-1.707529	0.682036
H	-4.785722	-4.009831	1.333574
H	0.002034	0.970812	-3.065459
H	2.400030	0.903974	-2.410891
H	-2.590222	-1.381142	-1.897877
H	-2.055959	-1.499951	-3.591264
H	-2.264951	0.106127	-2.838833
H	-0.662150	-2.821692	-1.110936
H	1.699037	-2.859529	-0.384023
H	3.652861	-1.597311	0.063717
H	3.707938	0.914981	-0.025402
H	4.484812	0.832040	-1.633959
H	5.316809	0.172158	-0.214213

```
 C    3.727060   -1.043651   -0.875904
 H    1.790129   -2.866249   -0.281685
 C    4.307255    0.340953   -0.641456
 C    4.573853   -1.844933   -1.862915
 H    3.719139   -1.582369    0.090326
 H    5.317489    0.253410   -0.211638
 H    3.683662    0.921937    0.056666
 H    4.409212    0.907397   -1.583443
 H    5.611478   -1.927999   -1.503363
 H    4.178775   -2.863467   -2.007235
 H    4.593259   -1.345754   -2.847372
*
```

TS(E-H)1•*S*

```
CPCM (MeOH)
M06 SCF (DZ) =            -1383.633117
G (1 atm) =               -1383.189114
qh-G (1 mol/L) =          -1383.180652
qh-G (24.56 mol/L) =      -1383.177629
Lowest Frequency =         -144.5168

HF SCF energy (TZ) =      -1375.895629
HF SCF energy (QZ) =      -1375.978873
Correlation energy (DZ) =    -5.098784
Correlation energy (TZ) =    -6.232027
DLPNO-CCSD(T1)/CBS =      -1382.898175

PBE0+D3BJ (ATZ) =         -1383.545672
M06-2X (ATZ) =            -1384.336327
wB97M-V (ATZ) =           -1384.403420
B2GP-PLYP (ATZ) =         -1383.605573
B2K-PLYP (ATZ) =          -1383.439911
PWPB95 (ATZ) =            -1383.964145
PWPB95+D3BJ (ATZ) =       -1384.010141
PWPB95+D4 (ATZ) =         -1384.026794

*xyz 0 1
 Ru   0.149185    0.037392   -0.633247
 C    1.330225    0.781726    0.892125
 N   -1.028412   -0.329101    1.130682
 C    0.818551    0.620444    2.202234
 C    2.582033    1.394885    0.776077
 O    2.406240   -1.471367   -0.824325
 O    0.222113   -2.703543   -0.207711
 C   -2.374663   -0.778583    1.117116
 C   -0.481611    0.014697    2.257257
 C    1.523152    1.033141    3.342823
 C    3.284530    1.816781    1.905490
 H    3.035148    1.542210   -0.210572
 C    3.358655   -1.548998    0.038228
 H    1.144705   -2.389188   -0.434892
 C    0.280159   -3.326060    1.055483
 C   -2.741635   -1.869956    0.321547
 C   -3.351666   -0.095294    1.851287
 H   -1.005992   -0.149461    3.210683
 C    2.763551    1.636515    3.191692
 H    1.090477    0.879315    4.336591
 H    4.258879    2.300215    1.783065
 H    4.087093   -2.939326   -1.996175
 H    4.596222   -1.463805   -2.858387
 H    5.548505   -2.064072   -1.474920
 H   -0.536086    1.839654   -0.768416
 O    1.601332   -0.105518    1.374027
 C    1.844276   -1.107030    2.156136
 C    2.658068   -0.720591    3.377947
 O    1.472618   -2.273534    1.987718
 H    3.554102   -0.160058    3.074716
 H    2.946295   -1.610587    3.950680
 H    2.053841   -0.056825    4.015422
 O   -1.482083    2.232412   -1.717619
 C   -2.671999    2.447606   -1.275134
 C   -3.662677    2.941346   -2.317417
 O   -3.049370    2.254101   -0.109075
 H   -4.086048    2.065109   -2.834656
 H   -4.487007    3.485859   -1.839174
 H   -3.169103    3.570903   -3.069401
*
```

TS(E-H)1•*S*

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1384.297459
G (1 atm) =               -1383.838839
qh G-E (1 mol/L) =            0.469618
qh G-E (24.56 mol/L) =        0.472641
Lowest Frequency =         -145.27

HF SCF energy (TZ) =      -1375.902684
HF SCF energy (QZ) =      -1375.984734
Correlation energy (DZ) =    -5.094933
Correlation energy (TZ) =    -6.227825
DLPNO-CCSD(T1)/CBS =      -1382.899271

PBE0+D3BJ (ATZ) =         -1383.546907
M06-2X (ATZ) =            -1384.349462
wB97M-V (ATZ) =           -1384.411347
B2GP-PLYP (ATZ) =         -1383.619050
B2K-PLYP (ATZ) =          -1383.442052
PWPB95 (ATZ) =            -1383.974137
PWPB95+D3BJ (ATZ) =       -1384.019845
PWPB95+D4 (ATZ) =         -1384.036265

SMD (MeOH)
HF SCF energy (TZ) =      -1375.920004
HF SCF energy (QZ) =      -1376.001758
Correlation energy (DZ) =    -5.090547
Correlation energy (TZ) =    -6.224286
DLPNO-CCSD(T1)/CBS =      -1382.913161

*xyz 0 1
 Ru   0.121913    0.070274   -0.630637
 C    1.312556    0.796426    0.892875
 N   -1.041633   -0.328824    1.117042
 C    0.830141    0.559826    2.200566
 C    2.561065    1.424536    0.791807
 C   -2.392111   -0.790498    1.100932
 C   -0.484039   -0.049370    2.247985
 C    1.549245    0.909629    3.351566
 C    3.282648    1.788291    1.930859
 C   -2.733457   -1.920918    0.352171
 C   -3.380047   -0.078410    1.787569
 C    2.785473    1.530829    3.213635
 C   -4.058065   -2.346978    0.315447
 C   -4.705752   -0.510997    1.740193
```

```
C    4.716577   -1.108829   -0.482102
O    3.255318   -1.962120    1.199770
H   -0.691521   -3.209419    1.567238
H    0.475297   -4.412273    0.963502
H    1.078189   -2.886493    1.678160
C   -4.068857   -2.283863    0.287652
H   -1.964383   -2.381833   -0.251675
C   -4.678804   -0.516163    1.806955
H   -3.072614    0.787357    2.434429
H    3.326804    1.971778    4.065690
H    4.631549   -0.155800   -1.027773
H    5.092202   -1.853950   -1.203017
H    5.446170   -1.010554    0.334412
C   -5.042179   -1.611947    1.028225
H   -4.347108   -3.143330   -0.327575
H   -5.434974    0.028808    2.377525
H   -6.084579   -1.937152    0.989799
C    0.489106    1.815688   -1.773178
C    1.057807    0.742134   -2.502792
C   -0.874171    1.776483   -1.346945
H    1.131261    2.642845   -1.459725
C    0.272489   -0.397757   -2.841129
H    2.126681    0.739666   -2.727818
C   -1.545853    2.879328   -0.565923
C   -1.641526    0.626324   -1.723357
C    0.913446   -1.565152   -3.512794
C   -1.101134   -0.422981   -2.493738
C   -0.603749    3.718202    0.281399
C   -2.322629    3.758513   -1.545234
H   -2.272966    2.382482    0.106646
H   -2.667398    0.540056   -1.347346
H    1.875706   -1.789178   -3.029194
H    1.101053   -1.326895   -4.572635
H    0.270881   -2.455931   -3.466871
H   -1.698921   -1.312446   -2.704844
H   -0.018845    3.103873    0.984863
H    0.101581    4.291327   -0.345129
H   -1.181581    4.451900    0.864697
H   -3.050057    3.175649   -2.132593
H   -1.630272    4.247763   -2.252589
H   -2.870845    4.547716   -1.007228
*
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```

```
C   -5.048688   -1.645308    1.006266
C    0.458566    1.840880   -1.785026
C    1.037491    0.764262   -2.499637
C   -0.905654    1.799050   -1.365636
C    0.262942   -0.386826   -2.820830
C   -1.590441    2.934658   -0.629270
C   -1.664947    0.641972   -1.730281
C    0.911056   -1.555633   -3.503489
C   -1.110977   -0.421830   -2.470038
C   -0.697126    3.670995    0.367086
C   -2.182441    3.895525   -1.669573
H    2.994600    1.631159   -0.190592
H   -0.999128   -0.253111    3.195635
H    1.136866    0.696374    4.341554
H    4.252252    2.281180    1.818395
H   -1.942700   -2.451974   -0.179928
H   -3.112230    0.827231    2.336974
H    3.362442    1.816915    4.095332
H   -4.319426   -3.235554   -0.263415
H   -5.474731    0.051448    2.274001
H   -6.087660   -1.979050    0.965397
H    1.091163    2.679003   -1.490302
H    2.100698    0.781176   -2.738262
H   -2.424167    2.479463   -0.068081
H   -2.690957    0.555945   -1.364689
H    1.883633   -1.762041   -3.039471
H    1.062960   -1.314394   -4.566737
H    0.281580   -2.452684   -3.435950
H   -1.707166   -1.310080   -2.680187
H   -0.281501    2.984118    1.118032
H    0.142394    4.179993   -0.132954
H   -1.282738    4.441632    0.890023
H   -2.853275    3.369306   -2.365535
H   -1.380884    4.369357   -2.259758
H   -2.757716    4.692110   -1.174623
O    2.361649   -1.568603   -0.792868
C    3.390509   -1.590933   -0.020641
C    4.675581   -1.066337   -0.648094
O    3.407549   -2.021627    1.141862
H    4.486705   -0.121256   -1.177086
H    5.033241   -1.792427   -1.395708
H    5.456841   -0.923091    0.109756
O    0.237897   -2.755830   -0.038861
C    0.347128   -3.275837    1.271368
H    1.140920   -2.405393   -0.305816
H   -0.607997   -3.134016    1.804081
H    0.564275   -4.360373    1.256947
H    1.154453   -2.773766    1.828011
*
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```

TS(E-H)1•S_2

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1500.010742
G (1 atm) =               -1499.502379
qh G-E (1 mol/L) =            0.521027
qh G-E (24.56 mol/L) =        0.524050
Lowest Frequency =          -133.93

SMD (MeOH)
HF SCF energy (TZ) =      -1491.018735
HF SCF energy (QZ) =      -1491.108410
Correlation energy (DZ) =    -5.471341
Correlation energy (TZ) =    -6.695887
DLPNO-CCSD(T1)/CBS =      -1498.546863
```

```
*xyz 0 1
Ru   0.210704   -0.032766   -0.529832
 C    1.509967    0.705693    0.892091
 C    2.816008    1.185860    0.721779
 C    1.031356    0.650380    2.221810
 C    3.595186    1.570342    1.815999
 C    1.806689    1.021068    3.328513
 C   -0.339104    0.201280    2.344321
 C    3.100484    1.485780    3.122171
 N   -0.966949   -0.091734    1.253045
 C   -2.363782   -0.380806    1.324377
 C   -3.208148    0.453749    2.065565
 C   -2.897305   -1.463648    0.618970
 C   -4.578175    0.197846    2.107846
 C   -4.266519   -1.712443    0.669425
 C   -5.112106   -0.884614    1.410594
 C    0.312652    1.750729   -1.654006
 C    1.205510    0.842162   -2.294022
 C   -1.058923    1.412134   -1.462138
 C    0.760005   -0.433367   -2.680312
 C   -2.058131    2.378008   -0.855485
 C   -1.519763    0.143390   -1.952648
 C    1.694347   -1.416623   -3.319351
 C   -0.626607   -0.772181   -2.504249
 C   -1.469690    3.305550    0.205945
 C   -2.712492    3.169710   -1.995413
 H    3.252609    1.256421   -0.277825
 H    4.609284    1.942945    1.647810
 H    1.392136    0.945258    4.337420
 H   -0.840702    0.129190    3.317678
 H    3.722501    1.785041    3.968057
 H   -2.795399    1.323663    2.581601
 H   -2.221138   -2.107764    0.055475
 H   -5.230142    0.858928    2.682712
 H   -4.676978   -2.564742    0.123543
 H   -6.186077   -1.080371    1.438361
 H    0.694701    2.701058   -1.281628
 H    2.259526    1.098743   -2.405996
 H   -2.838915    1.763777   -0.378205
 H   -2.559256   -0.144092   -1.784672
 H    1.465331   -2.444781   -3.014733
 H    1.577645   -1.342293   -4.412547
 H    2.737821   -1.197274   -3.062560
 H   -0.967305   -1.775335   -2.766370
 H   -2.276600    3.886937    0.675880
 H   -0.755888    4.024476   -0.226235
 H   -0.951678    2.742063    0.996384
 H   -3.180624    2.499292   -2.732150
 H   -1.964766    3.785576   -2.521123
 H   -3.490818    3.839411   -1.600194
 O    2.199364   -2.065041   -0.407104
 C    3.203996   -2.044204    0.411658
 C    4.551048   -1.779570   -0.241265
 O    3.126697   -2.237165    1.628743
 H    4.491999   -0.883408   -0.875915
 H    4.811974   -2.625257   -0.896318
 H    5.337373   -1.651061    0.513313
 O   -0.111965   -2.748531    0.452091
 C   -0.120001   -3.142167    1.809646
 H    0.837466   -2.581468    0.192166
 H   -1.067126   -2.824211    2.275884
 H   -0.045703   -4.240917    1.908947
 H    0.723033   -2.691349    2.357828
 O    1.831998   -4.383088   -1.824577
 C    3.070924   -4.812036   -2.345253
 H    2.001953   -3.554996   -1.326817
```

TS(E-H)2•*S*
CPCM (MeOH)
M06 SCF (DZ) = -1615.478232
G (1 atm) = -1615.079353
qh-G (1 mol/L) = -1615.071525
qh-G (24.56 mol/L) = -1615.068503
Lowest Frequency = -127.4500

HF SCF energy (TZ) = -1608.142414
HF SCF energy (QZ) = -1608.212753
Correlation energy (DZ) = -4.564008
Correlation energy (TZ) = -5.596404
DLPNO-CCSD(T1)/CBS = -1614.433616

PBE0+D3BJ (ATZ) = -1615.316916
M06-2X (ATZ) = -1616.084390
wB97M-V (ATZ) = -1616.129743
B2GP-PLYP (ATZ) = -1615.304934
B2K-PLYP (ATZ) = -1615.122314
PWPB95 (ATZ) = -1615.737300
PWPB95+D3BJ (ATZ) = -1615.780453
PWPB95+D4 (ATZ) = -1615.793820

*xyz 0 1
Ru -0.439749 -0.478092 0.331787
C -0.635109 -0.118422 2.409010
C -1.653879 1.145619 -0.065174
C 0.754050 -0.114458 2.065943
C -1.454481 -1.244170 2.119355
N 0.762888 0.711714 -0.997973
C -1.161780 2.046370 -1.040704
C -2.916556 1.428561 0.468766
C 1.666234 1.048296 2.368394
C 1.307019 -1.310220 1.494994
C -0.907491 -2.358803 1.443156
C 2.151036 0.532770 -1.247812
C 0.165416 1.751337 -1.500425
C -1.895898 3.157258 -1.483848
C -3.642773 2.544203 0.049356
C 0.980127 2.404390 2.337738
C 2.328694 0.802335 3.723048
C 0.501152 -2.402478 1.183390
C -1.769933 -3.499257 1.016208
C 2.664724 -0.735665 -1.534945
C 3.020434 1.627422 -1.147688
C -3.144027 3.407965 -0.932731
C 4.031199 -0.894404 -1.743866
C 4.386411 1.456141 -1.356153
C 4.897140 0.195741 -1.656908
H -1.091129 0.777664 2.838037
H -2.529195 -1.209605 2.314065
H -3.363288 0.764299 1.216374
H 2.455312 1.037363 1.591464
H 2.361284 -1.311800 1.198729
H 0.681135 2.396130 -2.227501
H -1.476527 3.817023 -2.250110
H -4.622350 2.744747 0.494117
H 0.441647 2.575861 1.391499
H 0.259130 2.513572 3.166174
H 1.727302 3.204560 2.456822
H 3.506473 -4.081772 -3.053866
H 2.908311 -5.754063 -2.890434
H 3.818253 -5.003904 -1.552712
*

TS(E-H)2•*S*
CPCM (MeOH)
wB97X-D3 SCF (DZ) = -1616.087577
G (1 atm) = -1615.676383
qh G-E (1 mol/L) = 0.421050
qh G-E (24.56 mol/L) = 0.424073
Lowest Frequency = -123.98

HF SCF energy (TZ) = -1608.149614
HF SCF energy (QZ) = -1608.218795
Correlation energy (DZ) = -4.559583
Correlation energy (TZ) = -5.592020
DLPNO-CCSD(T1)/CBS = -1614.434950

PBE0+D3BJ (ATZ) = -1615.317887
M06-2X (ATZ) = -1616.096228
wB97M-V (ATZ) = -1616.136113
B2GP-PLYP (ATZ) = -1615.319380
B2K-PLYP (ATZ) = -1615.139393
PWPB95 (ATZ) = -1615.746402
PWPB95+D3BJ (ATZ) = -1615.789164
PWPB95+D4 (ATZ) = -1615.802393

SMD (MeOH)
HF SCF energy (TZ) = -1608.158937
HF SCF energy (QZ) = -1608.228211
Correlation energy (DZ) = -4.557891
Correlation energy (TZ) = -5.590725
DLPNO-CCSD(T1)/CBS = -1614.443331

*xyz 0 1
Ru -0.416462 -0.459291 0.356249
C -0.592227 -0.102838 2.432951
C -1.663262 1.130052 -0.058848
C 0.790453 -0.114751 2.081171
C -1.431321 -1.216377 2.141921
N 0.768272 0.724477 -0.971161
C -1.181747 2.024644 -1.042866
C -2.931735 1.410694 0.468387
C 1.724209 1.037674 2.397259
C 1.324229 -1.311657 1.492213
C -0.909566 -2.327931 1.446646
C 2.163709 0.549473 -1.226819
C 0.164823 1.743054 -1.494246
C -1.918969 3.127024 -1.499430
C -3.667600 2.515956 0.036378
C 1.075285 2.417121 2.295800
C 2.331279 0.804146 3.786792
C 0.497415 -2.383654 1.166466
C -1.793921 -3.464220 1.020830
C 2.665298 -0.709435 -1.566722
C 3.034672 1.634779 -1.079144
C -3.172655 3.374178 -0.953048
C 4.032368 -0.871731 -1.776734
C 4.402334 1.461318 -1.289572
C 4.905485 0.209121 -1.638697
H -1.029897 0.790764 2.878631
H -2.498829 -1.168917 2.358704
H -3.370069 0.757381 1.227187
H 2.539846 0.986991 1.656678

```
 H    2.870615   -0.156691    3.745697
 H    1.569460    0.782506    4.524372
 H    3.045360    1.605838    3.954760
 H    0.912724   -3.246911    0.626896
 H   -1.449132   -3.879239    0.034202
 H   -1.676196   -4.320541    1.746192
 H   -2.826683   -3.205141    0.958653
 H    1.970123   -1.577373   -1.616798
 H    2.626647    2.610410   -0.871506
 H   -3.729483    4.272062   -1.255098
 H    4.424879   -1.886462   -1.979971
 H    5.055719    2.315453   -1.267806
 H    5.969941    0.060731   -1.814514
 O   -2.734640   -1.333750   -1.095614
 C   -3.229386   -0.602197   -2.192862
 H   -2.036370   -1.926823   -1.461000
 H   -3.869765   -1.224675   -2.846263
 H   -2.412106   -0.181578   -2.809949
 H   -3.836552    0.235671   -1.815468
 Cl  -0.248268   -2.498410   -2.208671
*
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```
 H    2.374697   -1.331047    1.194327
 H    0.678754    2.384554   -2.221487
 H   -1.503730    3.784950   -2.267719
 H   -4.648910    2.711901    0.477253
 H    0.614738    2.578646    1.309885
 H    0.299988    2.563277    3.064559
 H    1.837804    3.195159    2.448691
 H    2.831826   -0.174225    3.847130
 H    1.549387    0.836680    4.562960
 H    3.074114    1.582842    4.015508
 H    0.897793   -3.230520    0.609014
 H   -1.481199   -3.845987    0.039689
 H   -1.702517   -4.279932    1.754833
 H   -2.844510   -3.154697    0.965956
 H    1.968643   -1.542967   -1.679483
 H    2.645071    2.606848   -0.767741
 H   -3.762557    4.231035   -1.284477
 H    4.418501   -1.855763   -2.051496
 H    5.076970    2.311157   -1.166528
 H    5.977562    0.072580   -1.795156
 O   -2.784013   -1.390657   -1.173788
 C   -3.334560   -0.647188   -2.243439
 H   -2.042356   -1.915168   -1.550332
 H   -3.917183   -1.289933   -2.928276
 H   -2.554631   -0.127508   -2.827933
 H   -4.008990    0.113726   -1.824400
 Cl  -0.267054   -2.498964   -2.306683
*
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```

TS(E-H)2•S_2

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CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1731.801080
G (1 atm) =               -1731.341828
qh G-E (1 mol/L) =            0.472130
qh G-E (24.56 mol/L) =        0.475153
Lowest Frequency =          -116.45

SMD (MeOH)
HF SCF energy (TZ) =      -1723.256572
HF SCF energy (QZ) =      -1723.334302
Correlation energy (DZ) =    -4.938168
Correlation energy (TZ) =    -6.062795
DLPNO-CCSD(T1)/CBS =      -1730.077678

*xyz 0 1
 Ru  -0.416462   -0.459291    0.356249
 C   -0.592227   -0.102838    2.432951
 C   -1.663262    1.130052   -0.058848
 C    0.790453   -0.114751    2.081171
 C   -1.431321   -1.216377    2.141921
 N    0.768272    0.724477   -0.971161
 C   -1.181747    2.024644   -1.042866
 C   -2.931735    1.410694    0.468387
 C    1.724209    1.037674    2.397259
 C    1.324229   -1.311657    1.492213
 C   -0.909566   -2.327931    1.446646
 C    2.163709    0.549473   -1.226819
 C    0.164823    1.743054   -1.494246
 C   -1.918969    3.127024   -1.499430
 C   -3.667600    2.515956    0.036378
 C    1.075285    2.417121    2.295800
 C    2.331279    0.804146    3.786792
 C    0.497415   -2.383654    1.166466
 C   -1.793921   -3.464220    1.020830
 C    2.665298   -0.709435   -1.566722
```

TS(F-F^A)

CPCM (MeOH)

M06 SCF (DZ) =	-1663.658080
G (1 atm) =	-1664.099701
qh-G (1 mol/L) =	-1663.647700
qh-G (24.56 mol/L) =	-1663.644678
Lowest Frequency =	-66.20

HF SCF energy (TZ) =	-1655.136388
HF SCF energy (QZ) =	-1655.235195
Correlation energy (DZ) =	-5.812494
Correlation energy (TZ) =	-7.123236
DLPNO-CCSD(T1)/CBS =	-1663.162635

*xyz 0 1

Ru	-0.381062	-0.411227	0.160683
N	-1.375709	1.382681	-0.187429
N	2.398526	-1.279680	0.823363
C	-0.690518	2.545116	0.304196
C	-2.554401	1.613135	-0.679076
O	-1.846182	-0.777082	1.684064
O	1.028516	0.067815	-1.397450
O	-0.837027	-0.902441	-1.893768
O	-0.059942	0.353416	2.132330
C	1.206690	-1.997762	1.035881
C	3.102478	-1.496151	-0.221851
C	0.583426	2.870034	-0.165929
C	3.034672	1.634779	-1.079144
C	-3.172655	3.374178	-0.953048
C	4.032368	-0.871731	-1.776734
C	4.402334	1.461318	-1.289572
C	4.905485	0.209121	-1.638697
H	-1.029897	0.790764	2.878631
H	-2.498829	-1.168917	2.358704
H	-3.370069	0.757381	1.227187
H	2.539846	0.986991	1.656678
H	2.374697	-1.331047	1.194327
H	0.678754	2.384554	-2.221487
H	-1.503730	3.784950	-2.267719
H	-4.648910	2.711901	0.477253
H	0.614738	2.578646	1.309885
H	0.299988	2.563277	3.064559
H	1.837804	3.195159	2.448691
H	2.831826	-0.174225	3.847130
H	1.549387	0.836680	4.562960
H	3.074114	1.582842	4.015508
H	0.897793	-3.230520	0.609014
H	-1.481199	-3.845987	0.039689
H	-1.702517	-4.279932	1.754833
H	-2.844510	-3.154697	0.965956
H	1.968643	-1.542967	-1.679483
H	2.645071	2.606848	-0.767741
H	-3.762557	4.231035	-1.284477
H	4.418501	-1.855763	-2.051496
H	5.076970	2.311157	-1.166528
H	5.977562	0.072580	-1.795156
O	-2.784013	-1.390657	-1.173788
C	-3.334560	-0.647188	-2.243439
H	-2.042356	-1.915168	-1.550332
H	-3.917183	-1.289933	-2.928276
H	-2.554631	-0.127508	-2.827933
H	-4.008990	0.113726	-1.824400
Cl	-0.267054	-2.498964	-2.306683

*

TS(F-F^A)

CPCM (MeOH)

wB97X-D3 SCF (DZ) =	-1664.870652
G (1 atm) =	-1664.415274
qh G-E (1 mol/L) =	0.471048
qh G-E (24.56 mol/L) =	0.474071
Lowest Frequency =	-55.91

HF SCF energy (TZ) =	-1655.155464
HF SCF energy (QZ) =	-1655.254021
Correlation energy (DZ) =	-5.807349
Correlation energy (TZ) =	-7.117297
DLPNO-CCSD(T1)/CBS =	-1663.166465

SMD (MeOH)

HF SCF energy (TZ) =	-1655.175138
HF SCF energy (QZ) =	-1655.273466
Correlation energy (DZ) =	-5.800659
Correlation energy (TZ) =	-7.112093
DLPNO-CCSD(T1)/CBS =	-1663.181505

*xyz 0 1

Ru	-0.274496	0.092507	0.540139
N	-1.893982	1.022202	-0.203679
C	-2.021511	2.405105	0.190492
C	-2.826512	0.583597	-0.981035
C	-1.137230	3.355676	-0.319461

C	-1.297708	3.331916	1.285966
C	-3.592039	0.698064	-1.135912
H	-2.837325	2.674202	-0.774322
C	-1.165916	-0.123971	2.533406
C	0.248810	-0.382367	-2.292937
C	0.926626	-2.337862	2.396177
C	0.401528	-2.584328	0.022809
C	4.282147	-0.692144	-0.544549
H	2.859943	-2.295630	-0.950799
C	1.231798	3.994411	0.335725
H	1.051628	2.233334	-0.919193
C	-0.636420	4.450173	1.788416
H	-2.279898	3.043796	1.673334
C	-3.608875	-0.694617	-0.944254
C	-4.684104	1.301782	-1.786210
C	-1.623910	0.066019	3.936819
C	0.600731	-0.295259	-3.737071
C	-0.075253	-3.216816	2.716170
H	1.562584	-1.893387	3.166610
C	-0.626240	-3.500390	0.385890
H	0.726653	-2.573756	-1.019970
C	4.630018	0.429614	0.222558
C	5.067461	-1.032869	-1.652494
C	0.628572	4.786861	1.312869
H	2.225385	4.251810	-0.040592
H	-1.113303	5.056037	2.562950
C	-4.682674	-1.446914	-1.401068
H	-2.778619	-1.180687	-0.431150
C	-5.750961	0.543782	-2.251345
H	-4.687290	2.386937	-1.927346
H	-0.998516	-0.551277	4.601264
H	-1.487457	1.114885	4.237405
H	-2.673439	-0.230275	4.054502
H	-0.051508	-0.938011	-4.340648
H	1.653795	-0.575762	-3.881982
H	0.488211	0.746550	-4.074427
C	-0.871703	-3.803580	1.701307
H	-0.255828	-3.475135	3.763535
H	-1.210681	-3.970800	-0.410766
C	5.744015	1.187544	-0.112351
H	4.004605	0.691247	1.079903
C	6.185196	-0.272902	-1.986675
H	4.793104	-1.904603	-2.255453
H	1.148732	5.662815	1.708000
C	-5.751953	-0.836162	-2.058197
H	-4.687113	-2.528045	-1.241376
H	-6.586175	1.031051	-2.759460
H	-1.667532	-4.502816	1.969045
C	6.525301	0.837828	-1.217050
H	6.008875	2.061957	0.487784
H	6.792866	-0.547105	-2.852587
H	-6.590958	-1.438786	-2.415274
H	7.400608	1.437653	-1.479307

*

TS(F-F^A)
CPCM (MeOH)
M06 SCF (DZ) = -1663.658080

C	-3.016413	2.769411	1.097122
C	-3.012347	-0.783690	-1.485386
C	-1.259454	4.684285	0.081386
C	-3.126079	4.101170	1.497388
C	-2.635588	-1.934982	-0.779029
C	-3.647037	-0.916174	-2.729509
C	-2.248756	5.060195	0.992187
C	-2.859418	-3.192123	-1.331302
C	-3.852148	-2.175529	-3.286934
C	-3.455056	-3.316141	-2.588242
H	-3.564659	1.318034	-1.330170
H	-0.360038	3.040675	-1.016338
H	-3.690933	2.007450	1.494132
H	-0.571640	5.431740	-0.320079
H	-3.901023	4.386600	2.211930
H	-2.179223	-1.841536	0.205846
H	-3.968114	-0.021353	-3.269238
H	-2.334254	6.101849	1.308847
H	-2.565217	-4.084141	-0.773984
H	-4.330283	-2.266760	-4.264300
H	-3.619521	-4.306061	-3.019836
N	2.675005	-0.725515	0.942640
C	1.892673	-1.597972	1.736763
C	3.341812	-1.222591	-0.028355
C	1.826308	-1.343687	3.115443
C	1.171219	-2.676736	1.198167
C	4.126692	-0.393481	-0.957159
C	1.095059	-2.184704	3.947130
C	0.434213	-3.509092	2.040178
C	4.270767	0.988644	-0.770073
C	4.715230	-1.003912	-2.071089
C	0.402792	-3.274479	3.412389
C	4.986771	1.745196	-1.690348
C	5.428326	-0.243460	-2.996587
C	5.562927	1.131394	-2.807520
H	3.358017	-2.309514	-0.224047
H	2.369881	-0.486649	3.518477
H	1.174964	-2.848036	0.119928
H	1.061876	-1.987648	5.020932
H	-0.126754	-4.342576	1.611793
H	3.810317	1.457168	0.100638
H	4.600220	-2.081269	-2.217567
H	-0.178744	-3.927493	4.066561
H	5.097992	2.821432	-1.541722
H	5.878805	-0.724384	-3.867317
H	6.121696	1.730038	-3.530531
O	-1.478759	-0.866584	2.043833
O	-0.518276	1.033928	2.442521
C	-1.242322	0.076087	2.860701
C	-1.814080	0.080482	4.243256
H	-1.078004	0.477444	4.953848
H	-2.693951	0.741796	4.256458
H	-2.122021	-0.930274	4.535327
O	0.955305	1.093592	-0.894713
O	0.135794	-0.858452	-1.350563
C	0.825661	0.141317	-1.725037
C	1.421071	0.210952	-3.096498
H	1.693191	-0.793407	-3.443991
H	2.299191	0.868754	-3.100583
H	0.665211	0.622532	-3.782803

*

TS(F-F^A)
CPCM (MeOH)
wB97X-D3 SCF (DZ) = -1664.870652

```
G (1 atm) =               -1664.099701
qh-G (1 mol/L) =          -1663.647700
qh-G (24.56 mol/L) =      -1663.644678
Lowest Frequency =          -66.20

HF SCF energy (TZ) =      -1655.136388
HF SCF energy (QZ) =      -1655.235195
Correlation energy (DZ) =    -5.812494
Correlation energy (TZ) =    -7.123236
DLPNO-CCSD(T1)/CBS =      -1663.162635

*xyz 0 1
 Ru  -0.381062   -0.411227    0.160683
 N   -1.375709    1.382681   -0.187429
 N    2.398526   -1.279680    0.823363
 C   -0.690518    2.545116    0.304196
 C   -2.554401    1.613135   -0.679076
 O   -1.846182   -0.777082    1.684064
 O    1.028516    0.067815   -1.397450
 O   -0.837027   -0.902441   -1.893768
 O   -0.059942    0.353416    2.132330
 C    1.206690   -1.997762    1.035881
 C    3.102478   -1.496151   -0.221851
 C    0.583426    2.870034   -0.165929
 C   -1.297708    3.331916    1.285966
 C   -3.592039    0.698064   -1.135912
 H   -2.837325    2.674202   -0.774322
 C   -1.165916   -0.123971    2.533406
 C    0.248810   -0.382367   -2.292937
 C    0.926626   -2.337862    2.396177
 C    0.401528   -2.584328    0.022809
 C    4.282147   -0.692144   -0.544549
 H    2.859943   -2.295630   -0.950799
 C    1.231798    3.994411    0.335725
 H    1.051628    2.233334   -0.919193
 C   -0.636420    4.450173    1.788416
 H   -2.279898    3.043796    1.673334
 C   -3.608875   -0.694617   -0.944254
 C   -4.684104    1.301782   -1.786210
 C   -1.623910    0.066019    3.936819
 C    0.600731   -0.295259   -3.737071
 C   -0.075253   -3.216816    2.716170
 H    1.562584   -1.893387    3.166610
 C   -0.626240   -3.500390    0.385890
 H    0.726653   -2.573756   -1.019970
 C    4.630018    0.429614    0.222558
 C    5.067461   -1.032869   -1.652494
 C    0.628572    4.786861    1.312869
 H    2.225385    4.251810   -0.040592
 H   -1.113303    5.056037    2.562950
 C   -4.682674   -1.446914   -1.401068
 H   -2.778619   -1.180687   -0.431150
 C   -5.750961    0.543782   -2.251345
 H   -4.687290    2.386937   -1.927346
 H   -0.998516   -0.551277    4.601264
 H   -1.487457    1.114885    4.237405
 H   -2.673439   -0.230275    4.054502
 H   -0.051508   -0.938011   -4.340648
 H    1.653795   -0.575762   -3.881982
 H    0.488211    0.746550   -4.074427
 C   -0.871703   -3.803580    1.701307
 H   -0.255828   -3.475135    3.763535
 H   -1.210681   -3.970800   -0.410766
 C    5.744015    1.187544   -0.112351
 H    4.004605    0.691247    1.079903
 C    6.185196   -0.272902   -1.986675

G (1 atm) =               -1664.415274
qh G-E (1 mol/L) =            0.471048
qh G-E (24.56 mol/L) =        0.474071
Lowest Frequency =          -55.91

HF SCF energy (TZ) =      -1655.155464
HF SCF energy (QZ) =      -1655.254021
Correlation energy (DZ) =    -5.807349
Correlation energy (TZ) =    -7.117297
DLPNO-CCSD(T1)/CBS =      -1663.166465

SMD (MeOH)
HF SCF energy (TZ) =      -1655.175138
HF SCF energy (QZ) =      -1655.273466
Correlation energy (DZ) =    -5.800659
Correlation energy (TZ) =    -7.112093
DLPNO-CCSD(T1)/CBS =      -1663.181505

*xyz 0 1
 Ru  -0.274496    0.092507    0.540139
 N   -1.893982    1.022202   -0.203679
 C   -2.021511    2.405105    0.190492
 C   -2.826512    0.583597   -0.981035
 C   -1.137230    3.355676   -0.319461
 C   -3.016413    2.769411    1.097122
 C   -3.012347   -0.783690   -1.485386
 C   -1.259454    4.684285    0.081386
 C   -3.126079    4.101170    1.497388
 C   -2.635588   -1.934982   -0.779029
 C   -3.647037   -0.916174   -2.729509
 C   -2.248756    5.060195    0.992187
 C   -2.859418   -3.192123   -1.331302
 C   -3.852148   -2.175529   -3.286934
 C   -3.455056   -3.316141   -2.588242
 H   -3.564659    1.318034   -1.330170
 H   -0.360038    3.040675   -1.016338
 H   -3.690933    2.007450    1.494132
 H   -0.571640    5.431740   -0.320079
 H   -3.901023    4.386600    2.211930
 H   -2.179223   -1.841536    0.205846
 H   -3.968114   -0.021353   -3.269238
 H   -2.334254    6.101849    1.308847
 H   -2.565217   -4.084141   -0.773984
 H   -4.330283   -2.266760   -4.264300
 H   -3.619521   -4.306061   -3.019836
 N    2.675005   -0.725515    0.942640
 C    1.892673   -1.597972    1.736763
 C    3.341812   -1.222591   -0.028355
 C    1.826308   -1.343687    3.115443
 C    1.171219   -2.676736    1.198167
 C    4.126692   -0.393481   -0.957159
 C    1.095059   -2.184704    3.947130
 C    0.434213   -3.509092    2.040178
 C    4.270767    0.988644   -0.770073
 C    4.715230   -1.003912   -2.071089
 C    0.402792   -3.274479    3.412389
 C    4.986771    1.745196   -1.690348
 C    5.428326   -0.243460   -2.996587
 C    5.562927    1.131394   -2.807520
 H    3.358017   -2.309514   -0.224047
 H    2.369881   -0.486649    3.518477
 H    1.174964   -2.848036    0.119928
 H    1.061876   -1.987648    5.020932
 H   -0.126754   -4.342576    1.611793
 H    3.810317    1.457168    0.100638
 H    4.600220   -2.081269   -2.217567
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```
 H    4.793104   -1.904603   -2.255453
 H    1.148732    5.662815    1.708000
 C   -5.751953   -0.836162   -2.058197
 H   -4.687113   -2.528045   -1.241376
 H   -6.586175    1.031051   -2.759460
 H   -1.667532   -4.502816    1.969045
 C    6.525301    0.837828   -1.217050
 H    6.008875    2.061957    0.487784
 H    6.792866   -0.547105   -2.852587
 H   -6.590958   -1.438786   -2.415274
 H    7.400608    1.437653   -1.479307
*
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```

***cis*-TS(F-F^A)**

```
CPCM (MeOH)
M06 SCF (DZ) =            -1664.097149
G (1 atm) =               -1663.657701
qh-G (1 mol/L) =          -1663.646296
qh-G (24.56 mol/L) =      -1663.643274
Lowest Frequency =          -25.8462

HF SCF energy (TZ) =      -1655.150292
HF SCF energy (QZ) =      -1655.250935
Correlation energy (DZ) =    -5.803901
Correlation energy (TZ) =    -7.113431
DLPNO-CCSD(T1)/CBS =      -1663.159896

PBE0+D3BJ (ATZ) =         -1663.950620
M06-2X (ATZ) =            -1664.966681
wB97M-V (ATZ) =           -1665.067165
B2GP-PLYP (ATZ) =         -1664.041438
B2K-PLYP (ATZ) =          -1663.818000
PWPB95 (ATZ) =            -1664.492143
PWPB95+D3BJ (ATZ) =       -1664.539206
PWPB95+D4 (ATZ) =         -1664.560889

*xyz 0 1
 Ru  -0.526496   -1.314343   -0.230268
 N   -1.470259   -0.096414    1.110151
 N    1.235445    1.260731   -1.360091
 C   -2.852738    0.109470    0.783052
 C   -1.006028    0.685158    2.040549
 O   -1.195222   -0.626816   -2.110883
 O    0.256350   -2.247183   -2.027378
 O    0.084427   -2.563411    1.446147
 O   -1.620420   -3.011769    0.190246
 C    0.302784    2.313653   -1.314885
 C    2.450463    1.519047   -1.048912
 C   -3.788314   -0.911464    0.956914
 C   -3.247039    1.345595    0.265682
 C    0.364445    0.866335    2.500091
 H   -1.736507    1.341869    2.539268
 C   -0.399386   -1.410153   -2.721855
 C   -0.885576   -3.331212    1.188175
 C   -0.597310    2.462580   -2.378195
 C    0.216025    3.181111   -0.216036
 C    3.507233    0.511818   -0.971217
 H    2.771488    2.555999   -0.817800
 H   -0.178744   -3.927493    4.066561
 H    5.097992    2.821432   -1.541722
 H    5.878805   -0.724384   -3.867317
 H    6.121696    1.730038   -3.530531
 O   -1.478759   -0.866584    2.043833
 O   -0.518276    1.033928    2.442521
 C   -1.242322    0.076087    2.860701
 C   -1.814080    0.080482    4.243256
 H   -1.078004    0.477444    4.953848
 H   -2.693951    0.741796    4.256458
 H   -2.122021   -0.930274    4.535327
 O    0.955305    1.093592   -0.894713
 O    0.135794   -0.858452   -1.350563
 C    0.825661    0.141317   -1.725037
 C    1.421071    0.210952   -3.096498
 H    1.693191   -0.793407   -3.443991
 H    2.299191    0.868754   -3.100583
 H    0.665211    0.622532   -3.782803
*
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```

***cis*-TS(F-F^A)**

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1664.869319
G (1 atm) =               -1664.415288
qh G-E (1 mol/L) =            0.471078
qh G-E (24.56 mol/L) =        0.474100
Lowest Frequency =          -38.10

HF SCF energy (TZ) =      -1655.152168
HF SCF energy (QZ) =      -1655.251033
Correlation energy (DZ) =    -5.803910
Correlation energy (TZ) =    -7.114057
DLPNO-CCSD(T1)/CBS =      -1663.160446

PBE0+D3BJ (ATZ) =         -1663.949743
M06-2X (ATZ) =            -1664.987765
wB97M-V (ATZ) =           -1665.077539
B2GP-PLYP (ATZ) =         -1664.067735
B2K-PLYP (ATZ) =          -1663.849073
PWPB95 (ATZ) =            -1664.506833
PWPB95+D3BJ (ATZ) =       -1664.553560
PWPB95+D4 (ATZ) =         -1664.575425

SMD (MeOH)
HF SCF energy (TZ) =      -1655.169269
HF SCF energy (QZ) =      -1655.267942
Correlation energy (DZ) =    -5.796564
Correlation energy (TZ) =    -7.108349
DLPNO-CCSD(T1)/CBS =      -1663.172545

*xyz 0 1
 Ru  -0.574274   -1.283179   -0.037524
 N   -1.850516   -0.030626    0.965092
 N    1.759125    1.433258   -0.827602
 C   -3.239113   -0.131216    0.611541
 C   -1.557071    0.834694    1.875962
 O   -0.485936   -0.568108   -2.034479
 O    0.695122   -2.303330   -1.460116
 O   -0.721439   -2.613073    1.650756
 O   -1.967655   -2.801844   -0.112523
 C    0.923188    2.536113   -0.533608
 C    2.942431    1.662410   -1.246519
 C   -4.185027   -0.496309    1.569626
 C   -3.621881    0.105173   -0.710600
 C   -0.221534    1.115793    2.407947
```

C	-5.119875	-0.683532	0.622139
H	-3.464089	-1.875640	1.353421
C	-4.578940	1.558812	-0.080325
H	-2.496880	2.129763	0.121553
C	1.498348	0.215773	1.983819
C	0.550290	1.828125	3.510940
C	-0.191958	-1.291561	-4.190780
C	-1.209226	-4.528468	2.008338
C	-1.541538	3.482340	-2.358498
H	-0.534012	1.765655	-3.217042
C	-0.747393	4.188117	-0.194137
H	0.890138	3.038909	0.635977
C	4.782008	0.916324	-0.554810
C	3.275544	-0.838755	-1.272720
C	-5.519787	0.547108	0.099296
H	-5.854491	-1.479216	0.770556
H	-4.877510	2.526013	-0.494601
C	2.766053	0.519211	2.464825
H	1.395190	-0.537997	1.199493
C	1.819233	2.134559	3.985531
H	-0.322254	2.347606	3.918921
H	-1.055930	-0.817752	-4.674087
H	0.692057	-0.652449	-4.356334
H	0.015635	-2.272444	-4.638262
H	-0.311011	-4.905090	2.513430
H	-1.660490	-5.312464	1.386240
H	-1.944438	-4.242195	2.777475
C	-1.624663	4.347823	-1.265612
H	-2.227828	3.598912	-3.201587
H	-0.814108	4.850442	0.673392
C	5.810020	-0.012376	-0.422679
H	4.959124	1.971216	-0.321380
C	4.303903	-1.762826	-1.139483
H	2.283752	-1.156633	-1.608660
H	-6.565741	0.714713	-0.169010
C	2.933823	1.480157	3.461853
H	3.634119	0.000953	2.046153
H	1.940713	2.888360	4.766898
H	-2.378900	5.138611	-1.246067
C	5.569779	-1.354331	-0.711065
H	6.800251	0.310303	-0.092421
H	4.121269	-2.814747	-1.373116
H	3.934436	1.718832	3.830735
H	6.373396	-2.087832	-0.606798

*

TS(F-F^S)

CPCM (MeOH)

M06 SCF (DZ) =	-1223.415304
G (1 atm) =	-1223.115442
qh-G (1 mol/L) =	-1223.106496
qh-G (24.56 mol/L) =	-1223.103474
Lowest Frequency =	-8.73
HF SCF energy (TZ) =	-1216.935081
HF SCF energy (QZ) =	-1217.010753
Correlation energy (DZ) =	-4.157044
Correlation energy (TZ) =	-5.159743

H	-2.367927	1.452824	2.282766
C	0.367641	-1.460152	-2.351986
C	-1.650042	-3.231612	1.049825
C	-0.409908	2.492678	-0.960661
C	1.366091	3.620168	0.235075
C	3.919273	0.586156	-1.497273
H	3.295658	2.689583	-1.449754
C	-5.526490	-0.614570	1.202463
H	-3.865627	-0.706054	2.593008
C	-4.963715	-0.005364	-1.064983
H	-2.864390	0.369320	-1.450619
C	0.942341	0.421525	2.045795
C	-0.115897	2.178472	3.319059
C	0.988997	-1.470969	-3.712726
C	-2.378533	-4.382317	1.663003
C	-1.282701	3.527149	-0.635015
H	-0.738326	1.631818	-1.545058
C	0.483709	4.648459	0.565315
H	2.391779	3.634133	0.611635
C	5.144071	0.906361	-2.095167
C	3.649966	-0.744620	-1.147773
C	-5.919126	-0.366743	-0.111763
H	-6.265428	-0.907564	1.951381
H	-5.265128	0.188523	-2.096652
C	2.176326	0.783453	2.572674
H	0.912477	-0.441861	1.366188
C	1.118161	2.541239	3.849393
H	-1.016119	2.728684	3.603804
H	0.231129	-1.254883	-4.476719
H	1.745840	-0.671856	-3.748490
H	1.476353	-2.432573	-3.910625
H	-1.812114	-4.788280	2.508780
H	-2.557969	-5.159391	0.908995
H	-3.354930	-4.022123	2.021044
C	-0.841816	4.607925	0.132996
H	-2.320785	3.481917	-0.973754
H	0.834788	5.480984	1.179711
C	6.084955	-0.090286	-2.351521
H	5.358082	1.944747	-2.363143
C	4.588608	-1.737979	-1.404716
H	2.695916	-0.993585	-0.681410
H	-6.969054	-0.460543	-0.397104
C	2.267651	1.845357	3.474220
H	3.071512	0.234953	2.273150
H	1.184175	3.372549	4.553982
H	-1.532230	5.410816	0.400719
C	5.807537	-1.413273	-2.007753
H	7.037081	0.166751	-2.820659
H	4.369866	-2.773346	-1.134093
H	3.238828	2.129508	3.885339
H	6.543426	-2.195465	-2.207929

*

TS(F-F^S)

CPCM (MeOH)

wB97X-D3 SCF (DZ) =	-1223.920773
G (1 atm) =	-1223.609090
qh G-E (1 mol/L) =	0.324063
qh G-E (24.56 mol/L) =	0.327086
Lowest Frequency =	-201.15
HF SCF energy (TZ) =	-1216.937734
HF SCF energy (QZ) =	-1217.012360
Correlation energy (DZ) =	-4.156222
Correlation energy (TZ) =	-5.157644

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DLPNO-CCSD(T1)/CBS =      -1222.779210

PBE0+D3BJ (ATZ) =         -1223.285959
M06-2X (ATZ) =            -1223.988919
wB97M-V (ATZ) =           -1224.064012
B2GP-PLYP (ATZ) =         -1223.370835
B2K-PLYP (ATZ) =          -1223.212912
PWPB95 (ATZ) =            -1223.678360
PWPB95+D3BJ (ATZ) =       -1223.706055
PWPB95+D4 (ATZ) =         -1223.721115

*xyz 0 1
 Ru  -0.252470    0.855900    0.512370
 N   -0.308791   -1.035028   -0.068690
 O    0.768316    3.734761    0.075845
 C   -1.642642   -1.568984   -0.154770
 C    0.632018   -1.840792   -0.473580
 O   -0.783485    0.415434    2.539385
 O    0.243227    1.456087   -1.503935
 O    1.297517    0.441404    1.941445
 O   -1.824705    1.377215   -0.855925
 C   -0.147281    4.594582   -0.567771
 H    0.945926    3.005768   -0.543224
 C   -2.403992   -1.754323    0.999185
 C   -2.168170   -1.884975   -1.408684
 C    2.060266   -1.625524   -0.643501
 H    0.301010   -2.858445   -0.730657
 C    0.438841    0.264537    2.858508
 C   -0.995073    1.610550   -1.782299
 H    0.202718    4.902211   -1.570581
 H   -0.254793    5.501690    0.045063
 H   -1.151983    4.141229   -0.675601
 C   -3.692333   -2.269300    0.890302
 H   -1.976334   -1.486592    1.967347
 C   -3.462281   -2.390532   -1.507502
 H   -1.560290   -1.717399   -2.303130
 C    2.723395   -0.388291   -0.569366
 C    2.815744   -2.775361   -0.942804
 C    0.836913   -0.134919    4.235965
 C   -1.435091    2.025518   -3.141161
 C   -4.226315   -2.585577   -0.359203
 H   -4.286802   -2.424800    1.794140
 H   -3.874342   -2.630732   -2.490745
 C    4.094497   -0.316818   -0.778520
 H    2.154415    0.514819   -0.347175
 C    4.187724   -2.700365   -1.142922
 H    2.308614   -3.742417   -1.014647
 H    0.143730    0.286644    4.975519
 H    1.866961    0.177822    4.448287
 H    0.786077   -1.232385    4.314241
 H   -2.351821    2.626908   -3.079662
 H   -1.663041    1.123243   -3.730926
 H   -0.639428    2.581200   -3.653910
 H   -5.241233   -2.982882   -0.437024
 C    4.832192   -1.467054   -1.060920
 H    4.596338    0.652237   -0.721222
 H    4.755937   -3.605828   -1.367992
 H    5.911118   -1.400156   -1.221824
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DLPNO-CCSD(T1)/CBS =      -1222.777656

PBE0+D3BJ (ATZ) =         -1223.284757
M06-2X (ATZ) =            -1223.995054
wB97M-V (ATZ) =           -1224.065296
B2GP-PLYP (ATZ) =         -1223.372310
B2K-PLYP (ATZ) =          -1223.215691
PWPB95 (ATZ) =            -1223.678869
PWPB95+D3BJ (ATZ) =       -1223.708870
PWPB95+D4 (ATZ) =         -1223.721755

SMD (MeOH)
HF SCF energy (TZ) =      -1216.949642
HF SCF energy (QZ) =      -1217.024069
Correlation energy (DZ) =    -4.150360
Correlation energy (TZ) =    -5.152950
DLPNO-CCSD(T1)/CBS =      -1222.785295

*xyz 0 1
 Ru  -0.143113    0.922339    0.194050
 N   -0.345197   -1.028583   -0.290270
 C   -1.707021   -1.503334   -0.357249
 C    0.560852   -1.919288   -0.517941
 C   -2.498775   -1.507672    0.791467
 C   -2.219738   -1.931500   -1.581343
 C    2.009093   -1.698317   -0.623502
 C   -3.814423   -1.957846    0.707668
 C   -3.539922   -2.375526   -1.655306
 C    2.561876   -0.566264   -1.236670
 C    2.853489   -2.702688   -0.130667
 C   -4.338545   -2.390127   -0.512674
 C    3.944468   -0.430365   -1.319275
 C    4.236098   -2.551273   -0.195283
 C    4.782827   -1.412962   -0.788850
 H    0.222524   -2.957814   -0.632163
 H   -2.075343   -1.156533    1.733586
 H   -1.589102   -1.900003   -2.472607
 H   -4.436138   -1.970166    1.605458
 H   -3.943512   -2.708942   -2.613709
 H    1.906075    0.195631   -1.659863
 H    2.420561   -3.599348    0.320262
 H   -5.372917   -2.735126   -0.572000
 H    4.372310    0.451255   -1.801052
 H    4.888612   -3.327618    0.209288
 H    5.867201   -1.296374   -0.849753
 O    1.033563    3.597391   -0.002204
 C   -0.214658    3.956634    0.573788
 H    0.862395    3.188052   -0.865957
 H   -0.910480    4.383320   -0.166210
 H   -0.027346    4.703306    1.357466
 H   -0.719185    3.097165    1.071554
 O   -0.452801    0.475040    2.283068
 O    1.556890    0.545964    1.473191
 C    0.801710    0.371189    2.479839
 C    1.362293    0.084406    3.836205
 H    0.583122   -0.301920    4.503159
 H    1.763177    1.019847    4.254242
 H    2.189445   -0.632301    3.753224
 O    0.148933    1.569230   -1.870920
 O   -1.859557    1.418881   -1.057541
 C   -1.115957    1.666453   -2.051385
 C   -1.669080    2.037205   -3.388876
 H   -2.750340    2.203067   -3.330488
 H   -1.458723    1.219148   -4.093462
 H   -1.162212    2.937890   -3.760391
*
```

TS(F^c-F)
CPCM (MeOH)
M06 SCF (DZ) = -1496.953559
G (1 atm) = -1496.504730
qh-G (1 mol/L) = -1496.493474
qh-G (24.56 mol/L) = -1496.490451
Lowest Frequency = -40.95

HF SCF energy (TZ) = -1488.806656
HF SCF energy (QZ) = -1488.897019
Correlation energy (DZ) = -5.310318
Correlation energy (TZ) = -6.515314
DLPNO-CCSD(T1)/CBS = -1496.143682

PBE0+D3BJ (ATZ) = -1496.836035
M06-2X (ATZ) = -1497.723123
wB97M-V (ATZ) = -1497.796822
B2GP-PLYP (ATZ) = -1496.903168
B2K-PLYP (ATZ) = -1496.704348
PWPB95 (ATZ) = -1497.301181
PWPB95+D3BJ (ATZ) = -1497.344178
PWPB95+D4 (ATZ) = -1497.364941

*xyz 0 1
Ru 0.070136 0.119289 0.117012
C 3.110921 -1.254113 0.786954
C 2.214053 -2.271629 0.456608
C 3.779991 -0.530107 -0.206807
H 3.282067 -1.020309 1.843691
N -1.740620 0.912150 0.123235
O -0.297728 -0.582033 -1.881291
O 0.713612 1.304974 -1.547230
O -0.428188 -1.094715 1.824686
O 0.597794 0.796316 2.081881
C 1.965097 -2.615468 -0.877020
H 1.697430 -2.814645 1.255259
C 4.706875 0.609712 0.150314
C 3.532716 -0.879102 -1.538274
C -1.758667 2.345781 0.007673
C -2.915667 0.348178 0.138420
C 0.287406 0.435332 -2.368572
C 0.143085 -0.271131 2.601874
C 0.958420 -3.663685 -1.235960
C 2.648717 -1.904279 -1.867474
C 3.952891 1.726359 0.867653
C 5.896286 0.140283 0.982226
H 5.097104 1.016889 -0.801448
H 4.037867 -0.324125 -2.336743
C -1.267124 3.140187 1.043633
C -2.274931 2.930546 -1.150062
C -3.290522 -1.057627 0.137950
H -3.771193 1.040289 0.164792
C 0.461412 0.610396 -3.837746
C 0.331333 -0.572128 4.047351
H 1.383257 -4.430938 -1.903475
H 0.565569 -4.170372 -0.340520
H 0.107589 -3.204214 -1.769345
H 2.463244 -2.145016 -2.920576
H 3.096773 2.083849 0.271795
H 3.554529 1.375437 1.835581
H 4.617574 2.582389 1.070032
H 6.585160 0.977047 1.184653
H 5.567229 -0.257411 1.958138
H 6.463481 -0.653532 0.469853

TS(F^c-F) (Ru-C(*p*-cym) distance constrained at 4.43 Å)
CPCM (MeOH)
wB97X-D3 SCF (DZ) = -1497.650511
G (1 atm) = -1497.187056
qh G-E (1 mol/L) = 0.478519
qh G-E (24.56 mol/L) = 0.481541
Lowest Frequency = -33.14

HF SCF energy (TZ) = -1488.816636
HF SCF energy (QZ) = -1488.905892
Correlation energy (DZ) = -5.290877
Correlation energy (TZ) = -6.496312
DLPNO-CCSD(T1)/CBS = -1496.133477

PBE0+D3BJ (ATZ) = -1496.826507
M06-2X (ATZ) = -1497.730282
wB97M-V (ATZ) = -1497.794503
B2GP-PLYP (ATZ) = -1496.917804
B2K-PLYP (ATZ) = -1496.722460
PWPB95 (ATZ) = -1497.307115
PWPB95+D3BJ (ATZ) = -1497.345903
PWPB95+D4 (ATZ) = -1497.366946

SMD (MeOH)
HF SCF energy (TZ) = -1488.832961
HF SCF energy (QZ) = -1488.922055
Correlation energy (DZ) = -5.284457
Correlation energy (TZ) = -6.491225
DLPNO-CCSD(T1)/CBS = -1496.145282

*xyz 0 1
Ru 0.106638 0.332639 0.838824
N -1.724393 0.939621 0.311588
C -1.860716 2.377277 0.276480
C -2.786579 0.282311 -0.018368
C -1.969968 -2.109475 -0.363770
C -1.876869 3.102663 1.467636
C -1.961598 3.023304 -0.955204
C -2.987525 -1.164746 -0.157707
C -2.290825 -3.454716 -0.516227
C -2.005293 4.489283 1.418704
C -2.083868 4.412007 -0.993575
C -4.323994 -1.597544 -0.126464
C -3.619767 -3.878439 -0.454898
C -2.106144 5.147100 0.191367
C -4.638734 -2.946583 -0.258954
H -3.683719 0.884335 -0.213594
H -0.931750 -1.787935 -0.425428
H -1.781125 2.575663 2.417559
H -1.932602 2.436741 -1.876111
H -1.494389 -4.181171 -0.688813
H -2.026087 5.059950 2.349645
H -2.160436 4.919673 -1.957386
H -5.122280 -0.863422 0.011083
H -3.861124 -4.937290 -0.571510
H -2.201259 6.234489 0.159231
H -5.680987 -3.269148 -0.219780
C 3.201282 -2.836066 0.869161
C 4.091612 -1.798385 0.607967
C 2.544647 -3.506995 -0.172509
C 4.392195 -1.411842 -0.707265
C 1.544644 -4.595655 0.123227

```
 C   -1.316214    4.525836    0.922501
 H   -0.855130    2.658692    1.932934
 C   -2.309156    4.318509   -1.265960
 H   -2.636635    2.288648   -1.959192
 C   -2.430611   -2.138549   -0.124829
 C   -4.648480   -1.326573    0.393410
 H    1.497424    0.907819   -4.056931
 H   -0.194493    1.422699   -4.188630
 H    0.210966   -0.312252   -4.376244
 H    0.452955    0.350834    4.628019
 H    1.248622   -1.173232    4.159053
 H   -0.507427   -1.166485    4.432104
 C   -1.835235    5.118883   -0.229069
 H   -0.946750    5.150310    1.739876
 H   -2.711089    4.775070   -2.173952
 C   -2.920643   -3.437868   -0.120215
 H   -1.377449   -1.949135   -0.336392
 C   -5.130895   -2.628877    0.410658
 H   -5.329778   -0.492395    0.587802
 H   -1.868264    6.207554   -0.317581
 C   -4.265718   -3.690797    0.152361
 H   -2.241903   -4.268083   -0.333473
 H   -6.186340   -2.816281    0.621628
 H   -4.639990   -4.717625    0.158194
*
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 C    2.851252   -3.130565   -1.481783
 C    5.361558   -0.279721   -1.000164
 C    3.761989   -2.103759   -1.743592
 C    6.806162   -0.700295   -0.705122
 C    4.993761    1.003930   -0.247540
 H    2.988688   -3.112949    1.906105
 H    4.569562   -1.287078    1.448330
 H    2.018402   -5.442292    0.644489
 H    1.087343   -4.978988   -0.799677
 H    0.739788   -4.221930    0.775323
 H    2.361148   -3.639894   -2.316429
 H    5.284952   -0.070380   -2.080961
 H    3.977360   -1.828733   -2.780488
 H    7.509223    0.111254   -0.950932
 H    6.933720   -0.944849    0.362412
 H    7.089239   -1.588093   -1.291655
 H    3.945789    1.289243   -0.428808
 H    5.125411    0.883176    0.840090
 H    5.637872    1.837754   -0.567237
 O    0.534184   -0.243760   -1.180749
 O    1.088715    1.724789   -0.462221
 C    1.083436    0.879776   -1.413121
 C    1.717759    1.178309   -2.733701
 H    2.749904    0.795159   -2.718079
 H    1.747604    2.260369   -2.907850
 H    1.175988    0.668550   -3.539799
 O   -0.664798   -1.112385    2.225988
 O   -0.121147    0.877202    2.890270
 C   -0.560973   -0.282606    3.181248
 C   -0.909819   -0.654534    4.587151
 H   -1.557418   -1.538762    4.601048
 H    0.019649   -0.886065    5.128898
 H   -1.396492    0.190140    5.090777
*
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```

TS(F^C-F^S)

```
CPCM (MeOH)
M06 SCF (DZ) =            -1612.622302
G (1 atm) =               -1612.125063
qh-G (1 mol/L) =          -1612.113068
qh-G (24.56 mol/L) =      -1612.110045
Lowest Frequency =          -10.19

HF SCF energy (TZ) =      -1603.896805
HF SCF energy (QZ) =      -1603.995458
Correlation energy (DZ) =    -5.690289
Correlation energy (TZ) =    -6.987678
DLPNO-CCSD(T1)/CBS =      -1611.770972

*xyz 0 1
 Ru  -0.243436   -0.124735    0.329288
 C    2.858940   -1.157531    0.990132
 C    2.292179   -2.354825    0.564552
 C    3.860016   -0.514998    0.246301
 H    2.524333   -0.707245    1.933388
 N   -1.398205    1.308631   -0.399588
 O   -0.462117   -2.854889    2.434058
 O    0.340468    1.145507    1.985611
 O   -1.368054   -0.175189    2.169625
 O   -0.784472   -1.495439   -1.217943
 O    0.911226   -0.176770   -1.473134
 C    2.692047   -2.952845   -0.639174
 H    1.518669   -2.826856    1.182881
 C    4.407749    0.814941    0.716995
 C    4.272272   -1.126566   -0.937196
```

C	-0.667407	2.537617	-0.589931
C	-2.657276	1.366732	-0.721538
C	-1.111364	-3.722821	1.535990
H	-0.930197	-2.001227	2.426399
C	-0.616193	0.718299	2.692166
C	0.190710	-1.108689	-1.939473
C	2.046525	-4.223292	-1.104215
C	3.695265	-2.322214	-1.373227
H	5.059243	-0.668980	-1.544562
C	0.099959	2.721522	-1.739686
C	-0.750201	3.541396	0.374958
C	-3.701557	0.358413	-0.636715
H	-2.994294	2.330203	-1.134273
H	-0.458937	-4.597043	1.374188
H	-2.077018	-4.095806	1.929979
H	-1.293855	-3.254930	0.549203
C	-0.893039	1.249913	4.054150
C	0.461185	-1.707294	-3.275655
H	2.423012	-4.534867	-2.090588
H	2.222733	-5.052047	-0.397748
H	0.951930	-4.101844	-1.180986
H	4.038529	-2.774216	-2.310859
C	0.803112	3.910528	-1.910522
H	0.148308	1.923007	-2.481719
C	-0.038475	4.725247	0.198017
H	-1.369952	3.384758	1.261942
C	-3.572595	-0.903813	-0.033101
C	-4.939756	0.712373	-1.204326
H	-1.351407	0.477170	4.684893
H	-1.609755	2.082579	3.969009
H	0.024572	1.634767	4.516392
H	1.544826	-1.822619	-3.421007
H	0.086381	-1.028081	-4.057421
H	-0.045749	-2.675201	-3.380418
C	0.743133	4.911149	-0.941190
H	1.403332	4.055475	-2.812424
H	-0.099890	5.509782	0.956418
C	-4.651136	-1.778700	-0.010313
H	-2.620332	-1.184583	0.417453
C	-6.013163	-0.168410	-1.185238
H	-5.051516	1.696145	-1.670443
H	1.301164	5.840763	-1.077353
C	-5.870443	-1.419144	-0.586556
H	-4.541343	-2.757187	0.464285
H	-6.964693	0.122259	-1.636521
H	-6.712615	-2.115401	-0.565823
H	4.403783	0.787139	1.824317
C	5.832280	1.091026	0.258964
H	6.215016	2.010738	0.729775
H	6.517372	0.265964	0.513372
H	5.880917	1.246158	-0.833074
C	3.480834	1.949731	0.280238
H	2.450613	1.798190	0.643912
H	3.843648	2.921460	0.656737
H	3.443756	2.007272	-0.823030

*

TS(F^C-F^S)1

CPCM (MeOH)

M06 SCF (DZ) = -1612.620024

G (1 atm) = -1612.118435

qh-G (1 mol/L) = -1612.108549

qh-G (24.56 mol/L) = -1612.105526

Lowest Frequency = -125.60

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HF SCF energy (TZ) =      -1603.868371
HF SCF energy (QZ) =      -1603.966590
Correlation energy (DZ) =    -5.717552
Correlation energy (TZ) =    -7.016033
DLPNO-CCSD(T1)/CBS =      -1611.770967

*xyz 0 1
 Ru   0.155070   -0.181047    0.327231
 C    2.139627   -1.218500    1.038390
 C    1.095324   -2.106389    1.350080
 C    3.039566   -1.506911   -0.034194
 H    2.396053   -0.405066    1.723379
 N   -1.249346    1.174812   -0.363982
 O    2.122597    1.752238    1.397148
 O   -1.088846   -0.429949    2.005260
 O   -0.486047   -1.431031   -1.198310
 O    1.109851   -0.031624   -1.597723
 O   -0.177711    1.463990    2.735243
 C    0.916854   -3.308657    0.603708
 H    0.544231   -1.997217    2.288069
 C    4.121925   -0.502525   -0.346412
 C    2.856469   -2.681112   -0.730975
 C   -0.736751    2.501130   -0.599731
 C   -2.505451    1.051921   -0.663032
 C    2.597313    2.879988    0.707180
 H    1.281368    1.939513    1.860546
 C   -1.007355    0.539646    2.837582
 C    0.355723   -0.949163   -2.030739
 C   -0.238606   -4.199406    0.922317
 C    1.803837   -3.574494   -0.413146
 C    4.821598   -0.743791   -1.672961
 C    5.143529   -0.421970    0.786405
 H    3.606348    0.475799   -0.400320
 H    3.526544   -2.941752   -1.555240
 C   -0.227659    2.832223   -1.855971
 C   -0.815133    3.461581    0.408832
 C   -3.417215   -0.085982   -0.601795
 H   -2.989290    1.962084   -1.055309
 H    2.575064    3.796057    1.325874
 H    2.029008    3.077866   -0.222068
 H    3.647833    2.692545    0.428019
 C   -2.010633    0.530350    3.957118
 C    0.450350   -1.466108   -3.420732
 H   -1.184268   -3.719266    0.609203
 H   -0.322360   -4.388574    2.005351
 H   -0.168227   -5.167570    0.404512
 H    1.693381   -4.495699   -0.995902
 H    5.531079    0.071955   -1.885019
 H    5.402089   -1.683351   -1.659049
 H    4.107145   -0.798895   -2.510705
 H    5.895589    0.357530    0.578269
 H    5.675584   -1.383572    0.897684
 H    4.672259   -0.181680    1.752855
 C    0.196953    4.135801   -2.102268
 H   -0.175969    2.064396   -2.631733
 C   -0.387696    4.762110    0.151399
 H   -1.200204    3.172193    1.389263
 C   -3.166024   -1.331839   -0.001329
 C   -4.667424    0.126786   -1.211948
 H   -2.174714   -0.490426    4.329003
 H   -2.974748    0.896812    3.568338
 H   -1.690722    1.189581    4.774042
 H   -0.437431   -2.052520   -3.687884
 H    1.340756   -2.111720   -3.493296
 H    0.585533   -0.632517   -4.124210
 C    0.115936    5.103993   -1.102290
```

```
 H    0.586748    4.397359   -3.089255
 H   -0.456001    5.516456    0.939486
 C   -4.136288   -2.324865   -0.029018
 H   -2.218562   -1.506119    0.504561
 C   -5.630789   -0.873406   -1.246490
 H   -4.877822    1.096808   -1.672728
 H    0.444817    6.126813   -1.301539
 C   -5.365168   -2.105608   -0.653614
 H   -3.933679   -3.287475    0.447969
 H   -6.591507   -0.689205   -1.732617
 H   -6.119205   -2.896560   -0.670982
*
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```

TS(F^c-F^s)2

```
CPCM (MeOH)
M06 SCF (DZ) =            -1612.619686
G (1 atm) =               -1612.121567
qh-G (1 mol/L) =          -1612.110050
qh-G (24.56 mol/L) =      -1612.107027
Lowest Frequency =          -32.05

HF SCF energy (TZ) =      -1603.900002
HF SCF energy (QZ) =      -1603.998607
Correlation energy (DZ) =    -5.685052
Correlation energy (TZ) =    -6.982518
DLPNO-CCSD(T1)/CBS =      -1611.768990

*xyz 0 1
 Ru   0.528820   -0.259699    0.697396
 C   -3.114084   -0.580930    1.091218
 C   -2.738079    0.685331    1.534259
 C   -3.959261   -0.743158   -0.009388
 H   -2.715564   -1.465448    1.600624
 N    1.337319    0.832635   -0.809509
 O   -0.276615   -1.268314    2.475022
 O    1.015016    1.442915    1.989849
 O   -1.165157   -1.329558   -1.559887
 O    0.412052   -2.129202   -0.200482
 O    2.337183   -0.245579    1.684524
 C   -3.191886    1.842066    0.892759
 H   -2.070692    0.786951    2.397102
 C   -4.368044   -2.128925   -0.455497
 C   -4.429111    0.413051   -0.640222
 C    0.520295    1.973203   -1.130286
 C    2.526446    0.856944   -1.335626
 C    0.414330   -2.437747    2.926883
 H   -0.323768   -0.634268    3.206694
 C    2.134920    0.900382    2.216325
 C   -0.464630   -2.258913   -1.140181
 C   -2.775409    3.201475    1.366835
 C   -4.049760    1.679796   -0.198971
 C   -4.334714   -2.310616   -1.967185
 C   -5.743553   -2.480969    0.105986
 H   -3.630770   -2.828484   -0.015772
 H   -5.098966    0.329695   -1.502775
 C   -0.677182    1.789740   -1.823765
 C    0.933935    3.256815   -0.761787
 C    3.597408   -0.123738   -1.225807
 H    2.770982    1.733595   -1.956649
 H   -0.130618   -2.895276    3.765875
 H    1.445087   -2.195868    3.228530
 H    0.438688   -3.128909    2.075906
 C    3.204905    1.554193    3.016668
 C   -0.609890   -3.657207   -1.686383
 H   -2.751738    3.925716    0.537036
```

```
 H   -3.469544    3.597905    2.128579
 H   -1.773352    3.175389    1.826077
 H   -4.420458    2.568019   -0.722918
 H   -4.550222   -3.359391   -2.232849
 H   -5.098541   -1.689506   -2.467264
 H   -3.343235   -2.041387   -2.364337
 H   -6.035482   -3.508531   -0.169163
 H   -6.510485   -1.794408   -0.295568
 H   -5.765212   -2.400360    1.205407
 C   -1.442300    2.900466   -2.171149
 H   -0.988168    0.771075   -2.071284
 C    0.155590    4.358552   -1.106610
 H    1.861593    3.378760   -0.195215
 C    3.402619   -1.473163   -0.890210
 C    4.895229    0.323105   -1.526674
 H    2.774423    2.238969    3.758430
 H    3.842194    2.140706    2.334605
 H    3.837578    0.801553    3.505155
 H   -1.398352   -4.181049   -1.121302
 H   -0.917965   -3.629408   -2.740710
 H    0.318437   -4.234105   -1.574716
 C   -1.030223    4.185066   -1.819726
 H   -2.372558    2.756506   -2.727551
 H    0.480863    5.361188   -0.816992
 C    4.488984   -2.337564   -0.838170
 H    2.394270   -1.840815   -0.686403
 C    5.980688   -0.542204   -1.452587
 H    5.048770    1.369102   -1.810265
 H   -1.635583    5.051979   -2.097435
 C    5.779148   -1.877421   -1.106843
 H    4.327296   -3.389008   -0.586076
 H    6.986190   -0.175744   -1.672890
 H    6.627537   -2.564726   -1.056162
*
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TS(F^S-F^A)

```
CPCM (MeOH)
M06 SCF (DZ) =            -1779.770970
G (1 atm) =               -1779.281047
qh-G (1 mol/L) =          -1779.269863
qh-G (24.56 mol/L) =      -1779.266841
Lowest Frequency =          -40.7338

HF SCF energy (TZ) =      -1770.240924
HF SCF energy (QZ) =      -1770.349197
Correlation energy (DZ) =    -6.190395
Correlation energy (TZ) =    -7.592049
DLPNO-CCSD(T1)/CBS =      -1778.792907

*xyz 0 1
 Ru   0.380597   -0.109723    0.241820
 N    1.939529    0.581077   -0.757390
 O   -0.613677   -1.612815    2.665818
 C    1.666350    1.832395   -1.418321
 C    3.171051    0.168872   -0.848235
 N   -2.818350    0.201505    0.621469
 O   -0.748450   -0.412741   -1.563661
 O    1.435829    0.140143    2.113690
 O    0.449996   -2.011125   -0.731270
 O    0.251139    1.761097    1.299971
 C   -1.449419   -0.868132    3.522314
 H    0.277354   -1.226881    2.719073
 C    0.961535    1.855147   -2.621609
 C    2.120361    3.018903   -0.841273
 C    3.827361   -0.993795   -0.269559
```

H	3.833905	0.796324	-1.463842
C	-2.807914	1.607295	0.598476
C	-3.443113	-0.407773	-0.313595
C	-0.349278	-1.615000	-1.638285
C	0.994546	1.337029	2.226379
H	-1.358976	-1.191617	4.576153
H	-2.491022	-1.014191	3.195341
H	-1.241006	0.217974	3.472331
C	0.706879	3.075434	-3.241724
H	0.611333	0.916065	-3.052637
C	1.856158	4.234914	-1.465898
H	2.670698	2.978276	0.103012
C	3.237399	-1.930619	0.597038
C	5.181418	-1.160572	-0.617365
C	-2.496875	2.326422	-0.564188
C	-3.058851	2.303380	1.787307
C	-3.468357	-1.863755	-0.458814
H	-4.024605	0.151938	-1.075527
C	-0.776716	-2.523635	-2.737513
C	1.364121	2.186121	3.391542
C	1.147059	4.266925	-2.665403
H	0.161003	3.093619	-4.188525
H	2.209432	5.163526	-1.010652
C	3.984452	-2.992893	1.089658
H	2.190120	-1.817012	0.878309
C	5.923740	-2.225027	-0.123240
H	5.652201	-0.435577	-1.288437
C	-2.442951	3.717691	-0.532485
H	-2.246936	1.775689	-1.475939
C	-3.024251	3.693591	1.807101
H	-3.290068	1.731738	2.690887
C	-4.299049	-2.426848	-1.436389
C	-2.680311	-2.702769	0.343696
H	-1.529861	-2.042604	-3.373946
H	-1.184674	-3.452240	-2.309044
H	0.098269	-2.797800	-3.346428
H	2.348752	2.643472	3.204187
H	1.447130	1.574287	4.300065
H	0.629510	2.989659	3.531798
H	0.941731	5.221788	-3.155600
C	5.325021	-3.146431	0.734305
H	3.513439	-3.713220	1.763142
H	6.973038	-2.335712	-0.406401
C	-2.710671	4.407710	0.649228
H	-2.181191	4.267876	-1.441184
H	-3.236270	4.226766	2.738024
C	-4.351266	-3.806376	-1.611935
H	-4.909256	-1.768753	-2.063467
C	-2.733828	-4.079981	0.163058
H	-2.014563	-2.263017	1.093507
H	5.903741	-3.985735	1.128227
H	-2.668016	5.499703	0.671129
C	-3.567097	-4.635266	-0.811342
H	-5.003723	-4.236733	-2.375640
H	-2.116422	-4.732636	0.786157
H	-3.603326	-5.719436	-0.946688

*

***cis*-TS(F^A-G^A)1**
CPCM (MeOH)
M06 SCF (DZ) = -1664.113119
G (1 atm) = -1663.671374
qh-G (1 mol/L) = -1663.660703
qh-G (24.56 mol/L) = -1663.657681
Lowest Frequency = -85.62

***cis*-TS(F^A-G^A)1**
CPCM (MeOH)
wB97X-D3 SCF (DZ) = -1664.887603
G (1 atm) = -1664.428557
qh G-E (1 mol/L) = 0.473392
qh G-E (24.56 mol/L) = 0.476415
Lowest Frequency = -71.97

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HF SCF energy (TZ) =      -1655.145302
HF SCF energy (QZ) =      -1655.245906
Correlation energy (DZ) =    -5.830395
Correlation energy (TZ) =    -7.143540
DLPNO-CCSD(T1)/CBS =      -1663.187076

PBE0+D3BJ (ATZ) =         -1663.975662
M06-2X (ATZ) =            -1664.979338
wB97M-V (ATZ) =           -1665.088631
B2GP-PLYP (ATZ) =         -1664.059615
B2K-PLYP (ATZ) =          -1663.834922
PWPB95 (ATZ) =            -1664.508762
PWPB95+D3BJ (ATZ) =       -1664.559079
PWPB95+D4 (ATZ) =         -1664.580802

*xyz 0 1
 Ru   0.094399   -0.954469    0.115993
 C    2.583424   -1.641244   -1.038223
 N   -1.099537    0.342441    1.075850
 C    3.642068   -2.401656   -0.551462
 C    2.814930   -0.343007   -1.521906
 H    1.595867   -2.122108   -1.158800
 O   -0.060135   -3.335983   -1.451828
 N    0.527248    0.409558   -1.393676
 O    0.048489   -2.376705    1.728710
 O   -1.479596   -1.670188   -1.041051
 O    1.564160   -0.816152    1.754913
 C   -2.475138   -0.078389    1.156801
 C   -0.881657    1.526269    1.576040
 C    4.934893   -1.878773   -0.549559
 H    3.456800   -3.413625   -0.181558
 C    4.123793    0.157926   -1.557898
 C    1.713164    0.517217   -1.913364
 C   -1.176320   -2.805301   -1.566728
 C   -0.435668    1.378204   -1.841818
 C    1.069132   -1.856888    2.281785
 C   -2.823800   -1.223229    1.872361
 C   -3.452126    0.668598    0.497232
 C    0.289652    2.393674    1.573975
 H   -1.756900    1.995902    2.049807
 C    5.176942   -0.603567   -1.063405
 H    5.763988   -2.475233   -0.160638
 H    4.302909    1.163590   -1.950606
 H    1.909560    1.317978   -2.642290
 C   -2.283820   -3.450850   -2.356729
 C   -1.614597    0.956436   -2.460150
 C   -0.190217    2.742603   -1.662967
 C    1.693519   -2.481431    3.482569
 C   -4.157838   -1.614628    1.925839
 H   -2.041015   -1.798299    2.370330
 C   -4.783556    0.262293    0.547590
 H   -3.155046    1.553343   -0.074643
 C    1.587811    2.063372    1.149149
 C    0.042722    3.715070    1.993696
 H    6.192773   -0.201817   -1.076016
 H   -2.505141   -2.838752   -3.245815
 H   -3.204989   -3.490523   -1.756312
 H   -2.000606   -4.461348   -2.677339
 C   -2.536944    1.901147   -2.900661
 H   -1.797801   -0.112714   -2.572798
 C   -1.131019    3.679165   -2.085092
 H    0.729997    3.067713   -1.168803
 H    0.950217   -3.042993    4.062776
 H    2.469536   -3.187536    3.145742
 H    2.178375   -1.720692    4.107854

HF SCF energy (TZ) =      -1655.156379
HF SCF energy (QZ) =      -1655.255441
Correlation energy (DZ) =    -5.820983
Correlation energy (TZ) =    -7.133279
DLPNO-CCSD(T1)/CBS =      -1663.185391

PBE0+D3BJ (ATZ) =         -1663.976330
M06-2X (ATZ) =            -1665.008504
wB97M-V (ATZ) =           -1665.099868
B2GP-PLYP (ATZ) =         -1664.090789
B2K-PLYP (ATZ) =          -1663.873080
PWPB95 (ATZ) =            -1664.526026
PWPB95+D3BJ (ATZ) =       -1664.578527
PWPB95+D4 (ATZ) =         -1664.597565

SMD (MeOH)
HF SCF energy (TZ) =      -1655.173397
HF SCF energy (QZ) =      -1655.272205
Correlation energy (DZ) =    -5.814879
Correlation energy (TZ) =    -7.128243
DLPNO-CCSD(T1)/CBS =      -1663.197666

*xyz 0 1
 Ru  -0.368408   -0.523833   -0.367189
 C   -2.801546   -1.822687    0.501005
 N   -0.810885    0.082385    1.611348
 C   -3.836468   -2.393806   -0.235315
 C   -3.067088   -0.766973    1.383617
 N    0.802624    1.110858   -0.721650
 C    0.116729    0.803158    2.447601
 C   -1.986395   -0.095779    2.112721
 C   -5.139534   -1.914484   -0.095073
 C   -4.381889   -0.313406    1.548744
 C    2.148910    0.798948   -1.153564
 C    0.604954    2.377086   -0.542739
 C    1.403976    0.299476    2.645723
 C   -0.266054    2.002812    3.055474
 C   -5.411998   -0.878149    0.800390
 C    2.368447    0.177081   -2.382483
 C    3.223592    1.131541   -0.327406
 C   -0.550198    3.106871    0.000947
 C    2.295157    0.988463    3.465955
 C    0.635772    2.690503    3.865594
 C    3.672496   -0.109124   -2.781019
 C    4.524731    0.836466   -0.732285
 C   -1.876060    2.653003    0.040290
 C   -0.247590    4.369853    0.538495
 C    1.918379    2.185766    4.075981
 C    4.753451    0.215256   -1.959132
 C   -2.863046    3.432905    0.636522
 C   -1.233003    5.138859    1.149556
 C   -2.545234    4.668001    1.204291
 H   -1.795170   -2.268132    0.439847
 H   -3.622422   -3.217955   -0.918906
 H   -2.212036    0.292392    3.114282
 H   -5.950285   -2.358646   -0.676650
 H   -4.590026    0.499968    2.248348
 H    1.455106    3.031070   -0.776093
 H    1.694393   -0.619749    2.137563
 H   -1.259608    2.416884    2.871320
 H   -6.432915   -0.508876    0.916621
 H    1.517343   -0.086953   -3.009665
 H    3.035680    1.602753    0.639499
 H    3.298343    0.585205    3.621698
 H    0.330775    3.633635    4.324143
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 C   -5.140209   -0.879451    1.261278
 H   -4.433443   -2.506917    2.493868
 H   -5.545022    0.843598    0.021347
 C    2.587871    3.027027    1.128695
 H    1.811332    1.046124    0.839355
 C    1.041738    4.679625    1.961050
 H   -0.960811    3.988078    2.334002
 C   -2.305844    3.262772   -2.707354
 H   -3.452642    1.565941   -3.394849
 H   -0.937902    4.743264   -1.926145
 H   -6.184758   -1.198221    1.300673
 C    2.320521    4.338466    1.524012
 H    3.591022    2.748781    0.794280
 H    0.821979    5.701253    2.279423
 H   -3.040593    3.998701   -3.043071
 H    3.110881    5.092674    1.496835
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 H    3.843368   -0.590429   -3.746466
 H    5.362191    1.093642   -0.080174
 H   -2.138114    1.702009   -0.415645
 H    0.780533    4.738406    0.498210
 H    2.624334    2.727472    4.709139
 H    5.772869   -0.016734   -2.274725
 H   -3.892504    3.068853    0.658009
 H   -0.976370    6.108584    1.580565
 H   -3.323773    5.268369    1.680119
 O   -0.073622   -3.364493    0.095672
 O    1.273264   -1.608757    0.329175
 C    1.032225   -2.871043    0.380936
 C    2.181426   -3.735223    0.848188
 H    3.128814   -3.386631    0.416103
 H    2.262224   -3.648531    1.943051
 H    2.005650   -4.786372    0.589992
 O   -0.410875   -1.138058   -2.453414
 O   -1.974295    0.195106   -1.734031
 C   -1.483178   -0.492370   -2.679687
 C   -2.166013   -0.579336   -4.010330
 H   -2.762917    0.321402   -4.196203
 H   -2.840867   -1.448980   -3.994814
 H   -1.429587   -0.728634   -4.809337
*
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TS(F^A-G^A)1

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1664.889819
G (1 atm) =               -1664.428557
qh G-E (1 mol/L) =            0.471897
qh G-E (24.56 mol/L) =        0.474920
Lowest Frequency =          -75.41

HF SCF energy (TZ) =      -1655.165780
HF SCF energy (QZ) =      -1655.264686
Correlation energy (DZ) =    -5.813660
Correlation energy (TZ) =    -7.123642
DLPNO-CCSD(T1)/CBS =      -1663.183599

SMD (MeOH)
HF SCF energy (TZ) =      -1655.165781
HF SCF energy (QZ) =      -1655.281997
Correlation energy (DZ) =    -5.807311
Correlation energy (TZ) =    -7.118543
DLPNO-CCSD(T1)/CBS =      -1663.201757

*xyz 0 1
  Ru    -0.040317    0.079470    0.203910
  C     -2.855830    0.456917    0.909533
  N      0.204770   -1.948799   -0.283158
  C     -3.998516   -0.318166    0.731731
  C     -2.839148    1.791565    0.477180
  H     -2.016562    0.033142    1.482278
  N     -0.440702    2.113703    0.538914
  O     -0.785009   -0.878849    2.879139
  O      1.330876    0.621002   -1.258864
  O      1.081472   -0.103825    1.958616
  O     -0.748732    0.393606   -1.826688
  C     -1.070715   -2.622289   -0.305623
  C      1.187864   -2.653102   -0.725979
  C     -5.130311    0.230504    0.125898
  H     -4.002507   -1.355969    1.070730
  C     -3.991100    2.348522   -0.093862
  C     -1.628253    2.613115    0.553255
  C      0.653368    3.042096    0.519627
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  C      0.423733   -0.599048    2.946640
  C      0.437890    0.672247   -2.170058
  C     -1.541584   -3.244711    0.850625
  C     -1.824562   -2.639677   -1.480275
  C      2.602348   -2.262974   -0.823154
  H      0.959448   -3.663176   -1.096560
  C     -5.129377    1.566753   -0.278122
  H     -6.022059   -0.383459   -0.019275
  H     -3.983310    3.393141   -0.415565
  H     -1.756291    3.703753    0.585261
  C      1.686163    2.903221    1.449362
  C      0.706395    4.046344   -0.450111
  C      1.221141   -0.836114    4.208888
  C      0.804002    1.060243   -3.566997
  C     -2.771822   -3.901066    0.822609
  H     -0.949509   -3.195562    1.764941
  C     -3.056660   -3.291719   -1.495920
  H     -1.442789   -2.130522   -2.366594
  C      3.366157   -2.898135   -1.813624
  C      3.213801   -1.337181    0.033547
  H     -6.018548    2.001418   -0.739366
  C      2.758063    3.791920    1.421247
  H      1.644632    2.082664    2.166268
  C      1.788749    4.926216   -0.475375
  H     -0.085896    4.121915   -1.198632
  H      0.569011   -1.170269    5.024378
  H      1.985796   -1.603172    4.014841
  H      1.745685    0.084828    4.501025
  H     -0.052835    0.938690   -4.239072
  H      1.646800    0.444364   -3.909731
  H      1.130576    2.110546   -3.570027
  C     -3.531928   -3.926481   -0.347545
  H     -3.138197   -4.394892    1.725434
  H     -3.647257   -3.304692   -2.414628
  C      4.711754   -2.579163   -1.980070
  H      2.895772   -3.639047   -2.465855
  C      4.563744   -1.037261   -0.123948
  H      2.630326   -0.866296    0.826060
  C      2.813681    4.805532    0.461896
  H      3.561604    3.687139    2.153766
  H      1.830720    5.705451   -1.239528
  H     -4.496359   -4.438649   -0.363791
  C      5.312024   -1.646035   -1.134203
  H      5.294245   -3.066503   -2.764688
  H      5.037765   -0.319289    0.549188
  H      3.660843    5.494419    0.440025
  H      6.369555   -1.399983   -1.255397
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cis-TS(F^A-G^A)2

```
CPCM (MeOH)
M06 SCF (DZ) =            -1664.112029
G (1 atm) =               -1663.674318
qh-G (1 mol/L) =          -1663.664186
qh-G (24.56 mol/L) =      -1663.661164
Lowest Frequency =        -1224.78

HF SCF energy (TZ) =      -1655.100673
HF SCF energy (QZ) =      -1655.199453
Correlation energy (DZ) =    -5.876654
Correlation energy (TZ) =    -7.189370
DLPNO-CCSD(T1)/CBS =      -1663.185653

PBE0+D3BJ (ATZ) =         -1663.976735
M06-2X (ATZ) =            -1664.994049
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cis-TS(F^A-G^A)2

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1664.881340
G (1 atm) =               -1664.427266
qh G-E (1 mol/L) =            0.467178
qh G-E (24.56 mol/L) =        0.470200
Lowest Frequency =        -1201.08

HF SCF energy (TZ) =      -1655.107416
HF SCF energy (QZ) =      -1655.206079
Correlation energy (DZ) =    -5.869774
Correlation energy (TZ) =    -7.182639
DLPNO-CCSD(T1)/CBS =      -1663.185599

PBE0+D3BJ (ATZ) =         -1663.974902
M06-2X (ATZ) =            -1664.995384
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wB97M-V (ATZ) =           -1665.091724
B2GP-PLYP (ATZ) =         -1664.092813
B2K-PLYP (ATZ) =          -1663.874959
PWPB95 (ATZ) =            -1664.526447
PWPB95+D3BJ (ATZ) =       -1664.576851
PWPB95+D4 (ATZ) =         -1664.597740

*xyz 0 1
 Ru  -0.885225    0.130366    0.175705
 C   -2.501444   -1.098676   -0.297287
 N   -0.048430   -1.068370   -1.306664
 C   -2.127506   -2.145447   -1.189626
 H   -2.503757    0.248792   -0.753683
 C   -3.751955   -1.230442    0.338854
 N    0.991319    1.023872    0.873262
 O   -0.877157    1.658387   -1.262109
 O   -1.964622    0.993595    1.849445
 O   -0.996945   -0.940902    2.055347
 C    1.279511   -0.981432   -1.811834
 C   -0.816363   -2.026180   -1.753117
 C   -2.962142   -3.246757   -1.432784
 O   -3.049754    1.281977   -1.488148
 C   -4.568023   -2.333385    0.110279
 H   -4.094137   -0.436632    1.012332
 C    1.020395    2.453901    0.740393
 C    2.110532    0.518737    1.286089
 C   -2.013938    1.951661   -1.749064
 C   -1.707152   -0.020684    2.567153
 C    1.799486    0.261138   -2.183118
 C    2.081140   -2.124788   -1.907660
 H   -0.458005   -2.714280   -2.531423
 C   -4.182908   -3.343440   -0.781771
 H   -2.632247   -4.031479   -2.121261
 H   -5.531015   -2.407497    0.624407
 C    0.056723    3.241852    1.373772
 C    2.003325    3.061968   -0.046361
 C    2.538976   -0.867493    1.438898
 H    2.906765    1.236231    1.547672
 C   -2.086646    3.126102   -2.671666
 C   -2.257682   -0.155640    3.945068
 C    3.109985    0.352385   -2.644255
 H    1.158072    1.142852   -2.112078
 C    3.392114   -2.023797   -2.364001
 H    1.684544   -3.091548   -1.585102
 H   -4.837981   -4.199562   -0.959275
 C    0.086451    4.624557    1.223100
 H   -0.712834    2.757795    1.977033
 C    2.018831    4.446439   -0.201158
 H    2.742506    2.440695   -0.560234
 C    1.730891   -2.009174    1.312528
 C    3.907658   -1.040327    1.715246
 H   -1.727469    2.820887   -3.666697
 H   -1.426779    3.928032   -2.312687
 H   -3.117577    3.487204   -2.767633
 H   -2.422392    0.829747    4.399249
 H   -3.229954   -0.670885    3.882139
 H   -1.593019   -0.764395    4.571533
 C    3.913328   -0.784380   -2.730631
 H    3.507920    1.326971   -2.941193
 H    4.013681   -2.921277   -2.419694
 C    1.061465    5.233960    0.432892
 H   -0.665274    5.234743    1.730771
 H    2.785589    4.908969   -0.827979
 C    2.282951   -3.275167    1.462433
 H    0.667742   -1.899367    1.103844
 C    4.460244   -2.308183    1.844676
```

```
wB97M-V (ATZ) =           -1665.092658
B2GP-PLYP (ATZ) =         -1664.090324
B2K-PLYP (ATZ) =          -1663.872515
PWPB95 (ATZ) =            -1664.523993
PWPB95+D3BJ (ATZ) =       -1664.574528
PWPB95+D4 (ATZ) =         -1664.595306

SMD (MeOH)
HF SCF energy (TZ) =      -1655.122195
HF SCF energy (QZ) =      -1655.220673
Correlation energy (DZ) =    -5.863936
Correlation energy (TZ) =    -7.177996
DLPNO-CCSD(T1)/CBS =      -1663.196194

*xyz 0 1
 Ru  -0.889741    0.191328    0.209243
 C   -2.581135   -0.916446   -0.371448
 N   -0.052996   -1.107681   -1.203945
 C   -2.211725   -2.038274   -1.159583
 C   -3.881243   -0.929773    0.169527
 C    1.288216   -1.097845   -1.702268
 C   -0.851971   -2.025383   -1.653490
 C   -3.085867   -3.108870   -1.395937
 C   -4.747307   -1.999140   -0.048767
 C    1.843143    0.107844   -2.136791
 C    2.044586   -2.272671   -1.748863
 C   -4.358075   -3.090400   -0.837108
 C    3.148263    0.132667   -2.623631
 C    3.350689   -2.238691   -2.232755
 C    3.907542   -1.037851   -2.671983
 H   -4.220185   -0.080180    0.769519
 H   -0.504839   -2.759740   -2.390629
 H   -2.758105   -3.955767   -2.005094
 H   -5.748046   -1.982120    0.391104
 H    1.236217    1.012926   -2.090657
 H    1.622917   -3.206301   -1.371565
 H   -5.048902   -3.918145   -1.009749
 H    3.573853    1.077454   -2.969695
 H    3.940801   -3.157594   -2.249215
 H    4.933774   -1.012749   -3.044661
 H   -2.412262    0.393122   -0.969284
 N    1.028855    0.996150    0.984032
 C    1.091964    2.436009    0.919509
 C    2.152659    0.454517    1.306652
 C    0.256320    3.212481    1.722999
 C    1.985128    3.053638    0.040137
 C    2.513539   -0.967636    1.399344
 C    0.317190    4.602714    1.642055
 C    2.034104    4.444217   -0.042036
 C    1.611945   -2.015248    1.629401
 C    3.879784   -1.255889    1.257553
 C    1.199559    5.224617    0.757336
 C    2.074734   -3.326512    1.691254
 C    4.335087   -2.570219    1.297975
 C    3.430609   -3.609438    1.514720
 H    2.995087    1.131197    1.514066
 H   -0.445948    2.720810    2.394941
 H    2.626692    2.440798   -0.595991
 H   -0.334750    5.206150    2.277817
 H    2.728365    4.917025   -0.740321
 H    0.557551   -1.796776    1.787130
 H    4.588243   -0.439171    1.095685
 H    1.236298    6.314102    0.691198
 H    1.368109   -4.137684    1.879582
 H    5.397974   -2.782644    1.166897
 H    3.784334   -4.642082    1.557404
```

```
 H    4.545770   -0.157567    1.820162
 H    4.944703   -0.703757   -3.082545
 H    1.072818    6.319899    0.311196
 C    3.645092   -3.431659    1.720124
 H    1.641543   -4.155058    1.367317
 H    5.527484   -2.420007    2.049080
 H    4.070744   -4.432479    1.828217
*
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```

TS(F^A-G^A)2

```
CPCM (MeOH)
M06 SCF (DZ) =            -1664.111476
G (1 atm) =               -1663.674285
qh-G (1 mol/L) =          -1663.663828
qh-G (24.56 mol/L) =      -1663.660805
Lowest Frequency =        -1264.46

HF SCF energy (TZ) =      -1655.099952
HF SCF energy (QZ) =      -1655.200359
Correlation energy (DZ) =    -5.875218
Correlation energy (TZ) =    -7.187225
DLPNO-CCSD(T1)/CBS =      -1663.184490

*xyz 0 1
 Ru    -0.338553   -0.012652   -0.042207
 C      0.795600   -1.144801    1.277538
 N     -1.756676   -1.373145    0.602716
 H      0.261414    0.067778    1.761024
 C      0.116344   -2.362791    1.595693
 C      2.144315   -1.062912    1.684417
 N      1.226992    1.330041   -0.649957
 O     -1.395086    0.320905   -1.945775
 O     -1.213563    1.537235    1.045303
 O     -0.083285   -1.400078   -1.683011
 C     -3.110236   -1.375007    0.181454
 C     -1.271845   -2.400057    1.243694
 O      0.058650    0.987463    2.768979
 C      0.774577   -3.445693    2.198847
 C      2.793188   -2.138817    2.277163
 H      2.689372   -0.123717    1.542748
 C      0.777680    2.693057   -0.548730
 C      2.490411    1.239523   -0.927171
 C     -0.908316   -0.752004   -2.407675
 C     -0.817101    1.722954    2.237912
 C     -3.658701   -2.489462   -0.460867
 C     -3.885745   -0.227648    0.376077
 H     -1.916705   -3.245276    1.524646
 C      2.117838   -3.342414    2.526039
 H      0.218807   -4.366941    2.401409
 H      3.845437   -2.040921    2.562308
 C     -0.153380    3.190163   -1.459692
 C      1.254430    3.499679    0.484950
 C      3.354178    0.070235   -1.059557
 H      3.033170    2.193359   -1.042512
 C     -1.317878   -1.276694   -3.741797
 C     -1.427563    2.838628    3.022633
 C     -4.988045   -2.464397   -0.878094
 H     -3.031487   -3.365038   -0.653291
 O     -0.673824    1.736919   -1.200311
 O     -2.745708    1.307510   -1.833243
 C     -1.677640    1.985615   -1.926930
 C     -1.577349    3.085131   -2.940372
 H     -1.167590    2.657594   -3.868327
 H     -0.890067    3.863229   -2.587365
 H     -2.566152    3.505280   -3.157339
 O     -1.969025    1.119352    1.856806
 O     -1.222172   -0.912200    2.045582
 C     -1.854748    0.066751    2.553814
 C     -2.472496   -0.042145    3.913563
 H     -2.598806    0.950786    4.361174
 H     -3.463837   -0.508613    3.806070
 H     -1.859574   -0.682818    4.559630
*
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TS(F^A-G^A)2

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1664.880050
G (1 atm) =               -1664.426861
qh G-E (1 mol/L) =            0.467475
qh G-E (24.56 mol/L) =        0.470498
Lowest Frequency =        -1267.03

HF SCF energy (TZ) =      -1655.108552
HF SCF energy (QZ) =      -1655.207085
Correlation energy (DZ) =    -5.868614
Correlation energy (TZ) =    -7.180264
DLPNO-CCSD(T1)/CBS =      -1663.183482

SMD (MeOH)
HF SCF energy (TZ) =      -1655.123973
HF SCF energy (QZ) =      -1655.222333
Correlation energy (DZ) =    -5.862895
Correlation energy (TZ) =    -7.175678
DLPNO-CCSD(T1)/CBS =      -1663.194754

*xyz 0 1
  Ru    -0.315271   -0.036351   -0.029543
  C      0.798491   -1.168957    1.307068
  N     -1.752411   -1.386645    0.599744
  H      0.276255    0.054502    1.775980
  C      0.104454   -2.374203    1.623981
  C      2.152322   -1.119873    1.704339
  N      1.256155    1.342875   -0.637528
  O     -1.369531    0.300840   -1.909675
  O     -1.199108    1.520369    1.032842
  O     -0.059194   -1.422807   -1.690413
  C     -3.118123   -1.373635    0.192025
  C     -1.295450   -2.399642    1.264388
  O      0.043053    0.975022    2.776564
  C      0.738481   -3.472810    2.222786
  C      2.785498   -2.210161    2.291599
  H      2.717183   -0.195978    1.562385
  C      0.791874    2.708199   -0.561146
  C      2.511627    1.265691   -0.923886
  C     -0.888498   -0.765156   -2.398164
  C     -0.830940    1.706227    2.234073
  C     -3.659664   -2.450149   -0.514789
  C     -3.900979   -0.252067    0.478885
  H     -1.951915   -3.230246    1.552815
  C      2.086379   -3.397947    2.546763
  H      0.165689   -4.381458    2.427646
  H      3.840270   -2.133532    2.568777
  C     -0.119694    3.183263   -1.503209
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```
 C     -5.213248   -0.215751   -0.036061
 H     -3.424895    0.641220    0.852696
 H      2.640752   -4.181395    2.990953
 C     -0.605577    4.499774   -1.329027
 H     -0.527164    2.534298   -2.248918
 C      0.787968    4.806245    0.614542
 H      1.970385    3.083360    1.201315
 C      2.928255   -1.216391   -1.416951
 C      4.718165    0.290673   -0.801652
 H     -1.583447   -0.452373   -4.416219
 H     -2.212217   -1.906454   -3.608059
 H     -0.526108   -1.896661   -4.181356
 H     -2.150791    2.418503    3.739062
 H     -1.946933    3.546550    2.364696
 H     -0.651096    3.354869    3.604171
 C     -5.770224   -1.332477   -0.661842
 H     -5.410572   -3.336132   -1.384138
 H     -5.820730    0.677707    0.129452
 C     -0.143348    5.309756   -0.291173
 H     -1.330862    4.892302   -2.046554
 H      1.154422    5.431920    1.432648
 C      3.847058   -2.257265   -1.485097
 H      1.878123   -1.391859   -1.651882
 C      5.626934   -0.759789   -0.839416
 H      5.060216    1.298778   -0.547484
 H     -6.812129   -1.314572   -0.990656
 H     -0.509461    6.334364   -0.189780
 C      5.190830   -2.039492   -1.180976
 H      3.508998   -3.255576   -1.774719
 H      6.680497   -0.578134   -0.614316
 H      5.904001   -2.866680   -1.224476
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 C      1.241202    3.534666    0.469079
 C      3.385462    0.089088   -1.053603
 H      3.045455    2.217642   -1.060368
 C     -1.319087   -1.266082   -3.741905
 C     -1.473249    2.812301    3.016936
 C     -4.995398   -2.410749   -0.916073
 H     -3.028667   -3.306112   -0.764986
 C     -5.234404   -0.224911    0.080552
 H     -3.447191    0.587776    1.007479
 H      2.591199   -4.247035    3.011858
 C     -0.583063    4.493573   -1.407660
 H     -0.473116    2.513219   -2.287646
 C      0.765116    4.842427    0.562673
 H      1.942205    3.141667    1.209293
 C      2.962255   -1.190324   -1.432654
 C      4.745238    0.311435   -0.781981
 H     -1.616038   -0.428863   -4.385036
 H     -2.192472   -1.920610   -3.597525
 H     -0.519737   -1.851534   -4.211782
 H     -2.160228    2.367876    3.752817
 H     -2.033876    3.483845    2.357021
 H     -0.704806    3.369364    3.568605
 C     -5.786494   -1.302856   -0.615958
 H     -5.415582   -3.252353   -1.471025
 H     -5.848649    0.647386    0.314497
 C     -0.148339    5.325466   -0.373792
 H     -1.295293    4.866546   -2.147057
 H      1.108608    5.483667    1.377410
 C      3.884601   -2.229979   -1.514004
 H      1.913977   -1.367160   -1.667552
 C      5.659499   -0.736456   -0.838681
 H      5.083005    1.314010   -0.506346
 H     -6.831520   -1.274301   -0.931648
 H     -0.523656    6.348235   -0.298732
 C      5.228360   -2.011789   -1.205966
 H      3.548941   -3.224552   -1.815583
 H      6.711061   -0.554646   -0.607728
 H      5.943773   -2.835373   -1.263237
*
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```

TS(F^c-G^c)1

```
CPCM (MeOH)
M06 SCF (DZ) =            -1496.948782
G (1 atm) =               -1496.499343
qh-G (1 mol/L) =          -1496.488861
qh-G (24.56 mol/L) =      -1496,485838
Lowest Frequency =          -71.83

HF SCF energy (TZ) =      -1488.775095
HF SCF energy (QZ) =      -1488.865598
Correlation energy (DZ) =    -5.339143
Correlation energy (TZ) =    -6.545609
DLPNO-CCSD(T1)/CBS =      -1496.143458

PBE0+D3BJ (ATZ) =         -1496.833198
M06-2X (ATZ) =            -1497.716326
wB97M-V (ATZ) =           -1497.794599
B2GP-PLYP (ATZ) =         -1496.903294
B2K-PLYP (ATZ) =          -1496.705013
PWPB95 (ATZ) =            -1497.298074
PWPB95+D3BJ (ATZ) =       -1497.343420
PWPB95+D4 (ATZ) =         -1497.364029

*xyz 0 1
 Ru  -0.079692   -0.242430    0.349160
```

TS(F^c-G^c)1

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1497.654045
G (1 atm) =               -1497.187470
qh G-E (1 mol/L) =            0.479009
qh G-E (24.56 mol/L) =        0.482032
Lowest Frequency =          -37.28

HF SCF energy (TZ) =      -1488.778756
HF SCF energy (QZ) =      -1488.867757
Correlation energy (DZ) =    -5.338506
Correlation energy (TZ) =    -6.544363
DLPNO-CCSD(T1)/CBS =      -1496.143563

PBE0+D3BJ (ATZ) =         -1496.834655
M06-2X (ATZ) =            -1497.735544
wB97M-V (ATZ) =           -1497.802896
B2GP-PLYP (ATZ) =         -1496.921987
B2K-PLYP (ATZ) =          -1496.728697
PWPB95 (ATZ) =            -1497.310560
PWPB95+D3BJ (ATZ) =       -1497.356978
PWPB95+D4 (ATZ) =         -1497.376950

SMD (MeOH)
HF SCF energy (TZ) =      -1488.794978
```

```
 C    2.046044   -1.217820    0.471239
 C    1.121382   -2.099062    1.075677
 C    2.646523   -1.561108   -0.780248
 H    2.497737   -0.426451    1.082984
 C    0.985545    2.505192    0.796044
 H    0.676719    1.695087    1.475278
 O    0.801594    0.432722    3.110070
 N   -1.513643    1.226087   -0.099338
 O    0.297389   -0.119708   -1.794830
 O   -1.130349   -1.478623   -0.906361
 O   -0.988544   -0.532468    2.206374
 C    0.729468   -3.304004    0.420461
 H    0.899465   -2.007164    2.141189
 C    3.764998   -0.736880   -1.374112
 C    2.241854   -2.727980   -1.391181
 C    2.230645    3.088248    0.993653
 C    0.100549    3.037936   -0.152346
 C   -0.315496   -0.096319    3.215570
 C   -2.847198    0.807263   -0.402983
 C   -1.210648    2.453135   -0.372900
 C   -0.573772   -1.019095   -1.963614
 C   -0.279249   -4.186962    1.077674
 C    1.281378   -3.587420   -0.807744
 C    3.523674    0.763997   -1.309507
 C    5.087943   -1.091595   -0.695517
 H    3.843879   -1.030419   -2.438341
 H    2.693525   -3.008180   -2.349909
 C    2.615033    4.191835    0.230652
 H    2.902098    2.678952    1.753966
 C    0.479191    4.166163   -0.891995
 C   -0.988207   -0.265726    4.551995
 C   -3.596417    0.148306    0.573422
 C   -3.379348    1.023073   -1.676140
 H   -1.986390    3.108674   -0.799399
 C   -0.940212   -1.546319   -3.303782
 H   -1.255310   -3.673366    1.139159
 H    0.012689   -4.431393    2.112952
 H   -0.423800   -5.128263    0.527201
 H    0.991862   -4.504547   -1.331851
 H    2.561611    1.046319   -1.765708
 H    3.517510    1.119444   -0.265363
 H    4.331520    1.305014   -1.829506
 H    5.924145   -0.527620   -1.141597
 H    5.052483   -0.841992    0.380085
 H    5.311361   -2.167164   -0.783480
 C    1.739111    4.728044   -0.713166
 H    3.597881    4.645023    0.381732
 H   -0.217648    4.591293   -1.620153
 H   -1.881468    0.376699    4.596985
 H   -1.331298   -1.302906    4.678873
 H   -0.307916    0.007194    5.368468
 C   -4.891404   -0.264229    0.277370
 H   -3.140052   -0.038222    1.548365
 C   -4.672913    0.593915   -1.965679
 H   -2.767285    1.502804   -2.446245
 H   -0.810575   -0.768477   -4.067802
 H   -0.267929   -2.383942   -3.550070
 H   -1.972310   -1.920940   -3.305365
 H    2.036180    5.597039   -1.304612
 C   -5.433843   -0.044320   -0.989422
 H   -5.483413   -0.769289    1.044849
 H   -5.083475    0.755990   -2.965363
 H   -6.448373   -0.379877   -1.217545
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```
HF SCF energy (QZ) =      -1488.883762
Correlation energy (DZ) =    -5.331916
Correlation energy (TZ) =    -6.538885
DLPNO-CCSD(T1)/CBS =      -1496.154674

*xyz 0 1
 Ru  -0.432224    0.805777    0.132237
 C    2.045464   -0.474838   -1.715285
 O    0.945633    2.446215   -1.860747
 N   -0.795289   -1.049017   -0.775419
 O   -0.675353    2.756583    1.047649
 O   -2.264464    1.291065    0.942160
 O   -1.141324    1.729265   -1.569015
 C    3.413167   -0.395437   -1.963806
 C    1.422067   -1.722614   -1.622294
 C   -0.251189    2.428906   -2.188270
 C   -2.174229   -1.471908   -0.719993
 C   -0.012161   -1.880417   -1.374545
 C   -1.893059    2.475255    1.249674
 C    4.170659   -1.558818   -2.101982
 C    2.180630   -2.889341   -1.797601
 C   -0.761901    3.257598   -3.343258
 C   -3.168841   -0.629232   -1.221063
 C   -2.509308   -2.722115   -0.196791
 C   -2.867814    3.477518    1.774352
 C    3.552168   -2.808159   -2.017759
 C   -4.497531   -1.045396   -1.194966
 C   -3.843697   -3.126084   -0.164906
 C   -4.841260   -2.289869   -0.663634
 H    1.470925    0.455050   -1.648479
 H    3.888452    0.584006   -2.049872
 H   -0.450078   -2.813601   -1.752603
 H    5.245084   -1.492285   -2.286879
 H    1.690047   -3.864492   -1.742989
 H    0.050285    3.472492   -4.048713
 H   -1.586518    2.746002   -3.856435
 H   -1.146638    4.210446   -2.947948
 H   -2.885671    0.340706   -1.630298
 H   -1.726234   -3.373838    0.195118
 H   -2.346931    4.240423    2.364468
 H   -3.352203    3.965383    0.914896
 H   -3.642260    2.983001    2.373207
 H    4.139590   -3.721057   -2.134016
 H   -5.272526   -0.387623   -1.594367
 H   -4.100297   -4.100524    0.256129
 H   -5.886101   -2.606732   -0.639761
 C    0.994829    0.529114    1.954235
 C   -0.145785   -0.230100    2.286421
 C    2.213622   -0.122537    1.600250
 C   -0.090554   -1.651833    2.309988
 C    3.498503    0.666917    1.416822
 C    2.212931   -1.502299    1.542699
 C   -1.256834   -2.420350    2.868916
 C    1.075694   -2.263643    1.895173
 C    3.294027    2.042243    0.776933
 C    4.216701    0.803049    2.767508
 H    1.014269    1.589732    2.209605
 H   -0.997536    0.257570    2.764932
 H    4.143453    0.069060    0.750821
 H    3.128494   -2.024465    1.248407
 H   -2.210804   -2.045420    2.470784
 H   -1.293044   -2.303864    3.964571
 H   -1.180996   -3.493803    2.646674
 H    1.139955   -3.355113    1.880227
 H    2.714871    1.988675   -0.156632
 H    2.760466    2.726477    1.456761
```

TS(F^c-G^c)2
CPCM (MeOH)
M06 SCF (DZ) = -1496.948021
G (1 atm) = -1496.502568
qh-G (1 mol/L) = -1496.492655
qh-G (24.56 mol/L) = -1496.489632
Lowest Frequency = -1325.57

HF SCF energy (TZ) = -1488.719478
HF SCF energy (QZ) = -1488.809549
Correlation energy (DZ) = -5.394410
Correlation energy (TZ) = -6.602948
DLPNO-CCSD(T1)/CBS = -1496.145830

PBE0+D3BJ (ATZ) = -1496.838839
M06-2X (ATZ) = -1497.705880
wB97M-V (ATZ) = -1497.790158
B2GP-PLYP (ATZ) = -1496.905003
B2K-PLYP (ATZ) = -1496.707675
PWPB95 (ATZ) = -1497.299379
PWPB95+D3BJ (ATZ) = -1497.347416
PWPB95+D4 (ATZ) = -1497.366707

*xyz 0 1
Ru 0.148148 0.673374 0.097336
C -0.839627 -0.721451 1.324828
C -1.830331 0.480411 -1.365916
C -2.013697 -0.565469 2.085215
C -0.356385 -2.049675 1.154256
H 0.125579 0.054701 1.901680
C -0.759658 -0.170979 -2.013848
N 1.349919 -1.001402 -0.040606
O 0.711160 2.314267 -1.270822
O 1.682012 1.510434 1.217610
O -0.729791 2.643712 0.332193
C -2.954535 -0.261227 -0.913122
H -1.918244 1.565271 -1.436247
C -2.690687 -1.667843 2.593787
H -2.388991 0.443829 2.289556
C -1.037613 -3.161670 1.669517
C 0.896880 -2.117772 0.467104
O 0.988317 0.340437 2.969262
C -0.790088 -1.573776 -2.237061
H -0.035814 0.430332 -2.572406
C 2.686659 -0.935976 -0.509045
C -0.010426 3.116420 -0.601830
C 1.801370 1.131235 2.427562
C -4.189689 0.404226 -0.344332
C -2.932346 -1.632168 -1.085406
C -2.210752 -2.969351 2.383112
H -3.604547 -1.518128 3.176583
H -0.637847 -4.167618 1.507503
H 1.478799 -3.047367 0.395882
C 0.299229 -2.238482 -3.018309
C -1.869000 -2.279671 -1.741460
C 2.987839 -0.179797 -1.646670
C 3.717503 -1.580543 0.185823
C 0.003626 4.580744 -0.887096
C 2.982455 1.637675 3.191789
H 4.268197 2.502615 0.550968
H 5.178786 1.325966 2.648186
H 3.601770 1.382366 3.476542
H 4.413792 -0.182065 3.216873
*

TS(F^c-G^c)2
CPCM (MeOH)
wB97X-D3 SCF (DZ) = -1497.650864
G (1 atm) = -1497.190627
qh G-E (1 mol/L) = 0.474742
qh G-E (24.56 mol/L) = 0.477765
Lowest Frequency = -1275.87

HF SCF energy (TZ) = -1488.740922
HF SCF energy (QZ) = -1488.829788
Correlation energy (DZ) = -5.373448
Correlation energy (TZ) = -6.581538
DLPNO-CCSD(T1)/CBS = -1496.144032

PBE0+D3BJ (ATZ) = -1496.837185
M06-2X (ATZ) = -1497.727951
wB97M-V (ATZ) = -1497.796353
B2GP-PLYP (ATZ) = -1496.921694
B2K-PLYP (ATZ) = -1496.728527
PWPB95 (ATZ) = -1497.309272
PWPB95+D3BJ (ATZ) = -1497.356787
PWPB95+D4 (ATZ) = -1497.377166

SMD (MeOH)
HF SCF energy (TZ) = -1488.754719
HF SCF energy (QZ) = -1488.843438
Correlation energy (DZ) = -5.367819
Correlation energy (TZ) = -6.577095
DLPNO-CCSD(T1)/CBS = -1496.153888

*xyz 0 1
Ru 0.260953 0.718570 0.234627
C -0.766457 -0.663426 1.446818
C -1.964778 -0.513830 2.169042
C -0.326855 -1.992060 1.210735
N 1.425540 -0.986418 0.032451
O 1.783067 1.539384 1.349075
C -2.699473 -1.620815 2.586026
C -1.057960 -3.110277 1.635084
C 0.933002 -2.089249 0.506369
O 0.915247 0.539322 3.118191
C 2.738490 -0.982558 -0.520261
C 1.800485 1.272799 2.589167
C -2.251867 -2.922544 2.319316
C 3.011049 -0.161896 -1.619010
C 3.762474 -1.752542 0.043525
C 2.917277 1.812950 3.427626
C 4.287921 -0.146206 -2.174356
C 5.038808 -1.728513 -0.516172
C 5.305146 -0.931477 -1.629205
H -2.322579 0.490397 2.413867
H -3.632210 -1.473700 3.137069
H -0.690390 -4.117036 1.419114
H 1.459634 -3.044312 0.391477
H -2.835292 -3.782257 2.655454
H 2.218417 0.463692 -2.030073
H 3.568774 -2.350007 0.936876
H 3.708776 1.049305 3.471516
H 3.332160 2.722991 2.979792

```
 C   -5.335689    0.329530   -1.353810
 C   -3.983619    1.845555    0.093885
 H   -4.483691   -0.189179    0.545010
 H   -3.781703   -2.228522   -0.732569
 H   -2.752046   -3.824662    2.794440
 H    0.566101   -1.649272   -3.911567
 H    1.225330   -2.341144   -2.425816
 H    0.002366   -3.245499   -3.347062
 H   -1.916442   -3.363473   -1.893918
 C    4.298424   -0.108856   -2.106049
 H    2.185037    0.347397   -2.166186
 C    5.027509   -1.499925   -0.278292
 H    3.493191   -2.119471    1.110669
 H    0.205288    4.765822   -1.950192
 H   -0.944673    5.045172   -0.587502
 H    0.812959    5.046160   -0.302916
 H    3.852639    1.013343    2.933693
 H    3.216866    2.670381    2.903345
 H    2.809803    1.565135    4.272188
 H   -5.562823   -0.707846   -1.645619
 H   -6.253656    0.776700   -0.937661
 H   -5.073792    0.887291   -2.270578
 H   -3.127889    1.962895    0.775941
 H   -3.802682    2.505542   -0.773284
 H   -4.888446    2.219504    0.598905
 C    5.322278   -0.770321   -1.427962
 H    4.522407    0.473958   -3.002832
 H    5.825885   -2.001108    0.274550
 H    6.351708   -0.704681   -1.788120
*
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```

TS(F^S-G^S)1

```
CPCM (MeOH)
M06 SCF (DZ) =            -1223.418182
G (1 atm) =               -1223.117705
qh-G (1 mol/L) =          -1223.109067
qh-G (24.56 mol/L) =      -1223.106045
Lowest Frequency =          -96.9592

HF SCF energy (TZ) =      -1216.944599
HF SCF energy (QZ) =      -1217.020748
Correlation energy (DZ) =    -4.158022
Correlation energy (TZ) =    -5.160734
DLPNO-CCSD(T1)/CBS =      -1222.790347

PBE0+D3BJ (ATZ) =         -1223.295957
M06-2X (ATZ) =            -1224.001390
wB97M-V (ATZ) =           -1224.075544
B2GP-PLYP (ATZ) =         -1223.382940
B2K-PLYP (ATZ) =          -1223.225856
PWPB95 (ATZ) =            -1223.688115
PWPB95+D3BJ (ATZ) =       -1223.716849
PWPB95+D4 (ATZ) =         -1223.731590

*xyz 0 1
 Ru   0.131336    0.687770    0.386100
 C    2.553683   -0.602319   -0.591936
 O    0.648272    2.431594    1.598479
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 H    2.567545    2.004072    4.449012
 H    4.489525    0.490391   -3.038546
 H    5.833168   -2.328740   -0.067252
 H    6.307264   -0.911117   -2.062635
 C   -1.875004    0.479350   -1.455065
 C   -0.798085   -0.143242   -2.104059
 C   -2.967526   -0.274958   -0.980586
 C   -0.773519   -1.538502   -2.298568
 C   -4.201538    0.364806   -0.362440
 C   -2.910850   -1.655396   -1.141049
 C    0.359801   -2.202515   -3.035991
 C   -1.836152   -2.276388   -1.788832
 C   -5.404305    0.226182   -1.307108
 C   -4.009826    1.825425    0.042947
 H   -1.925303    1.567314   -1.431274
 H   -0.033095    0.478823   -2.573179
 H   -4.425216   -0.213952    0.551294
 H   -3.731449   -2.273786   -0.765705
 H    0.917007   -1.478704   -3.647297
 H    1.076226   -2.660719   -2.334837
 H   -0.010240   -3.001959   -3.694406
 H   -1.843601   -3.363546   -1.909982
 H   -5.600775   -0.825547   -1.564342
 H   -6.313428    0.637440   -0.840646
 H   -5.224335    0.776322   -2.245762
 H   -3.123018    1.966175    0.677195
 H   -3.891505    2.475285   -0.840091
 H   -4.892797    2.180901    0.595438
 H    0.197000    0.179578    2.091835
 O    0.811636    2.318189   -1.175812
 O   -0.667039    2.662315    0.389255
 C    0.032696    3.118022   -0.569212
 C   -0.043306    4.564800   -0.953329
 H    0.170470    4.688493   -2.021948
 H   -1.029626    4.975887   -0.706120
 H    0.718035    5.116433   -0.380950
*
---------------------------------------
```

TS(F^S-G^S)1

```
CPCM (MeOH)
wB97X-D3 SCF (DZ) =       -1223.933120
G (1 atm) =               -1223.620696
qh G-E (1 mol/L) =            0.323998
qh G-E (24.56 mol/L) =        0.327020
Lowest Frequency =          -82.11

HF SCF energy (TZ) =      -1216.950758
HF SCF energy (QZ) =      -1217.025753
Correlation energy (DZ) =    -4.153804
Correlation energy (TZ) =    -5.155707
DLPNO-CCSD(T1)/CBS =      -1222.789506

PBE0+D3BJ (ATZ) =         -1223.297479
M06-2X (ATZ) =            -1224.005619
wB97M-V (ATZ) =           -1224.076789
B2GP-PLYP (ATZ) =         -1223.385447
B2K-PLYP (ATZ) =          -1223.229121
PWPB95 (ATZ) =            -1223.689368
PWPB95+D3BJ (ATZ) =       -1223.719687
PWPB95+D4 (ATZ) =         -1223.732506

*xyz 0 1
 Ru   0.129112    0.701671    0.429491
 C    2.564247   -0.556938   -0.589024
 C    3.918355   -0.501888   -0.269229
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C	3.913494	-0.536462	-0.307586
C	1.917650	-1.850139	-0.707793
H	2.028459	0.331407	-0.853660
O	1.655282	2.281304	-1.484220
N	-0.346343	-0.996990	-0.635009
O	-0.514370	2.036781	-1.057226
O	-1.517058	0.450287	1.618589
O	0.335108	-0.533706	2.173342
C	-0.362307	3.417355	1.829456
H	1.014887	2.147522	2.449510
C	4.652327	-1.708309	-0.140842
H	4.402934	0.437954	-0.233407
C	2.677086	-3.022229	-0.579989
C	0.489026	-1.950044	-0.928705
C	0.472400	2.610450	-1.657757
C	-1.734129	-1.269662	-0.857638
C	-0.884486	-0.309732	2.430111
H	0.065608	4.276997	2.365813
H	-1.206042	2.995636	2.397331
H	-0.717018	3.737195	0.841518
C	4.034551	-2.950853	-0.287948
H	5.719825	-1.653062	0.086781
H	2.186204	-3.993915	-0.689299
H	0.098116	-2.887759	-1.349976
C	0.098854	3.747022	-2.571277
C	-2.503744	-0.354286	-1.577828
C	-2.320016	-2.422453	-0.329883
C	-1.581370	-0.914810	3.596153
H	4.615950	-3.868780	-0.173915
H	-0.811361	3.513494	-3.141374
H	-0.118869	4.638576	-1.960771
H	0.925089	3.986305	-3.253111
C	-3.852311	-0.616298	-1.796041
H	-2.028341	0.557889	-1.945868
C	-3.674750	-2.669013	-0.543624
H	-1.716335	-3.112740	0.266977
H	-2.144716	-1.797627	3.254496
H	-2.302540	-0.205089	4.022848
H	-0.857764	-1.234483	4.356137
C	-4.442321	-1.771795	-1.282127
H	-4.452022	0.094001	-2.370964
H	-4.131834	-3.568077	-0.122743
H	-5.504298	-1.967026	-1.449826

*

TS(F^S-G^S)2

CPCM (MeOH)

M06 SCF (DZ) =	-1223.422203
G (1 atm) =	-1223.125935
qh-G (1 mol/L) =	-1223.117742
qh-G (24.56 mol/L) =	-1223.114720
Lowest Frequency =	-1122.89
HF SCF energy (TZ) =	-1216.889216
HF SCF energy (QZ) =	-1216.964864
Correlation energy (DZ) =	-4.218356
Correlation energy (TZ) =	-5.221884
DLPNO-CCSD(T1)/CBS =	-1222.795939
PBE0+D3BJ (ATZ) =	-1223.304086
M06-2X (ATZ) =	-1223.992008
wB97M-V (ATZ) =	-1224.070939
B2GP-PLYP (ATZ) =	-1223.389409
B2K-PLYP (ATZ) =	-1223.232139
PWPB95 (ATZ) =	-1223.691911

C	1.925318	-1.798385	-0.731019
N	-0.351298	-0.975462	-0.654581
C	4.644941	-1.681010	-0.093240
C	2.668255	-2.977729	-0.587832
C	0.486735	-1.899583	-0.983414
C	-1.740453	-1.253849	-0.896049
C	4.020732	-2.918234	-0.260525
C	-2.484157	-0.392776	-1.704099
C	-2.342767	-2.358164	-0.290812
C	-3.834165	-0.657247	-1.922430
C	-3.697689	-2.608541	-0.507492
C	-4.445122	-1.762212	-1.325234
H	2.050343	0.385874	-0.837318
H	4.410302	0.467955	-0.170657
H	5.706515	-1.635158	0.159401
H	2.175206	-3.944758	-0.714929
H	0.111462	-2.823899	-1.441562
H	4.590533	-3.841290	-0.136962
H	-1.997837	0.481050	-2.139051
H	-1.752908	-3.006064	0.361757
H	-4.416933	0.009723	-2.561545
H	-4.169538	-3.469107	-0.028443
H	-5.505835	-1.959287	-1.494185
O	0.724050	2.397706	1.671115
C	-0.231762	3.436989	1.930373
H	1.070567	2.077322	2.516351
H	0.256363	4.262352	2.467316
H	-1.081266	3.049879	2.511573
H	-0.584882	3.785037	0.953204
O	1.594131	2.281006	-1.520769
O	-0.556235	2.046977	-1.007951
C	0.399552	2.591620	-1.675288
C	-0.004009	3.673988	-2.649827
H	-0.991108	3.467255	-3.083027
H	-0.066270	4.628834	-2.104727
H	0.748271	3.778190	-3.441450
O	-1.524814	0.428959	1.660246
O	0.334655	-0.544058	2.220748
C	-0.891380	-0.336269	2.465844
C	-1.597784	-0.981614	3.614252
H	-2.149278	-1.853826	3.231216
H	-2.323271	-0.285112	4.052805
H	-0.877091	-1.318046	4.368276

*

TS(F^S-G^S)2

CPCM (MeOH)

wB97X-D3 SCF (DZ) =	-1223.930745
G (1 atm) =	-1223.623374
qh G-E (1 mol/L) =	0.318628
qh G-E (24.56 mol/L) =	0.321651
Lowest Frequency =	-1202.57
HF SCF energy (TZ) =	-1216.895958
HF SCF energy (QZ) =	-1216.970248
Correlation energy (DZ) =	-4.212846
Correlation energy (TZ) =	-5.216409
DLPNO-CCSD(T1)/CBS =	-1222.795460
PBE0+D3BJ (ATZ) =	-1223.303512
M06-2X (ATZ) =	-1223.995465
wB97M-V (ATZ) =	-1224.072149
B2GP-PLYP (ATZ) =	-1223.391195
B2K-PLYP (ATZ) =	-1223.234825
PWPB95 (ATZ) =	-1223.692448

PWPB95+D3BJ (ATZ) = -1223.721519
PWPB95+D4 (ATZ) = -1223.735538

*xyz 0 1

Ru	0.339669	-0.589354	-0.038913
C	1.711159	0.919218	0.117810
H	1.186857	0.297792	1.317420
C	1.152059	2.205049	-0.147161
C	3.115882	0.840063	0.192832
N	-0.878006	1.055961	-0.238981
O	-1.146093	-2.057582	-0.844287
O	1.271001	-0.930004	-1.935443
O	1.809260	-2.177410	-0.232322
O	-0.541067	-0.963106	1.821165
O	1.024368	0.332737	2.701676
C	1.956811	3.340174	-0.322597
C	-0.273064	2.214496	-0.281426
C	3.908949	1.966838	0.001215
H	3.588616	-0.123036	0.414764
C	-2.280735	1.004588	-0.462622
C	-1.372324	-3.274674	-0.131786
H	-0.861634	-2.270078	-1.746722
C	1.980231	-1.875097	-1.450334
C	0.010910	-0.403620	2.823694
C	3.336810	3.222172	-0.250103
H	1.488237	4.307344	-0.531436
H	-0.843916	3.142391	-0.422721
H	4.997796	1.874038	0.056799
C	-3.089480	0.248068	0.391404
C	-2.853428	1.686659	-1.541248
H	-2.119740	-3.888864	-0.655713
H	-1.757081	-2.995239	0.856793
H	-0.436621	-3.843778	-0.009149
C	3.001246	-2.561613	-2.289471
C	-0.600118	-0.619994	4.170316
H	3.974644	4.098083	-0.389620
C	-4.463142	0.203181	0.179995
H	-2.620113	-0.288127	1.219407
C	-4.229611	1.630131	-1.748589
H	-2.212313	2.243398	-2.230341
H	2.675475	-2.607647	-3.336843
H	3.932561	-1.973623	-2.252035
H	3.212911	-3.566905	-1.904087
H	-1.359385	0.160287	4.337693
H	-1.101122	-1.594826	4.221582
H	0.157553	-0.530395	4.958649
C	-5.039093	0.892874	-0.887692
H	-5.092816	-0.378770	0.857978
H	-4.668992	2.161350	-2.596684
H	-6.118439	0.848285	-1.052426

*

PWPB95+D3BJ (ATZ) = -1223.721932
PWPB95+D4 (ATZ) = -1223.735907

*xyz 0 1

Ru	0.333664	-0.590218	-0.035686
C	1.709896	0.932128	0.165809
C	1.152875	2.200686	-0.156433
C	3.114652	0.866791	0.257287
N	-0.888192	1.061208	-0.278037
C	1.949131	3.335101	-0.371204
C	-0.283822	2.209504	-0.318907
C	3.907489	1.988285	0.025751
C	-2.301650	1.028271	-0.482995
C	3.331207	3.229294	-0.281182
C	-3.109433	0.339060	0.426352
C	-2.875351	1.663914	-1.587651
C	-4.489265	0.315896	0.243299
C	-4.258682	1.630970	-1.765975
C	-5.069659	0.962232	-0.850451
H	3.590895	-0.083908	0.513626
H	1.479213	4.289853	-0.622994
H	-0.845769	3.138295	-0.474917
H	4.995445	1.902283	0.092566
H	3.964049	4.102424	-0.452269
H	-2.640081	-0.167277	1.270779
H	-2.236765	2.171605	-2.314069
H	-5.117600	-0.214159	0.962570
H	-4.701815	2.127518	-2.631992
H	-6.152316	0.938279	-0.991545
H	1.171086	0.284199	1.397292
O	-1.149403	-2.029829	-0.836051
C	-1.300887	-3.321164	-0.231657
H	-0.976588	-2.149022	-1.781349
H	-2.124308	-3.863103	-0.717950
H	-1.545025	-3.145142	0.821945
H	-0.368417	-3.900319	-0.303442
O	1.319497	-0.923878	-1.908629
O	1.813956	-2.160590	-0.185634
C	2.005941	-1.874376	-1.406432
C	3.024966	-2.596692	-2.231453
H	2.685024	-2.674445	-3.271633
H	3.957102	-2.011226	-2.218146
H	3.226841	-3.590213	-1.814107
O	-0.574146	-0.977233	1.816701
O	1.035270	0.248996	2.699491
C	-0.003524	-0.465711	2.826208
C	-0.596791	-0.685819	4.184318
H	-1.375131	0.076108	4.344010
H	-1.068925	-1.674023	4.238447
H	0.165916	-0.573453	4.963101

*

TS(F^{2S}-G^{2S})1

CPCM (MeOH)
M06 SCF (DZ) = -1339.100810
G (1 atm) = -1338.748924
qh-G (1 mol/L) = -1338.739830
qh-G (24.56 mol/L) = -1338.736807
Lowest Frequency = -78.25

HF SCF energy (TZ) = -1332.042359
HF SCF energy (QZ) = -1332.126821
Correlation energy (DZ) = -4.543825
Correlation energy (TZ) = -5.639746
DLPNO-CCSD(T1)/CBS = -1338.432403

```
*xyz 0 1
 Ru  -0.030986    0.542899    0.027017
 C   -2.380443   -1.129642    0.752436
 O    1.643815    1.054042   -1.147788
 C   -1.884685   -2.230201    0.034195
 C   -3.751593   -0.951872    0.901562
 H   -1.702187   -0.459038    1.308812
 O   -1.008825    0.479154   -1.957940
 O   -0.982057    0.838046    2.751761
 N    0.394301   -1.436591   -0.082602
 O    1.020355    0.814608    1.774920
 O   -0.489340    2.635635    0.053252
 C    2.836666    1.505593   -0.507426
 H    1.255021    1.816577   -1.661889
 C   -2.785227   -3.160196   -0.504787
 C   -0.458458   -2.412553   -0.163864
 C   -4.641498   -1.863406    0.333062
 H   -4.126483   -0.100058    1.474826
 C   -2.426100    0.567353   -2.087847
 H   -0.644817    1.335243   -2.291895
 C    0.252002    0.946247    2.801525
 C    1.774365   -1.783877   -0.242985
 C   -0.360332    3.360543   -0.979988
 H    2.634282    2.378473    0.134143
 H    3.221233    0.683580    0.109843
 H    3.577094    1.765739   -1.279151
 C   -4.155658   -2.970159   -0.365417
 H   -2.399256   -4.026618   -1.049999
 H   -0.090904   -3.423138   -0.396943
 H   -5.718832   -1.719869    0.446783
 H   -2.691509    0.818681   -3.126477
 H   -2.843703    1.329136   -1.405544
 H   -2.855050   -0.411492   -1.836532
 C    0.962590    1.262544    4.091140
 C    2.602615   -1.827494    0.878276
 C    2.284603   -2.041380   -1.514269
 C   -0.775389    4.799664   -0.876838
 O    0.087122    2.946948   -2.091805
 H   -4.851667   -3.691573   -0.799924
 H    1.870276    0.650705    4.196578
 H    1.280911    2.317003    4.080113
 H    0.297445    1.105663    4.949979
 C    3.949515   -2.144190    0.721538
 H    2.180323   -1.597928    1.859371
 C    3.636092   -2.344149   -1.663161
 H    1.616712   -1.982658   -2.378828
 H   -1.605274    4.981744   -1.576842
 H    0.056653    5.443762   -1.197422
 H   -1.087716    5.065989    0.140117
 C    4.470056   -2.397992   -0.547412
 H    4.598935   -2.189058    1.599465
 H    4.039149   -2.540516   -2.659877
 H    5.529340   -2.638240   -0.666871
*
```

TS(F^{2S}-G^{2S})2

```
CPCM (MeOH)
M06 SCF (DZ) =            -1339.106590
G (1 atm) =               -1338.760354
qh-G (1 mol/L) =          -1338.750771
qh-G (24.56 mol/L) =      -1338.747748
Lowest Frequency =        -1188.18

HF SCF energy (TZ) =      -1331.993210
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HF SCF energy (QZ) =      -1332.077134
Correlation energy (DZ) =    -4.599512
Correlation energy (TZ) =    -5.696445
DLPNO-CCSD(T1)/CBS =      -1338.439843

*xyz 0 1
 Ru    0.279383   -0.336510   -0.021300
 C     1.417664    1.350490    0.322898
 N    -1.166117    1.116261   -0.038385
 C     2.815888    1.481517    0.409945
 C     0.665663    2.549305    0.143933
 H     1.072551    0.525719    1.411720
 O    -0.920056   -1.988461   -0.975257
 O     0.723018    0.004229   -2.146974
 O     1.897272   -1.743294    0.020685
 O    -0.340654   -1.113407    1.794701
 C    -2.547429    0.851617   -0.230491
 C    -0.748515    2.352244   -0.002290
 C     3.430143    2.723951    0.288044
 H     3.423854    0.585130    0.573803
 C     1.287998    3.800319    0.034445
 O     1.069925    0.276861    2.785060
 C    -1.474263   -3.035448   -0.187606
 H    -0.198234   -2.379205   -1.523120
 C     1.723036    0.866660   -2.678955
 H     1.004697   -0.927861   -2.350747
 C     2.153302   -2.506105   -0.961307
 C     0.211751   -0.641491    2.840583
 C    -3.243577    1.422964   -1.298847
 C    -3.202403   -0.011746    0.652500
 H    -1.455868    3.189991   -0.075825
 C     2.672016    3.887856    0.101584
 H     4.520322    2.795372    0.345938
 H     0.678259    4.695996   -0.121250
 H    -1.960926   -3.779109   -0.838219
 H    -2.226215   -2.596603    0.480728
 H    -0.700800   -3.529467    0.424535
 H     1.717176    0.798609   -3.777893
 H     2.725114    0.602859   -2.298626
 H     1.489988    1.898008   -2.381670
 C     3.317075   -3.446155   -0.823396
 O     1.498134   -2.526901   -2.044474
 C    -0.206826   -1.188484    4.167031
 C    -4.596740    1.139722   -1.472766
 H    -2.713556    2.072851   -2.000880
 C    -4.555081   -0.281810    0.475492
 H    -2.631439   -0.451144    1.474898
 H     3.168011    4.857183    0.012211
 H     4.060775   -3.212391   -1.600437
 H     2.975988   -4.475107   -1.011082
 H     3.785629   -3.381592    0.166040
 H     0.669789   -1.309342    4.817326
 H    -0.739140   -2.140846    4.057948
 H    -0.876663   -0.461445    4.651849
 C    -5.256120    0.290719   -0.586881
 H    -5.136584    1.583299   -2.313133
 H    -5.068293   -0.947005    1.174698
 H    -6.317092    0.069737   -0.726344
*
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TS(E^+-H)3

```
CPCM (MeOH)
M06 SCF (DZ) =            -1728.799344
G (1 atm) =               -1728.392004
qh-G (1 mol/L) =          -1728.384073
```

```
qh-G (24.56 mol/L) =      -1728.381051
Lowest Frequency =         -108.8494

HF SCF energy (TZ) =      -1720.956043
HF SCF energy (QZ) =      -1721.034278
Correlation energy (DZ) =    -4.873564
Correlation energy (TZ) =    -5.982501
DLPNO-CCSD(T1)/CBS =      -1727.688344

*xyz 0 1
 Ru   0.431775    0.071043   -0.627528
 C    0.081482    2.117715   -1.134372
 C    1.402906    1.759857   -1.542329
 C   -0.246046    3.288737   -0.240238
 C   -0.994734    1.324545   -1.653953
 C    1.619935    0.288591    1.062411
 N   -0.980111   -0.137536    1.005724
 O   -0.520315   -2.580885   -0.675121
 Cl   2.796895   -2.163841   -0.854065
 C    1.625840    0.643829   -2.380933
 H    2.263163    2.290392   -1.126249
 C   -0.695190    4.453024   -1.122896
 C    0.879675    3.720255    0.684664
 H   -1.107766    2.971568    0.380288
 C   -0.787631    0.257424   -2.555578
 H   -2.010516    1.532794   -1.298521
 C    0.948920    0.161455    2.302460
 C    2.993786    0.553685    1.118136
 C   -2.396248   -0.101721    0.873611
 C   -0.464823   -0.053361    2.196717
 C   -0.375336   -3.254079    0.338592
 H    1.488576   -2.940018    0.391388
 C    0.531454   -0.127349   -2.881076
 H    2.645900    0.313981   -2.586407
 H   -1.546034    4.177698   -1.766244
 H   -0.997633    5.312681   -0.504722
 H    0.132652    4.779102   -1.776462
 H    1.748317    4.095099    0.115894
 H    1.221366    2.901433    1.337750
 H    0.536030    4.547657    1.324777
 H   -1.631130   -0.353334   -2.884905
 C    1.605377    0.294496    3.536853
 C    3.648881    0.703972    2.340040
 H    3.572848    0.641460    0.193644
 C   -3.050919   -0.937843   -0.037763
 C   -3.139284    0.826225    1.615503
 H   -1.104899   -0.119155    3.089690
 C   -1.504012   -3.955664    1.024833
 O    0.782589   -3.400388    0.950294
 C    0.797776   -1.342433   -3.703938
 C    2.962873    0.574276    3.554088
 H    1.040585    0.185971    4.468288
 H    4.719804    0.929275    2.349988
 C   -4.432890   -0.861190   -0.177248
 H   -2.458758   -1.652229   -0.614567
 C   -4.522057    0.896568    1.465843
 H   -2.625182    1.516368    2.290919
 H   -1.154733   -4.839193    1.573979
 H   -1.952727   -3.257868    1.752007
 H   -2.280000   -4.228348    0.298338
 H    1.619314   -1.926224   -3.261267
 H    1.096891   -1.038392   -4.720835
 H   -0.095613   -1.977611   -3.782168
 H    3.493103    0.694283    4.501712
 C   -5.174998    0.052186    0.571583
 H   -4.936959   -1.525857   -0.883512
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 H   -5.088560    1.629388    2.045752
 H   -6.259172    0.112194    0.450249
*
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TS(E^{+}-H)4

```
CPCM (MeOH)
M06 SCF (DZ) =            -1268.416760
G (1 atm) =               -1268.011559
qh-G (1 mol/L) =          -1728.384073
qh-G (24.56 mol/L) =      -1728.381051
Lowest Frequency =          -57.63

HF SCF energy (TZ) =      -1261.294216
HF SCF energy (QZ) =      -1261.369040
Correlation energy (DZ) =    -4.690241
Correlation energy (TZ) =    -5.725121
DLPNO-CCSD(T1)/CBS =      -1267.721424

*xyz 0 1
 Ru  -0.113436   -0.443906    0.670661
 C    1.465395   -1.005528   -0.555687
 N   -0.331638    0.856952   -0.988401
 C    2.483743   -1.928079   -0.296537
 C    1.551360   -0.283065   -1.776276
 O    1.882273    2.295968    1.182982
 C    0.532054    0.722160   -1.946253
 C   -1.371962    1.819736   -1.095116
 C    3.521919   -2.133330   -1.216766
 H    2.492773   -2.500859    0.637017
 C    2.580989   -0.485930   -2.698385
 C    3.061228    2.255397    0.890537
 H    0.496234    1.375231   -2.830309
 C   -2.204267    1.843261   -2.216639
 C   -1.567235    2.727107   -0.050237
 C    3.571001   -1.423819   -2.415123
 H    4.302054   -2.865223   -0.990188
 H    2.609904    0.096455   -3.623891
 C    4.018111    3.393297    1.022280
 O    3.657024    1.162182    0.406646
 C   -3.226971    2.786371   -2.294094
 H   -2.058484    1.109467   -3.014779
 C   -2.587215    3.667722   -0.140601
 H   -0.895722    2.699552    0.813230
 H    4.383589   -1.597364   -3.123580
 H    4.460567    3.618643    0.040874
 H    4.844412    3.103073    1.687772
 H    3.507958    4.277513    1.418616
 H    2.984776    0.453716    0.328047
 C   -3.420284    3.698619   -1.259837
 H   -3.881293    2.800061   -3.168919
 H   -2.731361    4.386046    0.669869
 H   -4.225087    4.434700   -1.322527
 C   -0.362383   -2.442022    1.499307
 C   -0.203318   -1.551915    2.574126
 C   -1.324554   -2.184153    0.471690
 H    0.332453   -3.278282    1.379140
 C   -1.060494   -0.409883    2.723653
 H    0.622812   -1.691939    3.275960
 C   -1.445556   -3.123632   -0.700859
 C   -2.174504   -1.043997    0.644269
 C   -0.791951    0.573123    3.812974
 C   -2.088008   -0.206334    1.785393
 C   -2.367068   -4.273679   -0.297177
 C   -1.931359   -2.457727   -1.977622
 H   -0.432811   -3.531099   -0.880578
```

```
 H   -2.876055   -0.776228   -0.151162
 H   -1.292583    1.532835    3.623802
 H   -1.156442    0.176852    4.774862
 H    0.289376    0.748991    3.922191
 H   -2.719051    0.682762    1.853473
 H   -2.001466   -4.795184    0.601603
 H   -3.382278   -3.896511   -0.083708
 H   -2.442988   -5.008884   -1.113181
 H   -1.306216   -1.594256   -2.257496
 H   -2.976373   -2.115175   -1.887270
 H   -1.902449   -3.179081   -2.808284
*
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```

TS(E$^+$-H)5

```
CPCM (MeOH)
M06 SCF (DZ) =            -1499.786929
G (1 atm) =               -1499.439567
qh-G (1 mol/L) =          -1499.431204
qh-G (24.56 mol/L) =      -1499.428181
Lowest Frequency =          -18.24

HF SCF energy (TZ) =      -1493.058681
HF SCF energy (QZ) =      -1493.122159
Correlation energy (DZ) =    -4.152133
Correlation energy (TZ) =    -5.095264
DLPNO-CCSD(T1)/CBS =      -1498.787655

*xyz 0 1
 Ru  -0.298544   -0.505077   -0.428603
 C   -0.414327   -1.298517    1.529309
 N    0.500403    1.347416    0.186132
 C   -1.641461   -1.581109    0.849325
 C    0.839481   -1.801139    1.063612
 H   -0.430136   -0.679193    2.430593
 C   -1.753803    0.836218   -1.031319
 Cl   4.181815   -0.385505   -2.779286
 C    1.743838    1.434044    0.868942
 C   -0.238184    2.395125   -0.008578
 C   -2.986418   -1.188303    1.404763
 C   -1.552719   -2.300011   -0.382331
 C    0.925494   -2.460788   -0.164237
 H    1.753477   -1.550326    1.609756
 C   -1.497210    2.187435   -0.677531
 C   -2.929994    0.584783   -1.741683
 C    1.813834    1.980685    2.151933
 C    2.881544    0.900219    0.260083
 H    0.106952    3.390995    0.306356
 C   -2.971788    0.074803    2.249859
 C   -3.523998   -2.374897    2.204706
 H   -3.652615   -1.021963    0.538010
 C   -0.293622   -2.648328   -0.904143
 H   -2.456064   -2.481602   -0.970745
 C    2.232614   -2.864045   -0.757577
 C   -2.382999    3.225847   -0.982375
 C   -3.821866    1.620287   -2.048331
 H   -3.178614   -0.431578   -2.065383
 C    3.035334    1.995792    2.824116
 H    0.906248    2.365541    2.626839
 C    4.094982    0.928073    0.937249
 H    2.838503    0.473146   -0.750584
 H   -2.547985    0.933479    1.703464
 H   -2.397968   -0.064530    3.181886
 H   -4.000055    0.335131    2.544518
 H   -3.586201   -3.287907    1.591494
 H   -2.868445   -2.587614    3.067107
```

```
 H   -4.530708   -2.151843    2.590961
 H   -0.232586   -3.068302   -1.912444
 H    2.293695   -3.962288   -0.828537
 H    2.360672   -2.451091   -1.771712
 H    3.074315   -2.504285   -0.148761
 C   -3.559934    2.935683   -1.665414
 H   -2.145541    4.252025   -0.685914
 H   -4.743749    1.390042   -2.590334
 C    4.176118    1.469626    2.221401
 H    3.089926    2.414168    3.832120
 H    4.979789    0.515991    0.443564
 H   -4.269787    3.730530   -1.904532
 H    5.129648    1.477665    2.755067
*
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```

Cartesian coordinates (Å) and energies (a.u.) for IRC calculations on selected TS structures

Structures generated by IRC calculations at ωB97X-D3/cc-pVDZ-PP[Ru](CPCM) level are tabulated in two columns. The left column includes the cartesian coordinates and energies obtained by following the IRC path from the TS structure in the backward direction, while the right column includes the corresponding values by following the IRC path in the forward direction from the same TS structure. DZ is used as abbreviation for the basis sets cc-pVDZ-PP[Ru].

IRC backward from **TS(C^1-D^+)**

wB97X-D3 SCF (DZ) = -1729.437542

*xyz 0 1

Ru	-0.343397	0.651573	0.714665
C	1.545766	0.826203	1.802318
C	1.805661	0.960768	0.427602
C	0.569623	1.658304	2.439730
C	1.103785	1.899369	-0.394339
C	0.252606	1.500227	3.897157
C	-0.110854	2.597398	1.641535
C	1.401514	1.953151	-1.881047
C	0.149312	2.713205	0.240593
C	0.322198	2.663597	-2.693809
C	2.777002	2.596710	-2.096957
H	2.031502	0.035176	2.370496
H	2.521160	0.287017	-0.041301
H	0.392579	0.457797	4.206318
H	0.932238	2.137600	4.483695
H	-0.778658	1.810194	4.112161
H	-0.919771	3.182549	2.079729
H	1.461922	0.906480	-2.225960
H	-0.477617	3.380909	-0.348363
H	-0.677625	2.247311	-2.497593
H	0.294612	3.742318	-2.472261
H	0.530937	2.550841	-3.767641
H	3.569369	2.050717	-1.562689
H	2.779279	3.639567	-1.741125
H	3.031231	2.598931	-3.167390
C	2.096760	-2.222317	0.536668
N	-0.472785	-0.965914	-0.828766
C	1.803208	-1.957991	-0.804194
C	3.422939	-2.392903	0.929662
C	-1.736329	-1.110918	-1.516658
C	0.421446	-1.768552	-1.285832
C	2.833626	-1.912742	-1.752784
C	4.454433	-2.294713	-0.004977
C	-1.905851	-0.551912	-2.780588
C	-2.760193	-1.839169	-0.915096
C	4.158663	-2.056652	-1.348483
C	-3.123594	-0.708346	-3.442923
C	-3.969363	-1.999606	-1.587039
C	-4.158145	-1.428899	-2.847532
H	1.301564	-2.263406	1.282923
H	3.650681	-2.593307	1.978942
H	0.145485	-2.393123	-2.149133
H	2.596757	-1.734576	-2.804807
H	5.492829	-2.412754	0.312497
H	-1.086586	0.004891	-3.239858
H	-2.604853	-2.252400	0.082298
H	4.961943	-1.988351	-2.084734
H	-3.258897	-0.264359	-4.431600
H	-4.774077	-2.570434	-1.118444

IRC forward from **TS(C^1-D^+)**

wB97X-D3 SCF (DZ) = -1729.437542

*xyz 0 1

Ru	0.014848	0.273348	0.929553
C	1.699592	1.008311	2.037271
C	2.063189	1.016245	0.669428
C	0.537878	1.684441	2.509015
C	1.258410	1.683651	-0.293826
C	0.143879	1.647081	3.957526
C	-0.268828	2.315658	1.528507
C	1.720466	1.714057	-1.737506
C	0.070566	2.317565	0.146630
C	0.608612	1.712790	-2.782191
C	2.620375	2.950115	-1.892526
H	2.282074	0.398744	2.731520
H	2.942440	0.459950	0.343895
H	0.497218	0.722941	4.434215
H	0.598033	2.499800	4.484166
H	-0.946206	1.714418	4.070288
H	-1.235613	2.728938	1.824752
H	2.346359	0.820669	-1.890600
H	-0.634874	2.773640	-0.556436
H	0.004222	0.796322	-2.736680
H	-0.067919	2.574101	-2.670048
H	1.055528	1.767426	-3.785615
H	3.444646	2.945145	-1.163576
H	2.038160	3.874554	-1.749295
H	3.055507	2.971471	-2.902484
C	2.327097	-2.256999	0.372367
N	-0.319186	-1.082504	-0.729020
C	1.964177	-1.967496	-0.948973
C	3.671328	-2.408045	0.702888
C	-1.670329	-1.205250	-1.218282
C	0.557773	-1.796844	-1.345686
C	2.949625	-1.876198	-1.940793
C	4.655298	-2.259939	-0.276097
C	-2.411982	-0.064537	-1.529428
C	-2.241352	-2.473499	-1.342541
C	4.293931	-1.998092	-1.598788
C	-3.713838	-0.201389	-2.000809
C	-3.551951	-2.600116	-1.804475
C	-4.289124	-1.466399	-2.139677
H	1.554295	-2.374093	1.133406
H	3.951347	-2.637816	1.732801
H	0.242070	-2.321680	-2.258534
H	2.661627	-1.682366	-2.977289
H	5.709524	-2.363088	-0.010088
H	-1.988422	0.933669	-1.403677
H	-1.668441	-3.357889	-1.054526
H	5.061557	-1.895505	-2.368190
H	-4.282842	0.696256	-2.252092
H	-3.996623	-3.593382	-1.893402

H	-5.111148	-1.549923	-3.366947
O	0.323079	-1.670212	3.154911
O	-1.315017	-0.806304	1.868821
C	-0.849224	-1.611012	2.765071
C	-1.897983	-2.555866	3.325014
H	-2.807347	-2.003167	3.598253
H	-2.175533	-3.283757	2.547147
H	-1.506411	-3.094057	4.196551
Cl	-2.678610	1.303043	0.222297

*

IRC backward from **TS(C^1-D^+)•*S***

wB97X-D3 SCF (DZ) = -1845.159673

*xyz 0 1

Ru	-0.325873	0.677553	0.724838
C	2.175239	-2.138378	0.311557
C	0.477807	1.819924	2.420791
C	1.814110	1.025516	0.502452
H	1.931730	0.176964	2.492653
O	-0.520588	-2.707431	1.765330
N	-0.524063	-0.892683	-0.773845
Cl	-3.052977	1.727825	0.698092
O	-1.287817	-0.604392	2.011789
C	1.765381	-1.817322	-0.987928
C	3.534204	-2.273170	0.590725
C	1.462449	0.939461	1.868148
H	1.410749	-2.281917	1.079260
C	0.082643	1.725751	3.863588
C	-0.173425	2.691796	1.530420
C	1.166105	1.924154	-0.395202
H	2.571184	0.349052	0.110240
C	-1.356820	-1.890021	2.154054
C	-1.878511	-1.101324	-1.227040
C	0.334393	-1.676999	-1.325257
H	-2.618041	2.837608	-1.059288
C	2.712845	-1.679474	-2.010862
C	4.482601	-2.079434	-0.415137
H	3.855210	-2.522416	1.604560
H	0.112357	0.683113	4.206675
H	0.787995	2.309713	4.474065
H	-0.927311	2.125645	4.020754
C	0.131573	2.720252	0.132135
H	-1.023926	3.270791	1.887273
C	1.631963	2.012974	-1.838199
C	-2.622158	-2.338225	2.859032
C	-2.552457	-0.093045	-1.912648
C	-2.499888	-2.322275	-0.958777
H	-0.023405	-2.316169	-2.146779
C	4.071079	-1.785900	-1.716821
H	2.387700	-1.461857	-3.031566
H	5.547269	-2.169666	-0.187457
H	-0.492507	3.323766	-0.530242
C	0.519132	1.888627	-2.876687
C	2.412678	3.324822	-2.001283
H	2.337718	1.180314	-1.989886
H	-2.808729	-1.719031	3.747002
H	-3.471157	-2.194980	2.171858
H	-2.558858	-3.396832	3.137537
C	-3.854142	-0.319906	-2.350448
H	-2.077850	0.872468	-2.087529
C	-3.808794	-2.534706	-1.389884
H	-1.959385	-3.085623	-0.394647
H	4.811097	-1.647096	-2.507814
H	0.935616	2.047586	-3.882694
H	-0.284334	2.622957	-2.715541

H	-5.315177	-1.565651	-2.499723
O	-0.268754	-1.502707	2.122397
O	-1.961431	-0.292505	1.537718
C	-1.531613	-1.339467	2.114893
C	-2.456737	-2.350321	2.704031
H	-3.436743	-1.902979	2.903683
H	-2.577983	-3.164453	1.973502
H	-2.024938	-2.770644	3.620455
Cl	-2.739596	3.681531	-1.519154

*

IRC forward from **TS(C^1-D^+)•*S***

wB97X-D3 SCF (DZ) = -1845.156979

*xyz 0 1

Ru	-0.147844	0.507089	0.707565
C	2.223386	-2.109204	0.305531
C	0.463333	1.804533	2.374117
C	1.915533	1.120552	0.482782
H	2.091157	0.344195	2.503449
O	-0.578077	-2.712748	1.777501
N	-0.416445	-0.990384	-0.802415
Cl	-3.705028	2.261218	0.878912
O	-1.312617	-0.597654	1.916538
C	1.852385	-1.859647	-1.022006
C	3.574599	-2.202938	0.633493
C	1.552552	1.039192	1.854908
H	1.440853	-2.245773	1.057325
C	0.060267	1.697538	3.814513
C	-0.298702	2.541008	1.445135
C	1.179216	1.907758	-0.440164
H	2.737865	0.502784	0.118713
C	-1.438536	-1.890550	2.077321
C	-1.794017	-1.143819	-1.201633
C	0.433817	-1.751444	-1.393577
H	-2.869556	2.903686	-0.936482
C	2.826687	-1.737366	-2.020185
C	4.548709	-2.031521	-0.351738
H	3.868483	-2.405193	1.665774
H	0.252546	0.686571	4.200543
H	0.653060	2.411977	4.407327
H	-1.004122	1.937427	3.942365
C	0.030686	2.568140	0.054220
H	-1.247039	2.987992	1.753659
C	1.629294	1.999461	-1.885593
C	-2.758299	-2.287767	2.695990
C	-2.507810	-0.043835	-1.682076
C	-2.405563	-2.396257	-1.076301
H	0.081240	-2.363935	-2.235670
C	4.175242	-1.799201	-1.677717
H	2.526329	-1.566898	-3.057332
H	5.607073	-2.091327	-0.088038
H	-0.664102	3.064694	-0.631158
C	0.507415	1.852234	-2.911681
C	2.377519	3.329516	-2.052940
H	2.350778	1.180957	-2.042243
H	-2.916180	-1.727311	3.628570
H	-3.572539	-2.018351	2.005566
H	-2.781307	-3.365968	2.893936
C	-3.836337	-0.211006	-2.071218
H	-2.045798	0.941817	-1.767499
C	-3.736125	-2.548417	-1.459397
H	-1.842257	-3.234149	-0.655731
H	4.937741	-1.674805	-2.449154
H	0.914212	2.001163	-3.922774
H	-0.298680	2.585360	-2.756396

H	0.070946	0.885192	-2.855912
H	3.219037	3.408349	-1.256704
H	1.745541	4.194042	-1.883490
H	2.864540	3.374207	-3.003319
C	-4.486189	-1.536252	-2.089759
H	-4.380889	0.471298	-2.888219
H	-4.296194	-3.488223	-1.176594
H	-5.510538	-1.703431	-2.428722
C	-3.417645	4.146240	-2.265397
H	-3.104619	4.699824	-3.162460
H	-4.310402	3.549063	-2.524077
H	-3.705298	4.880624	-1.491836
O	-2.335331	3.335286	-1.855900

*

IRC backward from **TS(C^1-D^+)•S_2**

wB97X-D3 SCF (DZ) = -1960.874852

*xyz 0 1

Ru	-0.523526	0.493557	0.604505
C	1.200464	0.872360	1.842753
C	1.586120	1.005665	0.492111
C	0.120960	1.639045	2.375183
H	1.687350	0.125218	2.468494
C	-0.198077	2.595388	0.099342
C	-0.573698	2.469860	1.472106
C	0.910516	1.888955	-0.403338
C	1.864633	-2.174643	0.356880
O	0.153854	-1.666701	3.210388
Cl	-3.319900	1.140084	0.588143
N	-0.611838	-0.908889	-1.070630
O	-1.279254	-1.151990	1.553776
H	2.406040	0.396129	0.112636
C	-0.305004	1.513440	3.808912
H	-0.832218	3.185095	-0.564490
H	-1.490252	2.955308	1.807266
C	1.448406	2.055491	-1.812783
C	1.657060	-1.892682	-0.998233
C	3.158632	-2.372695	0.832683
H	1.020658	-2.218901	1.046099
C	-0.969054	-1.680094	2.703474
H	-3.473345	0.860912	2.744879
H	-2.992419	2.669964	-0.972875
C	-1.894309	-1.056933	-1.709074
C	0.306197	-1.680947	-1.546696
H	0.182036	0.653554	4.283558
H	-0.023793	2.427746	4.353035
H	-1.394328	1.381811	3.880526
C	0.393642	2.118066	-2.913175
C	2.334381	3.310981	-1.814333
H	2.096280	1.185294	-2.008099
C	2.747084	-1.857924	-1.878936
C	4.248064	-2.284562	-0.035281
H	3.315456	-2.586200	1.892005
C	-2.152186	-2.319913	3.397041
O	-3.566695	0.818838	3.717440
O	-2.688122	3.313828	-1.643353
C	-2.523238	0.036653	-2.301782
C	-2.510621	-2.309781	-1.707212
H	0.067584	-2.251283	-2.455862
H	0.875485	2.373442	-3.868626
H	-0.380864	2.873138	-2.710106
H	-0.101611	1.146213	-3.040942
H	3.108228	3.259018	-1.033573
H	1.728002	4.214198	-1.638347
H	2.835147	3.417995	-2.788058

H	0.063552	0.846955	-2.875575
H	3.194750	3.424792	-1.321867
H	1.692484	4.181823	-1.915142
H	2.809385	3.396170	-3.062508
C	-4.451707	-1.458137	-1.964359
H	-4.391150	0.650996	-2.452945
H	-4.214762	-3.525602	-1.358264
H	-5.494139	-1.580408	-2.266374
C	-3.354238	4.181368	-2.335269
H	-2.889968	4.592445	-3.245812
H	-4.316656	3.715832	-2.617326
H	-3.569191	5.022316	-1.650348
O	-2.459321	3.243533	-1.767856

*

IRC forward from **TS(C^1-D^+)•S_2**

wB97X-D3 SCF (DZ) = -1960.870189

*xyz 0 1

Ru	-0.331957	0.328779	0.548792
C	1.261507	0.933496	1.832920
C	1.679492	1.081313	0.482502
C	0.095149	1.587754	2.318274
H	1.808549	0.252399	2.485939
C	-0.261912	2.438846	0.011091
C	-0.676991	2.293832	1.368932
C	0.947621	1.872236	-0.443863
C	1.984105	-2.160440	0.326929
O	-0.018738	-1.721736	3.149149
Cl	-4.201286	1.760654	0.802923
N	-0.453605	-1.022374	-1.121752
O	-1.339008	-1.146094	1.442109
H	2.556309	0.530951	0.137666
C	-0.361837	1.445122	3.739059
H	-0.947093	2.934520	-0.682552
H	-1.671142	2.652939	1.646198
C	1.472147	2.045887	-1.856220
C	1.814831	-1.925155	-1.044533
C	3.266132	-2.310106	0.849632
H	1.118348	-2.227120	0.989757
C	-1.129461	-1.661254	2.634725
H	-3.806935	1.087831	2.800124
H	-3.251526	2.761936	-0.860532
C	-1.766114	-1.144865	-1.698321
C	0.476104	-1.754747	-1.627035
H	0.152557	0.614028	4.234880
H	-0.134294	2.376733	4.279416
H	-1.447739	1.274286	3.781939
C	0.398750	2.051645	-2.941579
C	2.303777	3.336955	-1.882858
H	2.151276	1.198248	-2.046212
C	2.930176	-1.885424	-1.891331
C	4.378882	-2.221306	0.011736
H	3.395288	-2.493687	1.918252
C	-2.375803	-2.175709	3.306968
O	-3.653375	0.892476	3.749331
O	-2.798553	3.225270	-1.597915
C	-2.503149	0.002310	-1.999218
C	-2.311005	-2.416093	-1.917386
H	0.260203	-2.302942	-2.555158
H	0.864812	2.255133	-3.916666
H	-0.366256	2.824135	-2.767766
H	-0.107582	1.078806	-3.011775
H	3.089473	3.325753	-1.112422
H	1.661417	4.214864	-1.706674
H	2.786045	3.455678	-2.864361

C	4.041324	-2.030057	-1.392173
H	2.581279	-1.669778	-2.942532
H	5.262215	-2.424125	0.345668
H	-2.817559	-1.508655	3.733721
H	-2.721368	-2.945176	2.695612
H	-1.828338	-2.911707	4.261002
C	-4.212566	2.010791	4.121841
C	-3.821933	3.987182	-2.156997
C	-3.749628	-0.139004	-2.935259
H	-2.078301	1.028517	-2.248156
C	-3.747772	-2.473804	-2.328729
H	-2.026033	-3.149242	-1.202584
H	4.891663	-1.972432	-2.074660
H	-4.415503	1.936611	5.201435
H	-5.178958	2.155399	3.601074
H	-3.590420	2.905427	3.950585
H	-4.405298	4.483625	-1.361374
H	-4.492284	3.307553	-2.710839
H	-3.465015	4.758969	-2.853617
C	-4.365345	-1.390788	-2.953092
H	-4.232860	0.720458	-3.405241
H	-4.226935	-3.454148	-2.322113
H	-5.332760	-1.518186	-3.442995

*

IRC backward from **TS(C^1-D^+)•S_3**

wB97X-D3 SCF (DZ) = -2076.588614

*xyz 0 1

Ru	-0.529321	0.480909	0.622870
C	1.183896	0.956975	1.845399
C	1.566208	1.053836	0.491358
C	0.077493	1.707200	2.349514
H	1.686418	0.241462	2.494738
C	-0.634011	2.492916	1.419705
C	-0.261845	2.579585	0.043308
C	0.863419	1.883269	-0.435346
Cl	-3.291877	0.944227	0.595326
C	2.013328	-2.114356	0.375574
N	-0.571550	-0.990497	-1.000125
O	0.301892	-1.570022	3.267371
O	-1.199001	-1.172234	1.638066
H	2.401591	0.453637	0.132558
C	-0.359276	1.608793	3.783231
H	-1.557262	2.976454	1.740266
H	-0.911205	3.128255	-0.641321
C	1.395445	2.019123	-1.850488
H	-3.006147	2.439995	-1.053405
H	-5.202607	1.027166	-0.812909
H	-3.431664	0.456793	2.749044
C	1.746187	-1.855308	-0.973613
C	3.331791	-2.238711	0.808468
H	1.195052	-2.199904	1.091647
C	-1.866963	-1.236236	-1.583808
C	0.364455	-1.734413	-1.475961
C	-0.808680	-1.707896	2.756859
H	-1.441181	1.423790	3.847340
H	-0.130269	2.551233	4.302821
H	0.161608	0.787203	4.289036
C	0.337783	1.996313	-2.950144
C	2.231624	3.307372	-1.900711
H	2.077804	1.168665	-2.013462
O	-2.783321	3.047711	-1.782548
O	-6.049775	1.212453	-1.251209
O	-3.540564	0.379943	3.715473
C	2.802433	-1.764042	-1.890035

IRC forward from **TS(C^1-D^+)•S_3**

wB97X-D3 SCF (DZ) = -2076.583824

*xyz 0 1

Ru	-0.252477	0.276060	0.575838
C	1.310966	1.007674	1.835159
C	1.722239	1.132095	0.479081
C	0.107048	1.608368	2.298868
H	1.893548	0.377536	2.508752
C	-0.700996	2.240514	1.325706
C	-0.290175	2.365028	-0.035526
C	0.948158	1.848222	-0.473272
Cl	-4.193509	1.556211	0.860097
C	2.166966	-2.091856	0.318725
N	-0.375075	-1.116477	-1.054268
O	0.157006	-1.680426	3.225847
O	-1.205375	-1.203822	1.520509
H	2.628746	0.618768	0.152331
C	-0.348807	1.485185	3.722467
H	-1.716427	2.548240	1.587521
H	-0.998477	2.801957	-0.745278
C	1.454255	2.003009	-1.894711
H	-3.256734	2.545963	-0.834421
H	-5.650315	1.270047	-0.746161
H	-3.693352	0.794635	2.832445
C	1.931370	-1.895574	-1.048831
C	3.474804	-2.132049	0.796533
H	1.330876	-2.214642	1.011468
C	-1.712774	-1.312394	-1.547234
C	0.559002	-1.830520	-1.574820
C	-0.950258	-1.722293	2.701377
H	-1.430119	1.288753	3.775126
H	-0.142981	2.434317	4.240834
H	0.186618	0.678811	4.236666
C	0.373314	1.900834	-2.968900
C	2.201783	3.342284	-1.974576
H	2.184132	1.193369	-2.060624
O	-2.913545	2.990803	-1.636623
O	-6.388061	1.329416	-1.383744
O	-3.586241	0.575800	3.779972
C	3.008312	-1.778111	-1.936554

C	4.385324	-2.096222	-0.096101
H	3.535791	-2.438373	1.862520
C	-2.537749	-0.231752	-2.279843
C	-2.449898	-2.492144	-1.415840
H	0.121905	-2.358521	-2.349434
C	-1.892751	-2.542019	3.408987
H	0.810677	2.216077	-3.918800
H	-0.458223	2.737744	-2.783192
H	-0.129750	1.005459	-3.026144
H	3.002299	3.319992	-1.114920
H	1.589848	4.193077	-1.765781
H	2.734829	3.393950	-2.875399
C	-3.947057	3.797132	-2.088718
C	-6.857762	1.909184	-0.322501
C	-4.555169	1.288399	4.096853
C	4.119725	-1.859955	-1.446122
H	2.592341	-1.592385	-2.948789
H	5.418144	-2.179654	0.249983
C	-3.783935	-0.501208	-2.835757
H	-2.112242	0.767632	-2.361068
C	-3.706904	-2.749082	-1.962377
H	-1.924341	-3.257926	-0.839986
H	-2.347269	-3.220972	2.674032
H	-2.677038	-1.852007	3.756997
H	-1.493360	-3.110567	4.257103
H	-4.164906	4.555498	-1.315057
H	-4.826497	3.141551	-2.196091
H	-3.770729	4.318548	-3.040315
H	-7.831437	2.095454	-0.799627
H	-7.034737	1.326483	0.599676
H	-6.425942	2.886207	-0.036411
H	-5.521629	1.065170	3.609273
H	-4.286036	2.335788	3.868505
H	-4.693191	1.200184	5.184256
H	4.942176	-1.758263	-2.157309
C	-4.374177	-1.755779	-2.678243
H	-4.309163	0.289398	-3.375331
H	-4.161931	-3.731835	-1.823816
H	-5.359105	-1.953945	-3.105322

*

IRC backward from **TS(C^1-D^+)•S_3^p**

wB97X-D3 SCF (DZ) = -2076.595330

*xyz 0 1

Ru	-0.552447	0.675482	0.672721
O	0.165515	-1.411725	3.307174
C	1.813908	-2.171769	0.518454
C	-0.953914	-1.545059	2.783167
H	0.975811	-2.206934	1.213161
H	1.245729	-2.715549	3.778205
N	-0.662106	-0.840078	-0.917730
Cl	-3.109855	1.279601	0.583813
O	-1.351685	-0.930570	1.725540
C	1.600647	-1.863456	-0.829195
C	3.103871	-2.414130	0.986203
C	-1.994010	-2.467494	3.379113
O	1.876530	-3.459142	3.870841
C	-1.950177	-1.035151	-1.534591
C	0.241574	-1.643755	-1.362965
H	-2.804360	2.754075	-1.096193
H	-3.310060	0.662120	2.746695
C	2.686871	-1.840475	-1.715119
C	4.189483	-2.335725	0.112843
H	3.238010	-2.666941	2.040555
H	-2.401631	-3.133475	2.605900

C	4.546037	-1.965876	-0.082796
H	3.656278	-2.288836	1.861819
C	-2.492766	-0.208913	-1.901575
C	-2.236189	-2.609026	-1.617015
H	0.324041	-2.434189	-2.463190
C	-2.143726	-2.386150	3.340108
H	0.820684	2.080062	-3.957337
H	-0.427867	2.642697	-2.825745
H	-0.083609	0.901250	-2.986065
H	2.995063	3.406163	-1.214382
H	1.507714	4.183991	-1.818020
H	2.665179	3.459354	-2.965442
C	-3.971106	3.778601	-2.158528
C	-7.412693	2.061674	-0.741962
C	-4.596026	1.271034	4.485758
C	4.312693	-1.790458	-1.448543
H	2.819745	-1.648894	-3.005116
H	5.570258	-1.984987	0.296263
C	-3.792353	-0.406263	-2.366501
H	-2.111464	0.811544	-1.826834
C	-3.538701	-2.795339	-2.076320
H	-1.633335	-3.461811	-1.288829
H	-2.641695	-3.047591	2.617618
H	-2.856623	-1.595875	3.624868
H	-1.838902	-2.953470	4.227513
H	-4.151284	4.685616	-1.552920
H	-4.906910	3.197671	-2.206778
H	-3.694862	4.093818	-3.175625
H	-8.262706	2.145438	-1.436316
H	-7.769985	1.565724	0.179578
H	-7.092229	3.084627	-0.469879
H	-5.611297	0.965848	4.173729
H	-4.515657	2.365192	4.356054
H	-4.485413	1.039096	5.555803
H	5.151309	-1.669929	-2.137082
C	-4.315269	-1.696379	-2.455537
H	-4.403114	0.459566	-2.638628
H	-3.945424	-3.808993	-2.124600
H	-5.339237	-1.841119	-2.807378

*

IRC forward from **TS(C^1-D^+)•S_3^p**

wB97X-D3 SCF (DZ) = -2076.583586

*xyz 0 1

Ru	-0.257082	0.366595	0.584579
O	-0.102174	-1.468802	3.266487
C	2.043039	-2.139766	0.465735
C	-1.198137	-1.520265	2.702428
H	1.173796	-2.188777	1.126200
H	1.155061	-2.638264	3.682764
N	-0.379526	-1.067505	-1.003392
Cl	-4.337550	2.224643	0.924943
O	-1.412802	-0.983918	1.535051
C	1.879575	-1.958943	-0.914368
C	3.319658	-2.271487	1.006116
C	-2.397118	-2.200848	3.305172
O	1.819980	-3.349666	3.740784
C	-1.716312	-1.182482	-1.515131
C	0.536499	-1.824426	-1.497198
H	-3.285331	2.835276	-0.878082
H	-3.770141	1.160083	2.734571
C	3.001731	-1.939550	-1.753705
C	4.437197	-2.200949	0.173333
H	3.417792	-2.446232	2.079261
H	-2.872746	-2.859813	2.566784

H	-2.815400	-1.837539	3.752777
H	-1.572107	-3.056123	4.202349
C	1.223546	-4.607986	3.375912
C	-2.559830	-0.018893	-2.266550
C	-2.581114	-2.268977	-1.375326
H	-0.018848	-2.260736	-2.236330
O	-2.533746	3.350464	-1.819101
O	-3.429060	0.542255	3.706948
C	3.979724	-2.048923	-1.237708
H	2.521731	-1.633704	-2.775377
H	5.202694	-2.511256	0.482385
H	1.939756	-5.443449	3.385114
H	0.355397	-4.899632	3.996679
H	0.868755	-4.479702	2.335581
C	-3.784784	-0.262076	-2.881807
H	-2.101137	0.966272	-2.339551
C	-3.817731	-2.498155	-1.979646
H	-2.106824	-3.041424	-0.767470
C	-3.688732	4.020303	-2.290983
C	-4.324366	1.541249	4.155860
H	4.827908	-1.997508	-1.923951
C	-4.416138	-1.499063	-2.742763
H	-4.252715	0.531015	-3.466996
H	-4.304572	-3.466715	-1.851580
H	-4.139241	4.671176	-1.519588
H	-4.460532	3.314654	-2.647735
H	-3.384548	4.652961	-3.137510
H	-5.309120	1.477789	3.657613
H	-3.923847	2.561706	4.007038
H	-4.478114	1.390871	5.234753
H	-5.379194	-1.677421	-3.226390
C	1.215592	0.985970	1.885944
C	1.600900	1.038094	0.533962
C	0.186543	1.841755	2.389360
H	1.651253	0.232020	2.538897
C	0.972737	1.919160	-0.398843
H	2.374952	0.360143	0.179329
C	-0.252255	1.792238	3.825570
C	-0.445455	2.690872	1.459798
C	1.514067	1.995900	-1.815349
C	-0.076518	2.726071	0.079183
H	-1.332231	1.598750	3.890589
H	-0.036050	2.752875	4.315761
H	0.270043	0.990358	4.360493
H	-1.307441	3.274219	1.784051
C	0.457549	2.047346	-2.913953
C	2.454799	3.209606	-1.880000
H	2.124586	1.090917	-1.968300
H	-0.671241	3.330961	-0.607187
H	0.944208	2.220591	-3.885178
H	-0.279872	2.847425	-2.751225
H	-0.085258	1.094888	-2.979788
H	3.222848	3.167094	-1.092727
H	1.889966	4.148113	-1.758970
H	2.965643	3.240989	-2.854080

*

IRC backward from **TS(C^2-D^+)**

wB97X-D3 SCF (DZ) = -1497.645249

*xyz 0 1

Ru	0.182042	-0.642478	0.061960
O	-0.028500	-0.759140	-1.953839
C	-0.444495	-1.824284	-2.593473
C	-1.412058	-1.502324	-3.710274
O	-0.134513	-2.980224	-2.322535
H	-3.117746	-1.413488	3.575719
H	-2.111755	-2.770876	4.195856
C	1.188295	-4.519396	3.265418
C	-2.453148	-0.023228	-1.766271
C	-2.299625	-2.440802	-1.682778
H	0.306156	-2.417416	-2.393958
O	-2.808591	3.153100	-1.674305
O	-3.623103	0.808177	3.636930
C	4.278398	-2.033303	-1.204490
H	2.871341	-1.824155	-2.832321
H	5.439170	-2.293203	0.598196
H	1.923848	-5.337314	3.281541
H	0.330511	-4.820055	3.895795
H	0.825224	-4.411006	2.225951
C	-3.765366	-0.120993	-2.222400
H	-2.022068	0.969251	-1.634884
C	-3.610752	-2.529185	-2.143870
H	-1.739877	-3.344482	-1.428101
C	-3.582512	4.172532	-2.274732
C	-4.331648	1.643583	4.529505
H	5.154207	-1.988152	-1.854980
C	-4.343145	-1.372114	-2.417976
H	-4.326827	0.796018	-2.415069
H	-4.059386	-3.514923	-2.273510
H	-3.757476	5.023287	-1.595565
H	-4.561169	3.797647	-2.617620
H	-3.030124	4.545022	-3.147513
H	-5.411225	1.674834	4.302485
H	-3.951343	2.679651	4.525316
H	-4.207168	1.239359	5.543462
H	-5.371945	-1.443613	-2.773944
C	1.302381	1.058459	1.865342
C	1.751099	1.148123	0.517787
C	0.114597	1.713371	2.296338
H	1.848091	0.417840	2.558985
C	1.023950	1.872986	-0.460742
H	2.645045	0.595975	0.220371
C	-0.374266	1.635474	3.711286
C	-0.655490	2.349366	1.297408
C	1.561698	1.983627	-1.874927
C	-0.210057	2.430544	-0.056584
H	-1.444560	1.381365	3.738789
H	-0.241391	2.621311	4.181914
H	0.187442	0.889094	4.283399
H	-1.671264	2.684866	1.524845
C	0.495528	1.914348	-2.966016
C	2.372514	3.285339	-1.962097
H	2.255593	1.138573	-2.016235
H	-0.899715	2.865295	-0.786221
H	0.966724	2.056438	-3.949287
H	-0.271673	2.695557	-2.849437
H	-0.008697	0.937746	-2.977237
H	3.158369	3.323526	-1.192700
H	1.717151	4.160732	-1.826482
H	2.854173	3.367837	-2.947748

*

IRC forward from **TS(C^2-D^+)**

wB97X-D3 SCF (DZ) = -1497.641965

*xyz 0 1

Ru	0.396100	-0.590969	0.020065
O	-0.196479	-0.701648	-1.869359
C	-0.558746	-1.780321	-2.547634
C	-1.656488	-1.504477	-3.541375
O	-0.066837	-2.887034	-2.384891

C	2.026236	-1.148685	1.064016
C	1.258203	-0.346724	1.949425
C	1.503463	-2.348402	0.503692
C	-0.074360	-0.676969	2.260487
C	2.352599	-3.187654	-0.401650
C	0.154963	-2.681099	0.795377
C	-0.955130	0.157823	3.168285
C	-0.616735	-1.839800	1.634468
C	-0.493886	1.606439	3.317688
C	-1.042752	-0.537997	4.532469
H	-1.087760	-0.621163	-4.279497
H	-2.369613	-1.257328	-3.224742
H	-1.546553	-2.363986	-4.375086
H	3.035986	-0.835361	0.798670
H	1.686933	0.593731	2.299769
H	3.127509	-2.578976	-0.886321
H	2.854746	-3.957341	0.205440
H	1.734006	-3.666656	-1.167069
H	-0.319216	-3.515475	0.280722
H	-1.958725	0.131939	2.713536
H	-1.691562	-2.001459	1.725652
H	-0.353693	2.101913	2.344751
H	0.454168	1.674840	3.874634
H	-1.247322	2.178250	3.878974
H	-1.428606	-1.564292	4.436220
H	-0.051767	-0.587268	5.012407
H	-1.718751	0.019413	5.197765
N	0.358437	1.476778	-0.443531
C	1.430871	2.187933	-0.474500
C	-0.877801	2.170063	-0.673590
C	2.798059	1.639529	-0.470811
C	-2.004623	1.815391	0.066420
C	-0.969393	3.161747	-1.656188
C	3.740849	2.136879	0.437126
C	3.167947	0.658403	-1.399712
C	-3.210340	2.477116	-0.142464
C	-2.179663	3.821761	-1.859743
C	5.031328	1.611656	0.454116
C	4.469688	0.163459	-1.401618
C	-3.301145	3.486682	-1.100108
C	5.396571	0.627263	-0.466101
H	1.338141	3.282814	-0.526146
H	-1.962382	1.002286	0.790568
H	-0.104067	3.401566	-2.278132
H	3.454526	2.916976	1.146700
H	2.429960	0.285290	-2.113296
H	-4.082029	2.181505	0.445121
H	-2.247301	4.593663	-2.628892
H	5.757737	1.978011	1.182475
H	4.758896	-0.596119	-2.130512
H	-4.249556	4.001238	-1.265539
H	6.411835	0.224665	-0.460136
O	-2.514545	-1.093932	-0.549917
C	-3.575998	-0.913128	0.126778
C	-4.900981	-0.921129	-0.648709
O	-3.628459	-0.686388	1.358899
H	-4.956718	-1.765349	-1.351648
H	-4.959124	0.006292	-1.242054
H	-5.768015	-0.947047	0.027613

*

IRC backward from ***cis*-TS(D^+-E^+)1**

wB97X-D3 SCF (DZ) = -1384.300159

* xyz 0 1

Ru	0.176936	0.085383	-0.644281

C	2.089369	-1.211707	1.170356
C	1.313421	-0.384696	2.016273
C	1.539637	-2.373908	0.543716
C	-0.062591	-0.634316	2.193874
C	2.399417	-3.228730	-0.337193
C	0.159898	-2.628614	0.722233
C	-0.958398	0.216390	3.071341
C	-0.635334	-1.737353	1.487417
C	-0.482897	1.656977	3.240016
C	-1.086534	-0.491925	4.428900
H	-1.464895	-0.569630	-4.085372
H	-2.578606	-1.385948	-2.950791
H	-1.767967	-2.342135	-4.240084
H	3.125119	-0.939155	0.961927
H	1.766806	0.519652	2.423855
H	3.190941	-2.630436	-0.808642
H	2.880257	-4.000091	0.283928
H	1.796632	-3.708264	-1.115509
H	-0.320931	-3.423248	0.152766
H	-1.953332	0.204922	2.598336
H	-1.728199	-1.810246	1.457089
H	-0.327824	2.154933	2.271051
H	0.458830	1.711475	3.808956
H	-1.237346	2.231587	3.796782
H	-1.492661	-1.508646	4.315475
H	-0.106987	-0.566519	4.928751
H	-1.763772	0.074663	5.085399
N	0.425692	1.528043	-0.454218
C	1.487651	2.253748	-0.448908
C	-0.832655	2.172517	-0.699760
C	2.843112	1.681696	-0.427944
C	-1.980510	1.685958	-0.071447
C	-0.926138	3.253351	-1.583852
C	3.789817	2.159496	0.485930
C	3.195679	0.682623	-1.346320
C	-3.201012	2.328337	-0.260039
C	-2.153562	3.884093	-1.776670
C	5.064801	1.600366	0.516648
C	4.483153	0.151085	-1.332542
C	-3.290696	3.435358	-1.103706
C	5.412350	0.598744	-0.392647
H	1.394254	3.347910	-0.483379
H	-1.952297	0.797581	0.563870
H	-0.049033	3.586368	-2.142924
H	3.516749	2.950580	1.188038
H	2.465763	0.337864	-2.082930
H	-4.079503	1.940974	0.259674
H	-2.218941	4.726340	-2.468731
H	5.794404	1.953121	1.248042
H	4.759064	-0.618357	-2.056188
H	-4.249655	3.935795	-1.252766
H	6.416897	0.170848	-0.374086
O	-3.106892	-1.743089	-0.589285
C	-3.910284	-1.099215	0.133354
C	-5.266721	-0.739544	-0.493407
O	-3.694868	-0.707476	1.313067
H	-5.667125	-1.592536	-1.061390
H	-5.117193	0.090894	-1.203532
H	-6.001026	-0.417101	0.259059

*

IRC forward from ***cis*-TS(D^+-E^+)1**

wB97X-D3 SCF (DZ) = -1384.300446

* xyz 0 1

Ru	0.073069	0.044254	-0.612379

C	1.310527	0.837384	0.896696
N	-1.012083	-0.363814	1.106994
C	0.831980	0.571854	2.199706
C	2.559364	1.463115	0.799490
C	-2.370451	-0.808339	1.093600
C	-0.472875	-0.055828	2.239936
C	1.553273	0.909055	3.353338
C	3.285015	1.806584	1.941057
C	-2.722911	-1.938115	0.350048
C	-3.355288	-0.084892	1.776672
C	2.788547	1.532884	3.221029
C	-4.051368	-2.353465	0.314100
C	-4.684859	-0.508111	1.732179
C	-5.037056	-1.642627	1.002665
C	0.458434	1.857764	-1.807830
C	1.031733	0.781323	-2.524597
C	-0.899553	1.804487	-1.362933
C	0.259930	-0.381200	-2.835237
C	-1.588692	2.938711	-0.628607
C	-1.644968	0.635517	-1.701615
C	0.912629	-1.548735	-3.513635
C	-1.100089	-0.428052	-2.457545
C	-0.697592	3.677609	0.367524
C	-2.182836	3.897347	-1.669747
H	2.988916	1.677358	-0.182992
H	-0.997816	-0.246375	3.185332
H	1.144117	0.680616	4.341353
H	4.256345	2.296176	1.832206
H	-1.931810	-2.477529	-0.173976
H	-3.085471	0.822214	2.323045
H	3.367289	1.807427	4.104950
H	-4.319863	-3.242058	-0.261377
H	-5.450473	0.060856	2.264860
H	-6.078635	-1.969389	0.963839
H	1.089493	2.701758	-1.527361
H	2.092558	0.801393	-2.773326
H	-2.421873	2.482094	-0.067573
H	-2.665121	0.541271	-1.320689
H	1.875360	-1.762359	-3.032061
H	1.088480	-1.303859	-4.571788
H	0.278192	-2.443323	-3.459897
H	-1.698542	-1.316882	-2.659554
H	-0.285783	2.992561	1.121930
H	0.144776	4.182212	-0.132266
H	-1.282960	4.451507	0.885775
H	-2.852551	3.368823	-2.365087
H	-1.382341	4.372118	-2.260647
H	-2.759612	4.693578	-1.175861
O	2.225587	-1.457097	-0.718996
C	3.303697	-1.549565	-0.005780
C	4.588071	-1.073261	-0.679313
O	3.362484	-2.015956	1.138057
H	4.421277	-0.130593	-1.218822
H	4.919756	-1.820333	-1.418678
H	5.390250	-0.941529	0.060600
O	0.214224	-2.954126	-0.027637
C	0.341396	-3.359672	1.318389
H	1.046774	-2.469826	-0.272062
H	-0.614614	-3.203302	1.848127
H	0.592214	-4.433946	1.383386
H	1.134657	-2.792476	1.831427

*

IRC backward from **TS(D⁺-E⁺)1•*S*ᵖ**
wB97X-D3 SCF (DZ) = -1384.776208

C	1.315165	0.751695	0.889881
N	-1.069935	-0.295253	1.129122
C	0.827937	0.547408	2.202065
C	2.562360	1.386362	0.785672
C	-2.412790	-0.772684	1.109212
C	-0.494520	-0.042150	2.257275
C	1.545078	0.911316	3.350344
C	3.279328	1.771182	1.921294
C	-2.743151	-1.903345	0.354654
C	-3.404428	-0.071875	1.798525
C	2.781964	1.529254	3.207304
C	-4.064011	-2.340161	0.316593
C	-4.726189	-0.513732	1.747908
C	-5.059717	-1.647796	1.009550
C	0.457875	1.821580	-1.758767
C	1.043427	0.744496	-2.471742
C	-0.911102	1.793353	-1.367471
C	0.266995	-0.394158	-2.806968
C	-1.592116	2.931079	-0.630204
C	-1.681372	0.648162	-1.755677
C	0.910037	-1.562713	-3.495106
C	-1.119089	-0.416426	-2.480488
C	-0.696864	3.664722	0.366813
C	-2.182146	3.894448	-1.669116
H	2.999859	1.585556	-0.196674
H	-1.000992	-0.258088	3.206298
H	1.129310	0.712624	4.341892
H	4.247649	2.266615	1.805169
H	-1.953473	-2.427166	-0.186111
H	-3.139020	0.832417	2.350879
H	3.357555	1.826292	4.086506
H	-4.318550	-3.228603	-0.265580
H	-5.498660	0.042148	2.282686
H	-6.096093	-1.988458	0.966553
H	1.091547	2.655217	-1.452613
H	2.108542	0.760908	-2.702629
H	-2.426358	2.477253	-0.068752
H	-2.714186	0.571502	-1.408552
H	1.891846	-1.761752	-3.048280
H	1.038480	-1.325981	-4.562697
H	0.285823	-2.462077	-3.412476
H	-1.715078	-1.302189	-2.701069
H	-0.277547	2.975859	1.114282
H	0.140017	4.178070	-0.133233
H	-1.282575	4.432134	0.894547
H	-2.853898	3.370359	-2.365797
H	-1.379426	4.367175	-2.258623
H	-2.756036	4.691512	-1.173329
O	2.494083	-1.685894	-0.860187
C	3.470979	-1.630569	-0.034275
C	4.755586	-1.059505	-0.617526
O	3.445735	-2.023671	1.144019
H	4.549636	-0.111792	-1.136223
H	5.142440	-1.763818	-1.370828
H	5.515737	-0.906047	0.158523
O	0.282091	-2.555340	-0.049194
C	0.354906	-3.185738	1.222380
H	1.231527	-2.338856	-0.343150
H	-0.601776	-3.059919	1.754307
H	0.535700	-4.273526	1.124760
H	1.171925	-2.757355	1.822526

*

IRC forward from **TS(D⁺-E⁺)1•*S*ᵖ**
wB97X-D3 SCF (DZ) = -1384.770132

```
*xyz 0 1
 Ru   -0.261722    1.024661    0.084789
 C     1.592422    0.064106    2.318851
 O    -0.865695    2.046056    2.393275
 C     2.819249    0.554873    2.750049
 C     1.468414   -1.264136    1.893925
 H     0.711646    0.709942    2.366493
 N    -0.630399   -1.015516    0.711976
 O    -2.194938    1.379026    0.789652
 C    -2.035838    1.872323    1.957252
 H    -0.868963    1.716371    4.265164
 C     3.931415   -0.287027    2.765389
 H     2.899835    1.594124    3.075474
 C     2.575275   -2.119840    1.956183
 C     0.195560   -1.759421    1.360052
 C    -1.857003   -1.639422    0.270467
 C    -3.256674    2.241069    2.749503
 O    -1.086468    1.308051    5.122063
 C     3.806384   -1.623771    2.379191
 H     4.897815    0.096900    3.098050
 H     2.477171   -3.164126    1.650132
 H    -0.052203   -2.819485    1.510340
 C    -1.880630   -2.356952   -0.926506
 C    -3.012887   -1.508396    1.040294
 H    -3.083784    2.046728    3.815344
 H    -3.440037    3.319074    2.621716
 H    -4.134658    1.691967    2.387838
 C    -1.047267   -0.091626    4.927173
 H     4.675267   -2.283549    2.410153
 C    -3.075293   -2.932274   -1.361029
 H    -0.966188   -2.473494   -1.511229
 C    -4.200758   -2.089097    0.599611
 H    -2.978174   -0.955907    1.979439
 H    -0.019350   -0.467130    4.767282
 H    -1.664263   -0.415464    4.067842
 H    -1.448302   -0.574002    5.830804
 C    -4.237916   -2.795102   -0.603536
 H    -3.091920   -3.495151   -2.296893
 H    -5.104500   -1.988164    1.204172
 H    -5.172599   -3.243049   -0.947842
 C    -0.789075    1.725494   -1.831497
 C    -0.037569    0.532765   -1.979756
 C    -0.274723    2.854312   -1.115120
 H    -1.822305    1.740271   -2.184030
 C     1.281920    0.413758   -1.437032
 H    -0.497935   -0.323803   -2.474040
 C    -1.143707    4.082018   -0.933462
 C     0.990393    2.692613   -0.517422
 C     2.078216   -0.846270   -1.601384
 C     1.758125    1.496169   -0.679449
 C    -0.752538    4.941079    0.267003
 C    -1.129756    4.891770   -2.236245
 H    -2.168480    3.707813   -0.770952
 H     1.372417    3.455017    0.161523
 H     1.438820   -1.736375   -1.529942
 H     2.539696   -0.846229   -2.601240
 H     2.878195   -0.912066   -0.852959
 H     2.703518    1.399142   -0.144423
 H    -0.727951    4.356119    1.198716
 H     0.234028    5.410591    0.125585
 H    -1.486438    5.749820    0.393539
 H    -1.458627    4.285526   -3.093794
 H    -0.116366    5.267239   -2.449323
 H    -1.805804    5.754800   -2.149701
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*xyz 0 1
 Ru   -0.069023    0.897793    0.066591
 C     1.328880    0.242537    1.969066
 O    -0.842432    2.296937    2.910100
 C     2.488247    0.886648    2.388882
 C     1.295756   -1.157318    1.838849
 H     0.392496    0.862291    2.022511
 N    -0.697430   -1.077061    0.571216
 O    -1.807911    1.409119    1.098745
 C    -1.851695    1.966453    2.258770
 H    -1.053262    1.745254    4.608320
 C     3.626334    0.131698    2.669298
 H     2.490454    1.972166    2.504712
 C     2.430510   -1.909464    2.143337
 C     0.078600   -1.777286    1.317807
 C    -1.940160   -1.657359    0.141462
 C    -3.236865    2.211925    2.805967
 O    -1.267494    1.170473    5.368702
 C     3.595262   -1.259094    2.548365
 H     4.538163    0.630572    3.000515
 H     2.405614   -2.996326    2.042046
 H    -0.168887   -2.817800    1.563159
 C    -1.989647   -2.399318   -1.038501
 C    -3.082368   -1.470079    0.920057
 H    -3.263410    1.906975    3.861055
 H    -3.442657    3.292338    2.763244
 H    -3.999216    1.676615    2.228440
 C    -0.997859   -0.149128    4.948811
 H     4.487591   -1.844619    2.775936
 C    -3.202620   -2.954809   -1.444770
 H    -1.080831   -2.551832   -1.624255
 C    -4.288644   -2.031372    0.504852
 H    -3.016166   -0.891752    1.842173
 H     0.079367   -0.327523    4.766287
 H    -1.544532   -0.421580    4.024281
 H    -1.323833   -0.836276    5.743829
 C    -4.352546   -2.770025   -0.677338
 H    -3.243595   -3.541779   -2.364611
 H    -5.183709   -1.893004    1.114742
 H    -5.300100   -3.207353   -0.998697
 C    -0.820319    1.643756   -1.787303
 C    -0.059177    0.480799   -2.043996
 C    -0.254321    2.766581   -1.094266
 H    -1.877755    1.654755   -2.055408
 C     1.293739    0.358119   -1.600118
 H    -0.549365   -0.375806   -2.509617
 C    -1.123950    3.975685   -0.827326
 C     1.070940    2.644998   -0.638940
 C     2.084168   -0.898974   -1.819769
 C     1.819926    1.451651   -0.882688
 C    -0.652781    4.844284    0.336005
 C    -1.221079    4.783835   -2.129509
 H    -2.126184    3.584596   -0.586194
 H     1.519849    3.425100   -0.024632
 H     1.435974   -1.784256   -1.765996
 H     2.547595   -0.875760   -2.817519
 H     2.882728   -0.995197   -1.071805
 H     2.811710    1.358914   -0.435720
 H    -0.539527    4.263212    1.263051
 H     0.306572    5.337246    0.112361
 H    -1.393100    5.636227    0.520755
 H    -1.608173    4.173781   -2.959477
 H    -0.231839    5.171138   -2.420688
 H    -1.898204    5.638650   -1.989712
*
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IRC backward from ***cis*-TS(D⁺-E⁺)2**
wB97X-D3 SCF (DZ) = -1269.052447
*xyz 0 1

Ru	-0.343380	-0.120375	-0.279600
C	-0.751992	1.984996	0.509516
H	-0.923130	1.048757	1.219138
C	-1.930430	2.722036	0.405830
C	0.486673	2.657559	0.523010
N	1.585676	0.586648	0.266884
O	-0.303203	-1.183322	1.533805
O	-1.287645	0.476253	2.656220
C	-1.878105	4.110709	0.308946
H	-2.893016	2.206436	0.439769
C	0.537667	4.049860	0.450452
C	1.691526	1.841046	0.543095
C	2.763150	-0.226221	0.222104
C	-0.835812	-0.679871	2.594681
C	-0.649367	4.773002	0.342191
H	-2.806203	4.679442	0.238116
H	1.502398	4.560179	0.470705
H	2.666264	2.286878	0.775068
C	2.763334	-1.459545	0.878405
C	3.882275	0.195602	-0.500533
C	-0.947887	-1.571755	3.795695
H	-0.617599	5.861981	0.285676
C	3.901681	-2.259072	0.827922
H	1.874377	-1.770126	1.428950
C	5.014161	-0.617680	-0.549218
H	3.861681	1.146405	-1.038002
H	-0.124433	-2.291552	3.839175
H	-1.896907	-2.122612	3.709998
H	-0.985610	-0.957603	4.703468
C	5.028290	-1.842953	0.115410
H	3.906816	-3.217601	1.350745
H	5.886206	-0.289553	-1.118351
H	5.916162	-2.477158	0.075414
C	-1.276534	0.592674	-2.128117
C	0.018977	0.140931	-2.441380
C	-2.211769	-0.230865	-1.424689
H	-1.546124	1.625981	-2.353224
C	1.016108	1.025700	-3.129079
C	0.364699	-1.193483	-2.036500
C	-1.865966	-1.530741	-1.013827
H	-3.173563	0.194363	-1.138080
H	2.040540	0.779683	-2.819591
H	0.944669	0.875145	-4.216578
H	0.818221	2.083710	-2.911763
C	-0.552087	-2.005989	-1.351582
H	1.384226	-1.554004	-2.189467
C	-2.784750	-2.413653	-0.195946
H	-0.221746	-2.976825	-0.977631
C	-3.822612	-1.639392	0.614116
C	-3.444198	-3.433088	-1.133302
H	-2.135736	-2.960628	0.507476
H	-3.357314	-0.867199	1.246079
H	-4.565322	-1.150564	-0.036120
H	-4.368674	-2.332975	1.269864
H	-2.694447	-4.022411	-1.682449
H	-4.086732	-2.923981	-1.869142
H	-4.068675	-4.127842	-0.553124

*

IRC backward from **TS(D⁺-E⁺)2•S^p**
wB97X-D3 SCF (DZ) = -1384.765172

IRC forward from ***cis*-TS(D⁺-E⁺)2**
wB97X-D3 SCF (DZ) = -1269.061925
*xyz 0 1

Ru	-0.350010	-0.064760	-0.300525
C	-0.724202	1.932199	0.379930
H	-1.078185	0.911632	1.707597
C	-1.906888	2.695658	0.385010
C	0.487472	2.657510	0.491569
N	1.585315	0.593463	0.258234
O	-0.309247	-1.168704	1.538120
O	-1.266710	0.503387	2.626361
C	-1.866758	4.093544	0.336102
H	-2.884723	2.202977	0.402099
C	0.536465	4.055320	0.469961
C	1.693775	1.851789	0.527788
C	2.759113	-0.222786	0.219744
C	-0.815852	-0.710464	2.581207
C	-0.647250	4.775969	0.352978
H	-2.798300	4.661467	0.254334
H	1.502281	4.565279	0.489285
H	2.668764	2.288986	0.774476
C	2.763702	-1.457005	0.876343
C	3.881686	0.194896	-0.501158
C	-0.957142	-1.549631	3.797134
H	-0.620899	5.864696	0.279292
C	3.901621	-2.258132	0.826944
H	1.879238	-1.774144	1.429125
C	5.014154	-0.617725	-0.549115
H	3.861904	1.145905	-1.038294
H	-0.133627	-2.270211	3.832279
H	-1.901575	-2.107412	3.705885
H	-0.990781	-0.937443	4.704493
C	5.028897	-1.843201	0.114974
H	3.906476	-3.216801	1.350061
H	5.886292	-0.289547	-1.118260
H	5.916689	-2.477626	0.075038
C	-1.281165	0.594806	-2.130773
C	0.020046	0.138390	-2.435925
C	-2.217432	-0.225617	-1.427168
H	-1.547563	1.628014	-2.357411
C	1.015592	1.024008	-3.127567
C	0.365437	-1.203872	-2.045647
C	-1.855811	-1.522558	-1.011311
H	-3.181564	0.193488	-1.142935
H	2.041154	0.780493	-2.819266
H	0.944231	0.874877	-4.215443
H	0.818261	2.082511	-2.910856
C	-0.549177	-2.012498	-1.362950
H	1.385726	-1.560510	-2.200609
C	-2.779666	-2.409976	-0.195983
H	-0.224945	-2.984653	-0.986631
C	-3.822125	-1.640417	0.613623
C	-3.441668	-3.430456	-1.132999
H	-2.135967	-2.963327	0.507831
H	-3.362508	-0.866035	1.246568
H	-4.564341	-1.150845	-0.036484
H	-4.368506	-2.333935	1.269363
H	-2.693774	-4.021655	-1.682557
H	-4.085696	-2.922992	-1.868857
H	-4.067064	-4.125815	-0.553219

*

IRC forward from **TS(D⁺-E⁺)2•S^p**
wB97X-D3 SCF (DZ) = -1384.770742

```
*xyz 0 1
 Ru   -0.611745   -0.111818   -0.311400
 C    -1.257261    0.442976   -2.332306
 C     0.416438   -1.251090   -1.855226
 C    -2.259422   -0.383012   -1.730032
 C     0.087744    0.036488   -2.403000
 H    -1.529727    1.444754   -2.668715
 C    -0.568978   -2.063919   -1.273322
 C    -1.337833    1.977353    0.304108
 N     1.143780    0.828786    0.448372
 H    -1.462392    1.066710    1.020201
 O    -0.738700   -1.092875    1.547028
 H     1.459675   -1.571277   -1.822845
 C    -1.937944   -1.637812   -1.181924
 H    -3.269972    0.013308   -1.630720
 C     1.148138    0.924113   -2.982623
 H    -0.266704   -2.992264   -0.785370
 C    -2.567638    2.565475    0.019326
 C    -0.186774    2.780090    0.428290
 C     2.396421    0.154144    0.611997
 C     1.081176    2.099766    0.652138
 O    -1.879544    0.556082    2.525147
 C    -1.346601   -0.573800    2.550699
 C    -2.941399   -2.514426   -0.463801
 H     2.120279    0.739813   -2.506903
 H     1.250062    0.708168   -4.056615
 H     0.882955    1.983201   -2.865978
 C    -2.652632    3.946513   -0.140076
 H    -3.464108    1.942818   -0.032248
 C    -0.277715    4.165012    0.291025
 C     2.429090   -1.062408    1.298158
 C     3.563548    0.690009    0.060543
 H     1.964804    2.663349    0.976269
 H    -1.329320    1.547922    4.019034
 C    -1.436657   -1.365043    3.818238
 C    -4.092430   -1.738613    0.173719
 C    -3.448217   -3.581029   -1.442235
 H    -2.382379   -3.018806    0.341253
 C    -1.515369    4.742454    0.009503
 H    -3.621494    4.403324   -0.344603
 H     0.615533    4.781662    0.403511
 C     3.641816   -1.728906    1.450342
 H     1.504655   -1.467690    1.711972
 C     4.770977    0.009789    0.213982
 H     3.525727    1.623743   -0.504938
 O    -0.736705    1.798829    4.750278
 H    -0.802638   -2.256014    3.803848
 H    -2.490875   -1.650436    3.951599
 H    -1.168545   -0.690662    4.643258
 H    -3.729947   -0.938115    0.837369
 H    -4.752356   -1.287430   -0.583834
 H    -4.707300   -2.423382    0.775435
 H    -2.617656   -4.165343   -1.866530
 H    -3.997685   -3.112630   -2.274425
 H    -4.127435   -4.274909   -0.925973
 H    -1.597464    5.824988   -0.088068
 C     4.814382   -1.197085    0.910185
 H     3.669023   -2.674199    1.996071
 H     5.680918    0.426882   -0.222182
 C     0.545673    1.968764    4.184078
 H     5.761500   -1.727761    1.026150
 H     0.586089    2.828230    3.488538
 H     0.894509    1.069901    3.639401
 H     1.256743    2.163041    5.000354
*
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```

```
*xyz 0 1
 Ru   -0.620913   -0.056487   -0.336779
 C    -1.262056    0.445464   -2.335605
 C     0.419014   -1.262979   -1.865576
 C    -2.266467   -0.377836   -1.734009
 C     0.087420    0.034638   -2.395978
 H    -1.530380    1.446727   -2.675023
 C    -0.563561   -2.069228   -1.283542
 C    -1.286573    1.911617    0.177176
 N     1.143636    0.834660    0.438034
 H    -1.645018    0.950977    1.534987
 O    -0.739846   -1.086626    1.545849
 H     1.463265   -1.579774   -1.835632
 C    -1.929571   -1.627240   -1.178251
 H    -3.279021    0.011657   -1.637435
 C     1.147088    0.922366   -2.980308
 H    -0.268506   -2.999745   -0.794443
 C    -2.535321    2.534820    0.001047
 C    -0.183287    2.773746    0.396263
 C     2.391968    0.156986    0.608097
 C     1.084302    2.110305    0.634351
 O    -1.861742    0.579097    2.466276
 C    -1.324082   -0.606567    2.529060
 C    -2.936413   -2.509672   -0.463332
 H     2.120652    0.740755   -2.505884
 H     1.248940    0.707445   -4.054709
 H     0.882823    1.982096   -2.864656
 C    -2.641355    3.926014   -0.106755
 H    -3.448624    1.935568   -0.073229
 C    -0.283121    4.166448    0.313539
 C     2.429028   -1.059739    1.295870
 C     3.562885    0.689121    0.059670
 H     1.966386    2.666340    0.975010
 H    -1.338952    1.600413    4.032613
 C    -1.450494   -1.338528    3.813727
 C    -4.092121   -1.739259    0.173467
 C    -3.445463   -3.577689   -1.441646
 H    -2.382308   -3.020374    0.341691
 C    -1.515441    4.743074    0.024000
 H    -3.612510    4.381136   -0.322140
 H     0.611288    4.783625    0.425547
 C     3.641459   -1.727660    1.449394
 H     1.509429   -1.471042    1.712552
 C     4.770703    0.009778    0.214330
 H     3.526102    1.623166   -0.505311
 O    -0.729437    1.789511    4.760335
 H    -0.815118   -2.227947    3.793822
 H    -2.502330   -1.631730    3.944133
 H    -1.176900   -0.665512    4.637306
 H    -3.735008   -0.936571    0.836701
 H    -4.751502   -1.287664   -0.584212
 H    -4.707273   -2.424245    0.775038
 H    -2.616833   -4.164252   -1.866493
 H    -3.996615   -3.111330   -2.273950
 H    -4.125437   -4.272127   -0.925676
 H    -1.600931    5.824681   -0.094507
 C     4.814819   -1.197241    0.910147
 H     3.668143   -2.673030    1.995565
 H     5.680745    0.426981   -0.221672
 C     0.549858    1.968001    4.184207
 H     5.761871   -1.728157    1.026340
 H     0.582328    2.828310    3.490738
 H     0.898295    1.070008    3.638204
 H     1.259037    2.161755    5.000888
*
----------------------------------------
```

IRC backward from **TS(E-H)1**

wB97X-D3 SCF (DZ) = -1269.063447

```
*xyz 0 1
 Ru   -0.104402    0.859799   -0.133357
 C     1.582853   -0.435824    2.005210
 H     0.735688    0.249458    2.103171
 C     2.822449   -0.056525    2.506956
 C     1.400234   -1.709698    1.453057
 N    -0.635153   -1.210772    0.249006
 O    -0.695147    1.730734    2.211048
 O    -2.044375    1.176936    0.579627
 C     3.883036   -0.961390    2.478551
 H     2.952050    0.942758    2.927824
 C     2.453087   -2.632562    1.470352
 C     0.112085   -2.068306    0.853505
 C    -1.947826   -1.659028   -0.145874
 C    -1.864148    1.602411    1.777064
 C     3.694315   -2.250657    1.973957
 H     4.857588   -0.664653    2.870867
 H     2.306684   -3.636966    1.066315
 H    -0.224960   -3.111785    0.927904
 C    -2.333992   -1.649280   -1.487204
 C    -2.848013   -2.069563    0.839041
 C    -3.093650    1.932507    2.578601
 H     4.522285   -2.961451    1.974924
 C    -3.619199   -2.057802   -1.839099
 H    -1.633020   -1.340459   -2.261477
 C    -4.133531   -2.472952    0.479711
 H    -2.545164   -2.048178    1.887864
 H    -3.767946    1.063872    2.584152
 H    -3.628909    2.757594    2.085116
 H    -2.843049    2.219684    3.605510
 C    -4.523942   -2.466713   -0.858538
 H    -3.914139   -2.055405   -2.890785
 H    -4.835350   -2.785293    1.255643
 H    -5.532915   -2.777214   -1.138238
 C     1.884027    1.636037   -0.620062
 C     0.946017    2.715048   -0.580647
 C     1.696550    0.511371   -1.443631
 H     2.740707    1.661945    0.055002
 C    -0.237962    2.679264   -1.339754
 H     1.121949    3.523206    0.128027
 C     2.703907   -0.598879   -1.517522
 C     0.468380    0.446503   -2.166950
 C    -1.303009    3.751430   -1.283173
 C    -0.483219    1.494374   -2.110992
 H     3.325091   -0.631523   -0.612927
 H     3.366127   -0.425312   -2.380479
 H     2.214749   -1.572298   -1.656671
 H     0.239441   -0.457637   -2.733905
 C    -1.178591    4.684909   -0.082211
 C    -1.275970    4.526394   -2.607228
 H    -2.266285    3.219537   -1.211456
 H    -1.447052    1.366612   -2.607720
 H    -1.135692    4.132214    0.868278
 H    -0.279017    5.316611   -0.152711
 H    -2.051032    5.352788   -0.046118
 H    -1.414459    3.857970   -3.470326
 H    -0.315306    5.050988   -2.729824
 H    -2.082333    5.273592   -2.621834
*
```

IRC backward from **TS(E-H)2**

wB97X-D3 SCF (DZ) = -1616.090705

IRC forward from **TS(E-H)1**

wB97X-D3 SCF (DZ) = -1269.056327

```
*xyz 0 1
 Ru    0.058873    0.718665   -0.145890
 C     1.372096   -0.273075    1.721590
 H     0.477055    0.395895    1.819281
 C     2.559880    0.225969    2.250447
 C     1.261806   -1.633466    1.383284
 N    -0.701434   -1.268247    0.108594
 O    -0.733550    1.975155    2.746640
 O    -1.681214    1.123753    0.898769
 C     3.643136   -0.632084    2.434304
 H     2.627502    1.280627    2.524311
 C     2.342558   -2.492804    1.592401
 C     0.012121   -2.097610    0.785203
 C    -2.027340   -1.666435   -0.261508
 C    -1.724427    1.677299    2.073999
 C     3.533561   -1.985852    2.107958
 H     4.575419   -0.244895    2.848393
 H     2.254296   -3.549129    1.331240
 H    -0.321416   -3.132633    0.934368
 C    -2.428555   -1.656268   -1.597264
 C    -2.921423   -2.042157    0.743570
 C    -3.136024    1.951572    2.545068
 H     4.383229   -2.653792    2.258449
 C    -3.726188   -2.042377   -1.925737
 H    -1.726249   -1.374265   -2.381458
 C    -4.218786   -2.422620    0.406350
 H    -2.601884   -2.014398    1.787404
 H    -3.765141    1.063553    2.395488
 H    -3.561455    2.760492    1.932128
 H    -3.145857    2.252723    3.598523
 C    -4.623807   -2.424654   -0.927720
 H    -4.035519   -2.046752   -2.972787
 H    -4.916438   -2.711931    1.194813
 H    -5.641138   -2.720975   -1.190802
 C     1.939894    1.624966   -0.738589
 C     0.980793    2.664559   -0.604079
 C     1.748141    0.504103   -1.588070
 H     2.838717    1.665734   -0.120487
 C    -0.251151    2.585697   -1.291469
 H     1.181315    3.476106    0.093337
 C     2.787214   -0.572400   -1.720263
 C     0.498137    0.421428   -2.246514
 C    -1.332677    3.636013   -1.171639
 C    -0.500125    1.421975   -2.081543
 H     3.421486   -0.615806   -0.824304
 H     3.431760   -0.357959   -2.586091
 H     2.318724   -1.553801   -1.874361
 H     0.265128   -0.474786   -2.825032
 C    -1.169001    4.569975    0.024245
 C    -1.365328    4.423588   -2.491486
 H    -2.285942    3.092279   -1.069163
 H    -1.481236    1.284614   -2.539031
 H    -1.071658    4.019646    0.971270
 H    -0.285605    5.218236   -0.089213
 H    -2.049719    5.223862    0.099114
 H    -1.544355    3.766030   -3.355129
 H    -0.411489    4.950638   -2.652641
 H    -2.170092    5.172131   -2.459384
*
```

IRC forward from **TS(E-H)2**

wB97X-D3 SCF (DZ) = -1616.090336

```
* xyz 0 1
 Ru  -0.466622   -0.444565    0.369264
 C   -0.593781   -0.111150    2.454298
 C   -1.662487    1.175277   -0.021117
 C    0.782910   -0.111703    2.078631
 C   -1.432108   -1.224186    2.163938
 N    0.742927    0.713258   -0.984274
 C   -1.187577    2.043492   -1.030959
 C   -2.930330    1.455119    0.503602
 C    1.721274    1.037130    2.397680
 C    1.306995   -1.297772    1.464140
 C   -0.913582   -2.328217    1.447127
 C    2.141274    0.540218   -1.234625
 C    0.151320    1.745353   -1.494932
 C   -1.930467    3.134046   -1.504210
 C   -3.673753    2.545662    0.048810
 C    1.075498    2.418128    2.298033
 C    2.329968    0.801599    3.786154
 C    0.485528   -2.377581    1.143924
 C   -1.798986   -3.463471    1.022474
 C    2.646431   -0.716495   -1.577697
 C    3.013221    1.625245   -1.079102
 C   -3.183241    3.386327   -0.957425
 C    4.015271   -0.876824   -1.782492
 C    4.382198    1.454168   -1.285650
 C    4.887802    0.203668   -1.637529
 H   -1.028136    0.776689    2.914655
 H   -2.496536   -1.183757    2.395477
 H   -3.361598    0.809057    1.272763
 H    2.536461    0.986307    1.656501
 H    2.354200   -1.309917    1.152637
 H    0.669605    2.386551   -2.219284
 H   -1.521146    3.777616   -2.287589
 H   -4.656254    2.742619    0.485501
 H    0.619454    2.582701    1.310635
 H    0.296610    2.562649    3.063536
 H    1.838111    3.194947    2.456692
 H    2.828613   -0.177887    3.845169
 H    1.549336    0.835149    4.563592
 H    3.074825    1.578505    4.015078
 H    0.885781   -3.220023    0.580006
 H   -1.499526   -3.834271    0.032816
 H   -1.691190   -4.286155    1.746375
 H   -2.851946   -3.159484    0.989207
 H    1.950798   -1.550535   -1.696955
 H    2.624714    2.596816   -0.764580
 H   -3.777153    4.234275   -1.303324
 H    4.404028   -1.859318   -2.059168
 H    5.056352    2.304057   -1.157587
 H    5.960826    0.068498   -1.790754
 O   -2.543033   -1.313068   -1.136171
 C   -3.232543   -0.639275   -2.182794
 H   -1.897829   -1.918436   -1.573875
 H   -3.868300   -1.334581   -2.760704
 H   -2.530415   -0.147486   -2.876255
 H   -3.881310    0.129409   -1.739668
 Cl  -0.233563   -2.634824   -2.426521
*
```

IRC backward from **TS(F-F^{A})**

```
wB97X-D3 SCF (DZ) =       -1664.871123
* xyz 0 1
Ru  -0.599990   -1.543528   -0.021557
 N   -1.734920   -0.155587    0.946127
 C   -3.142493   -0.087149    0.673467
```

```
* xyz 0 1
 Ru  -0.375059   -0.482749    0.333202
 C   -0.590070   -0.094413    2.409383
 C   -1.663694    1.083671   -0.098355
 C    0.796523   -0.116882    2.082784
 C   -1.430109   -1.208596    2.117319
 H   -1.030865    0.803827    2.842573
 N    0.791615    0.733691   -0.960277
 O   -3.010634   -1.470011   -1.230465
 Cl  -0.310118   -2.352241   -2.176191
 C   -1.175224    2.005509   -1.054716
 C   -2.932768    1.366224    0.432644
 C    1.727048    1.038075    2.397327
 C    1.337677   -1.322318    1.516489
 C   -0.905809   -2.329654    1.445559
 H   -2.499939   -1.154496    2.322341
 C    2.184600    0.558482   -1.219523
 C    0.178105    1.741345   -1.493616
 C   -3.429877   -0.653262   -2.300555
 H   -2.184157   -1.907947   -1.523313
 C   -1.907364    3.119661   -1.493600
 C   -3.661084    2.485992    0.024376
 H   -3.378207    0.705758    1.181045
 C    1.075371    2.416106    2.293940
 C    2.332942    0.806827    3.787727
 H    2.543141    0.987551    1.657306
 C    0.507411   -2.390295    1.187542
 H    2.392178   -1.350422    1.235621
 C   -1.789280   -3.466576    1.020108
 C    2.683817   -0.702343   -1.556230
 C    3.055181    1.643895   -1.079140
 H    0.688450    2.383600   -2.222249
 H   -3.947112   -1.240098   -3.081789
 H   -2.587878   -0.113910   -2.772020
 H   -4.130909    0.098281   -1.908009
 C   -3.162105    3.361479   -0.948161
 H   -1.486549    3.791397   -2.246901
 H   -4.641447    2.680520    0.469185
 H    0.610334    2.574014    1.309479
 H    0.303414    2.563764    3.065747
 H    1.837575    3.195544    2.441049
 H    2.835385   -0.170462    3.849301
 H    1.549812    0.838175    4.562663
 H    3.073814    1.587300    4.016437
 H    0.910328   -3.241694    0.638766
 H   -1.463644   -3.859138    0.047819
 H   -1.714794   -4.275239    1.763311
 H   -2.836973   -3.150909    0.943650
 C    4.049310   -0.866496   -1.771022
 H    1.986927   -1.535787   -1.661885
 C    4.421801    1.468388   -1.293304
 H    2.665164    2.616737   -0.770785
 H   -3.748180    4.226785   -1.265267
 C    4.922902    0.214670   -1.639786
 H    4.433020   -1.851982   -2.043788
 H    5.097017    2.318185   -1.175279
 H    5.994131    0.076909   -1.799421
*
```

IRC forward from **TS(F-F^{A})**

```
wB97X-D3 SCF (DZ) =       -1664.873500
* xyz 0 1
Ru  -0.326457   -0.007699    0.597707
 N   -1.895086    1.001711   -0.187747
 C   -2.001721    2.388763    0.198003
```

C	-1.260948	0.742334	1.742566	C	-2.820767	0.582298	-0.984028
C	-4.069438	-0.196616	1.709550	C	-1.095291	3.323390	-0.302967
C	-3.564953	0.089834	-0.646248	C	-3.005492	2.774391	1.086220
C	0.147889	0.858944	2.113558	C	-3.025897	-0.782244	-1.490739
C	-5.432753	-0.112198	1.422666	C	-1.206362	4.657074	0.085690
C	-4.926528	0.184832	-0.920043	C	-3.103101	4.110183	1.475685
C	1.169555	0.073726	1.558655	C	-2.676367	-1.941587	-0.783269
C	0.490752	1.838984	3.059319	C	-3.643792	-0.903246	-2.744477
C	-5.863184	0.083489	0.111585	C	-2.205226	5.053560	0.977154
C	2.492327	0.240945	1.957945	C	-2.904820	-3.193786	-1.343905
C	1.813509	2.018455	3.452649	C	-3.855820	-2.158284	-3.309586
C	2.815546	1.215807	2.904581	C	-3.481711	-3.306214	-2.610445
H	-1.943475	1.494560	2.156664	H	-3.537372	1.330449	-1.350737
H	-3.722127	-0.358843	2.732340	H	-0.310460	2.993299	-0.984231
H	-2.821877	0.159476	-1.443109	H	-3.697440	2.024624	1.476333
H	-6.159484	-0.203214	2.232668	H	-0.503047	5.393111	-0.310380
H	-5.259272	0.339096	-1.948716	H	-3.885574	4.411174	2.175550
H	1.015185	-0.737120	0.816152	H	-2.234379	-1.859500	0.208549
H	-0.296412	2.468377	3.483606	H	-3.945504	-0.003254	-3.286612
H	-6.930191	0.152848	-0.109638	H	-2.282578	6.098853	1.283901
H	3.272787	-0.382819	1.517649	H	-2.627976	-4.090784	-0.785710
H	2.061869	2.788301	4.187078	H	-4.320836	-2.240394	-4.293984
H	3.855378	1.351789	3.212153	H	-3.649479	-4.292629	-3.048689
N	1.684521	1.749348	-1.042787	N	2.880742	-0.675663	0.951290
C	0.708785	2.733590	-0.773569	C	1.966602	-1.456212	1.695562
C	2.920600	2.053171	-1.120576	C	3.395858	-1.172988	-0.106910
C	-0.582132	2.517324	-1.278475	C	1.923878	-1.266742	3.090832
C	0.949376	3.844545	0.048024	C	1.125704	-2.421811	1.112563
C	3.956649	1.008509	-1.251918	C	4.229594	-0.371757	-1.017327
C	-1.610142	3.415251	-0.998169	C	1.126190	-2.080655	3.883153
C	-0.086067	4.733521	0.333853	C	0.336939	-3.244664	1.923467
C	5.307053	1.373338	-1.288883	C	4.424379	1.000189	-0.805312
C	3.613539	-0.351690	-1.292125	C	4.769878	-0.978068	-2.156682
C	-1.364704	4.528415	-0.190037	C	0.344092	-3.087318	3.301865
C	6.300283	0.395992	-1.363615	C	5.143450	1.752653	-1.725944
C	4.601921	-1.325522	-1.368491	C	5.493555	-0.223054	-3.078566
C	5.949797	-0.953146	-1.403280	C	5.677182	1.142719	-2.865914
H	3.284729	3.095754	-1.069140	H	3.210142	-2.216770	-0.419694
H	-0.760304	1.622711	-1.879751	H	2.549162	-0.488683	3.533937
H	1.937697	3.992611	0.492943	H	1.115691	-2.557331	0.031179
H	-2.612562	3.237758	-1.399480	H	1.114816	-1.937283	4.965700
H	0.112090	5.590661	0.982170	H	-0.295981	-4.001060	1.455418
H	5.581504	2.431240	-1.251720	H	3.988098	1.466018	0.079259
H	2.561388	-0.634402	-1.245207	H	4.606758	-2.045657	-2.327097
H	-2.173601	5.226653	0.038950	H	-0.278115	-3.729203	3.928786
H	7.351926	0.690147	-1.387612	H	5.285216	2.823213	-1.562799
H	4.321034	-2.381103	-1.394874	H	5.908691	-0.700067	-3.968643
H	6.727223	-1.718656	-1.461101	H	6.236549	1.737956	-3.591199
O	-0.445383	-0.782100	-2.013303	O	-1.629394	-0.890165	2.079711
O	0.611905	-2.614671	-1.501541	O	-0.564547	0.952189	2.480009
C	0.313339	-1.740268	-2.372875	C	-1.343459	0.038204	2.897136
C	0.854707	-1.796707	-3.769496	C	-1.911787	0.075392	4.281020
H	0.044310	-1.629268	-4.491639	H	-1.163473	0.460319	4.985614
H	1.587398	-0.984974	-3.895213	H	-2.773477	0.760028	4.288121
H	1.343629	-2.759040	-3.958796	H	-2.247092	-0.922700	4.586320
O	-0.934632	-2.885084	1.612581	O	0.968690	0.988488	-0.777708
O	-2.140420	-2.935698	-0.188955	O	0.084797	-0.908390	-1.331077
C	-1.910752	-3.395161	0.982000	C	0.813023	0.081525	-1.653585
C	-2.791226	-4.440495	1.589789	C	1.420313	0.187761	-3.018108
H	-2.263277	-4.972226	2.390522	H	1.710965	-0.806546	-3.380758
H	-3.140976	-5.141905	0.822525	H	2.288074	0.858352	-3.006885
H	-3.671012	-3.939928	2.023264	H	0.661518	0.595253	-3.703386

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