Supporting Information

On the mechanism of gold(I)-catalyzed Meyer-Schuster rearrangement of 1-phenyl-2-propyn-1-ol via 4-*endo*-dig cyclization

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Contents

Computational details

Complexes NHC'-Au-X (NHC' = 1,3-dimethylimidazol-2-ylidene; X = OTf^- Trifluoromethanesulfonate or triflate anion, OTs^- Toluenesulfonyl or tosylate anion, BF_4^- Tetrafluoroborate, TFA Trifluoroacetate) and 1-phenyl-2-propyn-1-ol have been used in the calculations as a model for the catalysts and the substrate, respectively.
The computational analysis has been carried out with ADF related QUantum-regions Interconnected by Local Description (QUILD) program[1], to identify reactant complexes, intermediates, product complexes and transition states of the carbene-gold(I) catalyzed Meyer-Schuster rearrangement of the 1-phenyl-2-propyn-1-ol, assisted by the OTf^-, OTs^-, BF_4^- and TFA^- counterions. A TZ2P basis set with the core small approximation, the GGA BP86 functional[2,3] and the scalar zeroth-order regular approximation ZORA Hamiltonian[4,5] for the inclusion of relativistic effects were used. This protocol is hereafter labeled as "BP86/ZORA".
The stationary points and transition states have also been optimized including Grimme's D3 dispersion correction[6,7], in order to evaluate the effect of the dispersion on the geometries and, indirectly, on the reaction energies (this protocol is labeled as "BP86/ZORA/D3"). Frequency calculations have been carried out at the same level of theory in order to identify the stationary points (zero imaginary frequencies) and the transition states (one imaginary frequency). The same protocol (BP86/ZORA/D3) has been used for calculating the geometries of stationary points and transition states (with relative frequencies) for two model reactions that account for experimental conditions, i.e. traces of acid (where the OTf^- anion was protonated) and in presence of an explicit molecule of ɣ-valerolactone, in substitution of the anion.
With the BP86/ZORA protocol, other structures were optimized for modeling the preequilibrium step with the OTf^-. OTs^- and TFA^- counterions, a gold-hydroxy mechanism similar to the one reported in Ref. 8.
Final energies have been calculated at several levels of theory. For all optimized structures, final energies have been calculated with the same computational setup as that used for the optimizations, i.e. either "//BP86/ZORA" and "//BP86/ZORA/D3" when dispersion was included. In addition to this, single-point energy calculations were carried out using the ORCA program package[9] by single-point B2PLYP perturbatively corrected double hybrid functional[10] DFT calculations, with Ahlrich's def2-TZVP basis set[11] and an effective core potential (ECP) for gold[12], in order to account for relativistic effects. This setup is labeled as "//B2PLYP". The BP86/ZORA//B2PLYP protocol has been proven to be very accurate when analyzing reaction paths involving gold complexes as reactive species, as reported in previous benchmark studies[13].
Nonetheless, for the reaction profiles of the intramolecular rearrangement of the substrate assisted by the three counterions (i.e. OTf^-, OTs^- and BF_4^-) and the acid- and ɣ-valerolactone-assisted reactions, we also calculated final energies using the DLPNO-CCSD(T) approach[14,15] (labeled as "//DLPNO-CCSD(T)"), which has been shown to yield very accurate results (comparable to the regular Coupled-Cluster approach[16]) by keeping the computational cost relatively low (it has been estimated that its computational cost is only two to four times the cost of DFT[17]). The calculations have been carried out with the ORCA program package, by using the def2-TZVP basis set and an effective core potential (ECP) for gold. The default "NormalPNO" DLPNO settings were used as recommended for obtaining a reasonable balance between computational cost and accuracy[18].

The solvent effect has been taken into account for both the preequilibrium and the nucleophilic attack steps by using the Conductor-like Polarizable Continuum Model (CPCM)[19–21] as implemented in the ORCA package. Since the solvent used in the experiments (i.e. p-cymene) is not included in the list of solvents available for such model, we used toluene, since they have very similar dielectric constant (2.24 vs 2.38 for p-cymene and toluene, respectively) and dimension. In order to assess the solvation effect on the geometries, optimization calculations have been also performed with the Conductor like Screening Model COSMO[22-24] using toluene as solvent.

All the energies calculated with the methods described above are presented as electronic energy differences. However, for a full description of the mechanism of this reaction, enthalpies and Gibbs free energies have been calculated for the intramolecular rearrangement of the substrate assisted by the three counterions, in order to evaluate the effect of the entropic contributions on the energy profiles. These calculations have been carried out with the QUILD program, with the BP86/ZORA/D3//BP86/ZORA/D3 protocol.

EXPERIMENTAL PROCEDURES

GENERAL PROCEDURES AND MATERIALS

1-phenyl-2-propyn-1-ol, $AgBF_4$, AgOTf, AgOTs and AgTFA were purchased from Sigma Aldrich. All the solvents (Table S1) were used as delivered without any further purification, unless otherwise stated. NHC-Au-Cl (**1**-Cl)[23] and (NHC)-Au-OTf (**1**-OTf)[24] were synthesized according to the literature. All compounds were characterized in solution by ^1H and ^{13}C NMR spectroscopies. The spectra were recorded on a Bruker AVANCE III HD 400 MHz spectrometer. Referencing is relative to TMS (^1H and ^{13}C).

NHC-Au-OTf (1-OTf) catalysed Meyer-Schuster rearrangement of 1-phenyl-2-propyn-1-ol to cinnamaldehyde (Table S1 and S2).

NHC-Au-OTf (1.8 mg, 0.0025 mmol), the appropriate solvent (200 µL), and 1-phenyl-2-propyn-1-ol (61 µL, 0.5 mmol) were added into a 2 mL glass screw-top vial. The vial was placed in a bath oil at 50°C with magnetic stirring. The reactions were checked by NMR: 10 µL of the reaction mixture was added to a 500 mL of non-anhydrous $CDCl_3$. The progress of the reaction was monitored integrating the signal of 1-phenyl-2-propyn-1-ol and cinnamaldehyde. Conversion was calculated from the integral intensities of the corresponding signals (conversion [%] = (n cinnamaldehyde) / (n 1-phenyl-2-propyn-1-ol + n cinnamaldehyde) x 100). Reported yields are an average of three runs.

^1H NMR (400 MHz, $CDCl_3$, 298 K) δ(ppm): 9.74 (d, 1 H, $^3J_{HH}$ = 7.7 Hz), 7.60 (dd, 2H, $^3J_{HH}$ = 6.8, $^4J_{HH}$ = 2.9 Hz), 7.55 – 7.39 (m, 4H), 6.75 (dd, 1H, $^3J_{HH}$ = 15.9, $^4J_{HH}$ = 7.7Hz).

Table S1. 1-X catalyzed Meyer-Schuster rearrangement of 1-phenyl-2-propyn-1-ol to cinnamaldehyde at 50°C.[a]

Entry	Solvent	Catalytic system	Conv.[b] %	TOF[c] (h^{-1})	ε_r[d]
	VOS				
1	Chloroform	**1**-OTf	75	300	4.81
2	Dichloromethane	**1**-OTf	12	53	8.93
3	Acetone	**1**-OTf	13	50	21
	Green				
4	p-Cymene	**1**-OTf	91	394	2.24
5	p-Cymene[e]	**1**-Cl/ AgOTs	11	44	2.24
6	p-Cymene[f]	**1**-Cl/ AgTFA	0.4	2	2.24
7	p-Cymene[g]	**1**-Cl/$AgBF_4$	7	28	2.24
8	p-Cymene[h]	**1**-Cl/AgOTf	30	115	2.24
9	p-Cymene[i]	**1**-OTf/HOTf	100	400	2.24
10	p-Cymene[j]	**1**-OTf/HOTs	93	371	2.24
11	p-Cymene[k]	**1**-OTf/P.S.	0	0	2.24
12	Limonene	**1**-OTf	67	246	2.4
13	Anisole	**1**-OTf	85	368	4.3
14	Ethyl Lactate	**1**-OTf	24	106	15.4
15	Furfuryl alcohol	**1**-OTf	37	161	16.9
16	γ-Valerolactone	**1**-OTf	23	105	36.9
17	DMSO	**1**-OTf	0	0	46.7
18	Methyl levulinate	**1**-OTf	17	74	-
19	-	**1**-OTf	74	296	-

[a]Catalysis conditions: NHC-Au-OTf (0.0025 mmol, 1.8 mg), 1-phenyl-2-propyn-1-ol (0.5 mmol, 61 μL), solvent (200 μL). [b]Determined by ^1H NMR; average value of three measurements after 30 minutes. [c]TOF = ($mol_{product}/mol_{catalyst}$)/t calculated after 30 minutes. [d]ε_r = dielectric constant. [e]NHC-Au-Cl (0.0025 mmol, 1.6 mg), 1.1 eq AgOTs. [f]NHC-Au-Cl (0.0025 mmol, 1.6 mg), 1.1 eq AgTFA. [g]NHC-Au-Cl (0.0025 mmol, 1.6 mg), 1.1 eq $AgBF_4$. [h]NHC-Au-Cl (0.0025 mmol, 1.6 mg), 1.1 eq AgOTf. [i]NHC-Au-OTf (0.0025 mmol, 1.8 mg), 10% (respect to substrate) HOTf. [j]NHC-Au-OTf (0.0025 mmol, 1.8 mg), 10% (respect to substrate) HOTs. [k]NHC-Au-OTf (0.0025 mmol, 1.8 mg), 10% (respect to substrate) proton sponge (1,8-Bis(dimethylamino)naphthalene). [l]no solvent was used.

Figure S1. Plot of conversion against time for **1**-OTf catalysed Meyer-Schuster rearrangement of 1-phenyl-2-propyn-1-ol to cinnamaldehyde at 50°C. See Table S1 and S2 for details.

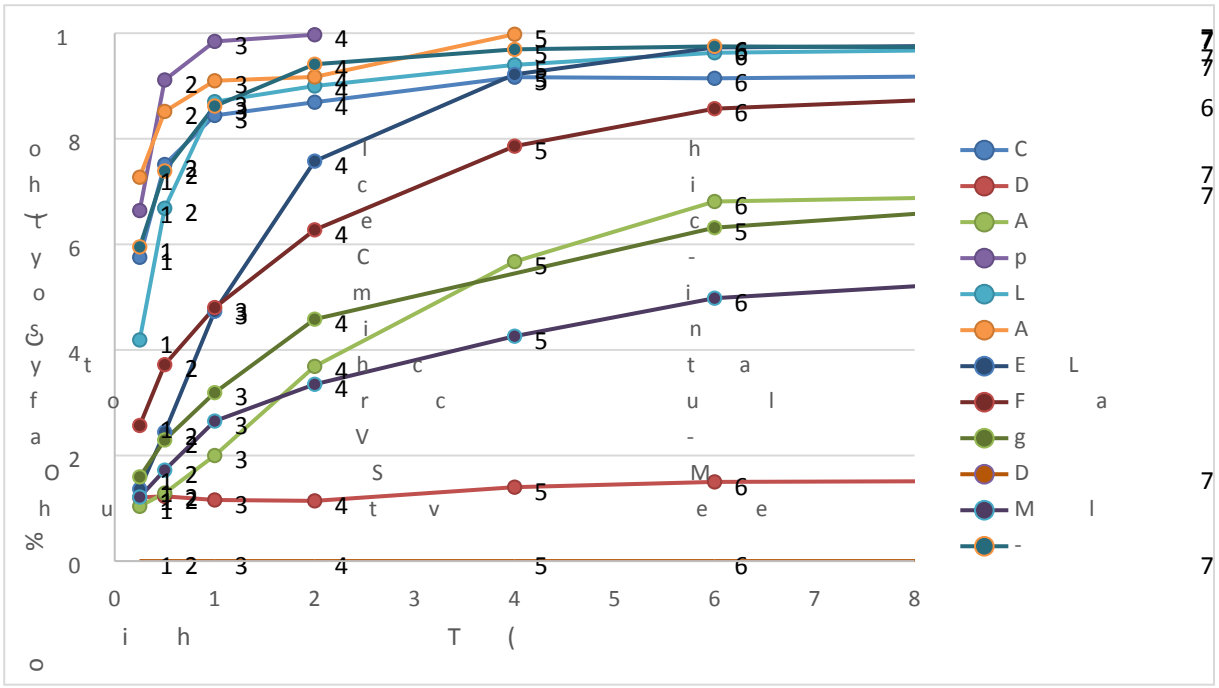


Figure S2. Plot of conversion against time for **1**-X catalysed Meyer-Schuster rearrangement of 1-phenyl-2-propyn-1-ol to cinnamaldehyde at 50°C. See Table S1 and S2 for details.

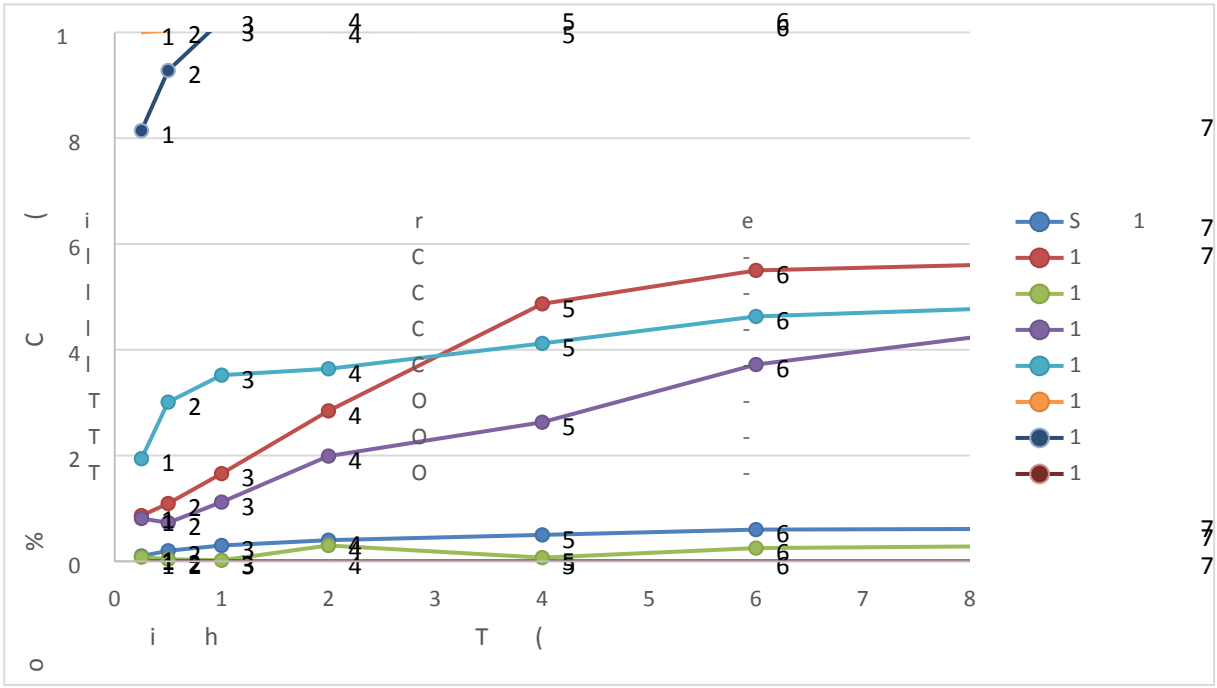


Table S2. **1**-X catalysed Meyer-Schuster rearrangement of 1-phenyl-2-propyn-1-ol to cinnamaldehyde at 50°C.

		TIME (h):	0.25		0.5		1		2		4		6		24	
ENTRY	SOLVENT	CAT	Conv. (%)	TOF (h^{-1})	Conv. (%)	TOF (h^{-1})	Conv. (%)	TOF (h^{-1})	Conv. (%)	TOF (h^{-1})	Conv. (%)	TOF (h^{-1})	Conv. (%)	TOF (h^{-1})	Conv. (%)	TOF (h^{-1})
1	Chloroform	**1**-OTf	57.5	460	75.1	300	84.4	169	86.9	87	91.7	46	91.5	30	94.3	8
2	Dichloromethane	**1**-OTf	12.1	104	12.3	53	11.6	25	11.4	12	14.0	6	15.0	1	16.0	0
3	Acetone	**1**-OTf	10.4	80	12.9	50	20.0	39	36.9	36	56.7	27	68.1	22	74.0	6
4	p-Cymene	**1**-OTf	66.4	574	91.1	394	98.4	213	99.7	108						
5	p-Cymene[e]	**1**-Cl/ AgOTs	8.6	69	10.9	44	16.6	33	28.4	28	48.7	24	55.0	18	64.0	5
6	p-Cymene[f]	**1**-Cl/ AgTFA	0.8	6	0.4	2	0.2	0	3.0	3	0.7	0	2.5	2	5.3	0
7	p-Cymene[g]	**1**-Cl/ $AgBF_4$	8.1	62	7.3	28	11.2	21	19.9	19	26.3	10	37.2	6	82.8	7
8	p-Cymene[h]	**1**-Cl/ AgOTf	19.4	149	30.1	115	35.2	67	36.4	35	41.2	20	46.3	10	58.6	5
9	p-Cymene[i]	**1**-OTf/ HOTf	100.0	800	100.4	402	100.8	202	100.4	100	100.5	50	101.6	34		
10	p-Cymene[j]	**1**-OTf/ HOTs	81.4	651	92.8	371	102.3	205	102.9	103	103.2	52	103.1	34		
11	p-Cymene[k]	**1**-OTf/ P.S.	0.0	0	0.0	0	0.0	0	0.0	0	0.0	0	0.0	0	0.0	0
12	Limonene	**1**-OTf	41.9	308	66.8	246	87.0	160	90.0	79	94.0		96.3	29	100.0	8
13	Anisole	**1**-OTf	72.7	628	85.2	368	91.0	197	91.7	99	99.8	50				
14	Ethyl Lactate	**1**-OTf	13.6	118	24.4	106	47.3	102	75.8	82	92.2	44	97.3	6	99.5	0
15	Furfuryl alcohol	**1**-OTf	25.7	222	37.2	161	48.0	104	62.7	68	78.6	9	85.7	2	99.6	0
16	γ-Valerolactone	**1**-OTf	16.0	147	22.9	105	31.9	73	45.8	53			63.2	24	86.7	8
17	DMSO	**1**-OTf	0.0	0	0.0	0	0.0	0	0.0	0	0.0		0.0		0.0	
18	Methyl levulinate	**1**-OTf	12.1	105	17.2	74	26.5	57	33.5	36	42.6	18	49.8	9	70.1	2
19	-	**1**-OTf	59.5	476	73.9	296	86.2	172	94.1	94	96.9	48	97.5	33	96.2	8

[a]Catalysis conditions: NHC-Au-OTf (0.0025 mmol, 1.8 mg), 1-phenyl-2-propyn-1-ol (0.5 mmol, 61 µL), solvent (200 µL). [b]Determined by 1H NMR; average value of three measurements after 30 minutes. [c]TOF = (molproduct/molcatalyst)/t calculated after 30 minutes. [d]ε_r = dielectric constant. [e]NHC-Au-Cl (0.0025 mmol, 1.6 mg), 1.1 eq AgOTs. [f]NHC-Au-Cl (0.0025 mmol, 1.6 mg), 1.1 eq AgTFA. [g]NHC-Au-Cl (0.0025 mmol, 1.6 mg), 1.1 eq AgBF4. [h]NHC-Au-Cl (0.0025 mmol, 1.6 mg), 1.1 eq AgOTf. [i]NHC-Au-OTf (0.0025 mmol, 1.8 mg), 10% (respect to substrate) HOTf. [j]NHC-Au-OTf (0.0025 mmol, 1.8 mg), 10% (respect to substrate) HOTs. [k]NHC-Au-OTf (0.0025 mmol, 1.8 mg), 10% (respect to substrate) proton sponge (1,8-Bis(dimethylamino)naphthalene). [l]no solvent was used.

Stoichiometric reaction of 1-phenyl-2-propyn-1-ol with 1-OTf

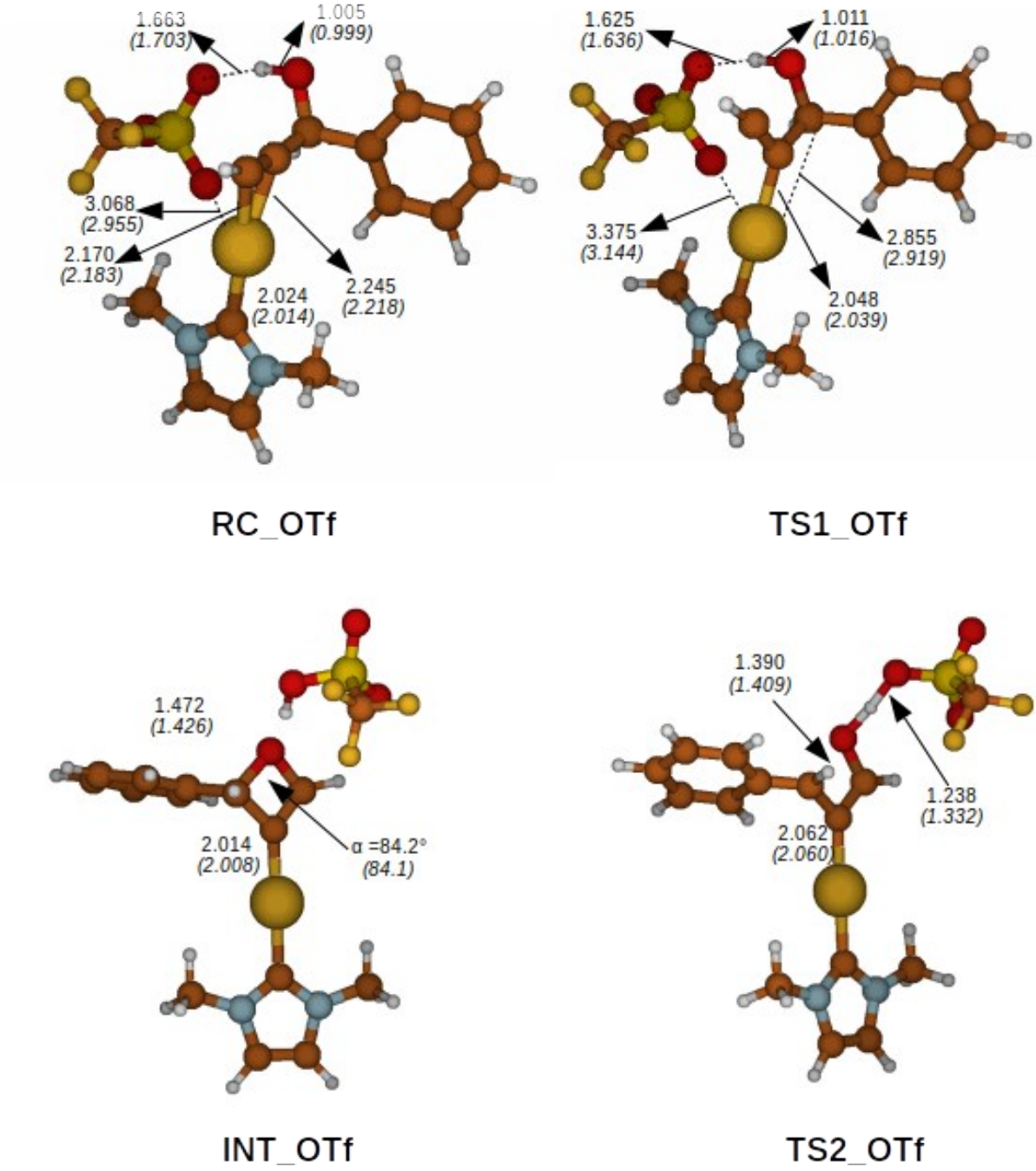
In a NMR tube, 3.6 μL (0.027mmol) of 1-phenyl-2-propyn-1-ol and 8.6 mg (0.0401 mmol) of protonsponge [1,8-Bis(dimethylamino)naphthalene] were dissolved into 500 μL of $CDCl_3$. Then, 20 mg (0.027 mmol) of **1**-OTf was added and the solution was shaken. The formation of the sigma bonded species was observed, which was completely characterized by multinuclear NMR techniques.

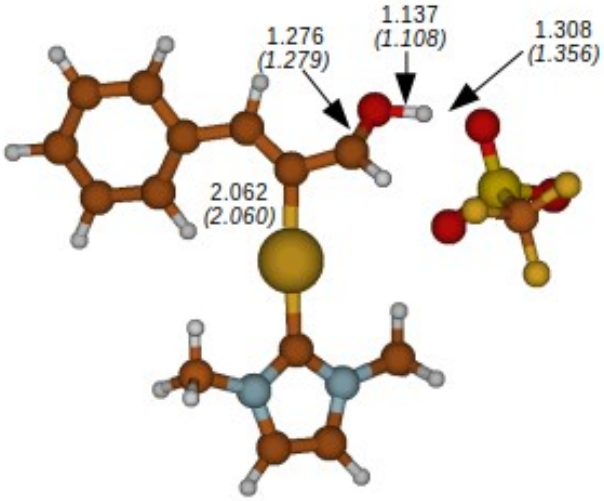
^{1}H NMR (400 MHz, $CDCl_3$, 298 K) δ(ppm): 7.50 (m), 7.26 (m), 5.41 (d, 1H, $^3J_{HH}$ = 5.5), 2.60 (hept, 4H, $^3J_{HH}$ = 6.8), 2.16 (d, 1H, $^3J_{HH}$ = 5.9, H8), 1.37 (d, 12H, $^3J_{HH}$ = 6.9), 1.24 (d, 12H, $^3J_{HH}$ = 6.8).
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$, 298 K) δ(ppm) = 190.77, 145.62, 142.58 (1C, C4), 134.26, 130.51 (2C, C2), 128.03, 127.35 (1C, C1), 127.03 (2C, C3), 125.43, 124.18, 123.22, 121.63, 102.97 (1C, C6), 65.32 (1C, C5), 28.81, 24.58, 24.03.

Stoichiometric reaction of 3-hexyn-2-ol and 1,3-diphenyl-2-propyn-1-ol with 1-X

0.030 mmol of the internal alkyne (3-hexyn-2-ol or 1,3-diphenyl-2-propyn-1-ol) was mixed with 0.04 mmol of base (1,8-Bis(dimethylamino)naphthalene or potassium bicarbonate) in 0.5 mL of deuterated solvent ($CDCl_3$ or CD_3OD) and the ^{1}H-NMR spectrum was recorded at 298 K. Then, 0.027 mmol of the gold complex (**1**-OTf or **1**-TFA) was added to the solution, while the temperature was lowered to 223 K. Mono and bidimensional multinuclear NMR experiments were then recorded in order to possibly detect the formation of the oxetene intermediate. Unfortunately, the presence in solution of this species was not observed.

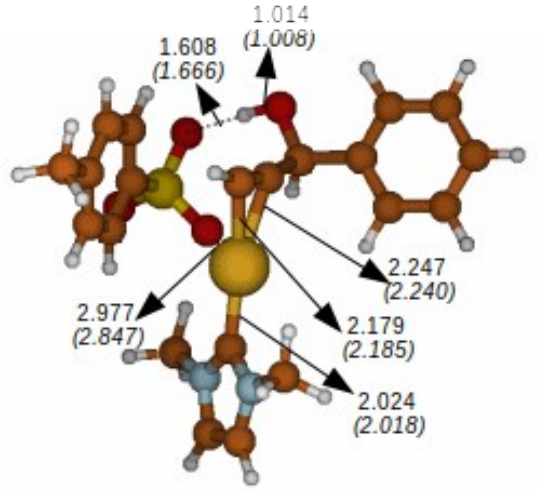
Figure S3. Optimized geometries of stationary points for the intramolecular nucleophilic attack in the 1-phenyl-2-propyn-1-ol assisted by the OTf^- counterion. The most relevant bond lengths and angles at the BP86/ZORA level are reported (value in parenthesis refer to BP86/ZORA/D3 results).



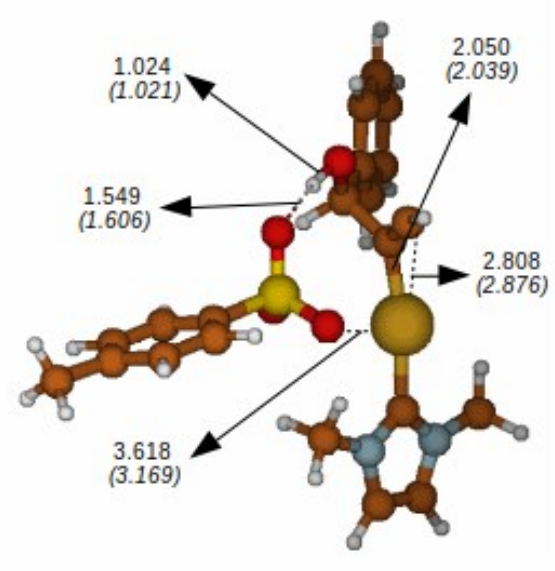


PC_OTf

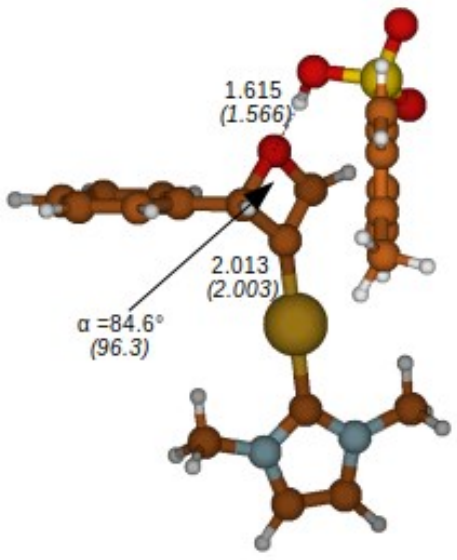
Figure S4. Optimized geometries of stationary points for the intramolecular nucleophilic attack in the 1-phenyl-2-propyn-1-ol assisted by the OTs^- counterion. The most relevant bond lengths and angles at the BP86/ZORA level are reported (value in parenthesis refer to BP86/ZORA/D3 results).



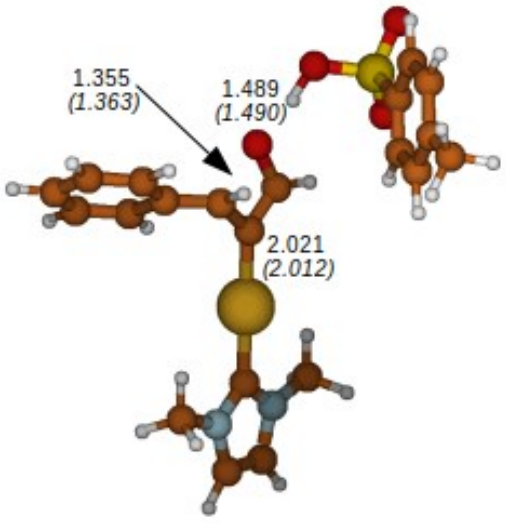
RC_OTs



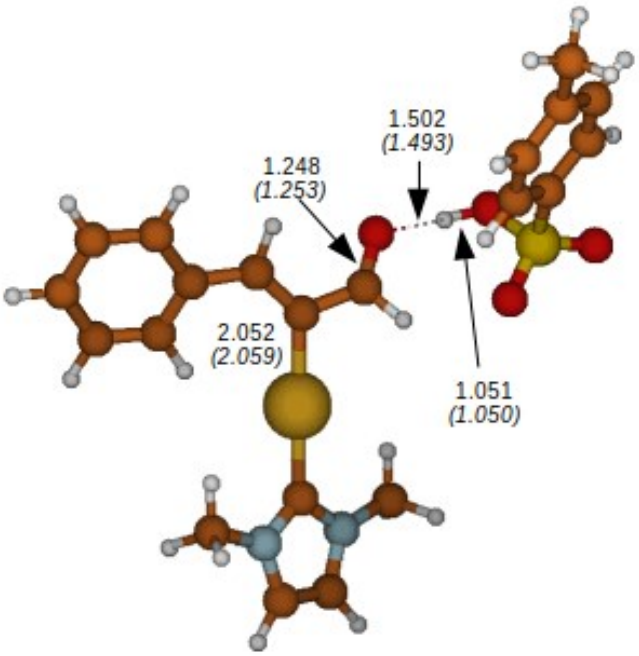
TS1_OTs



INT_OTs

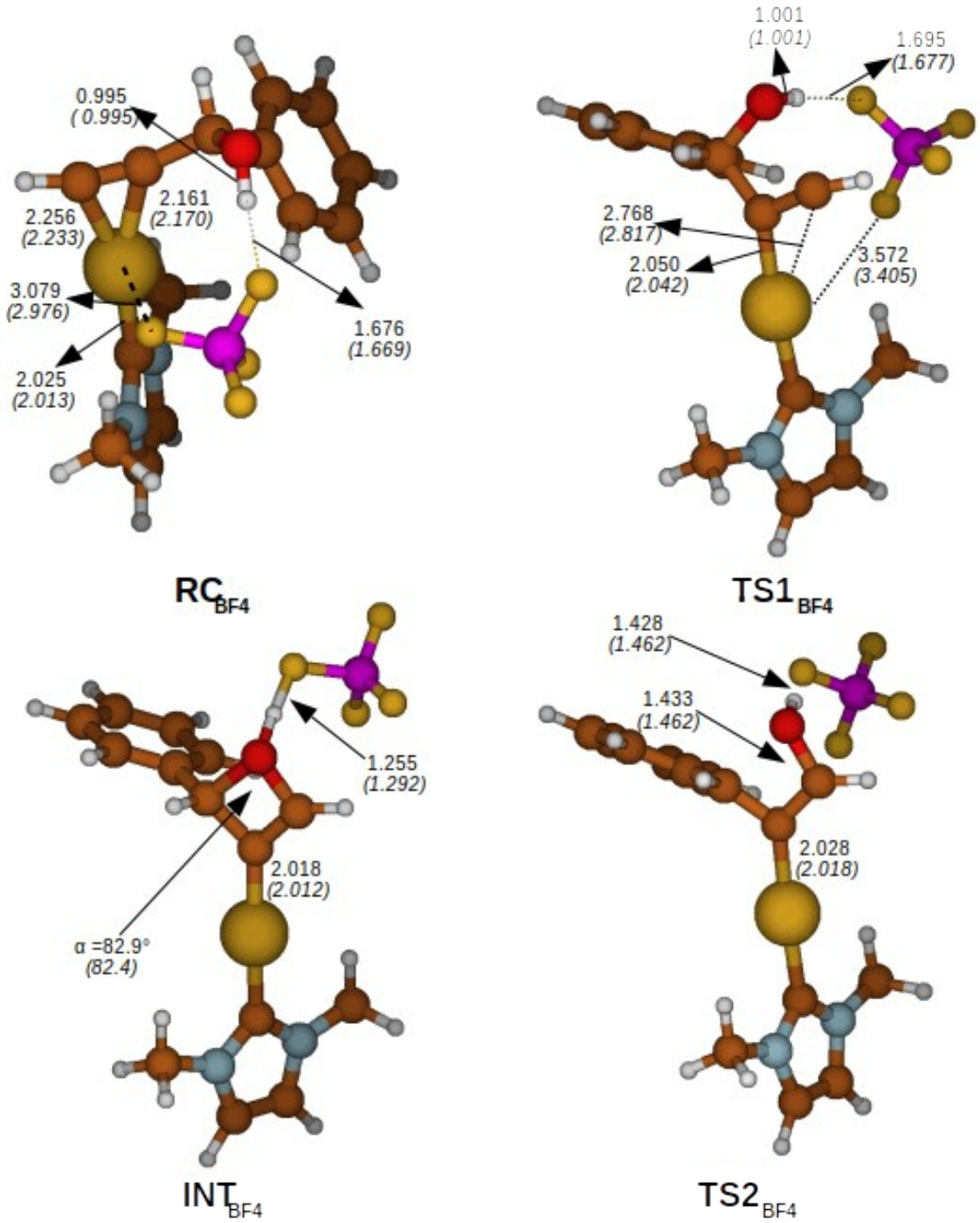


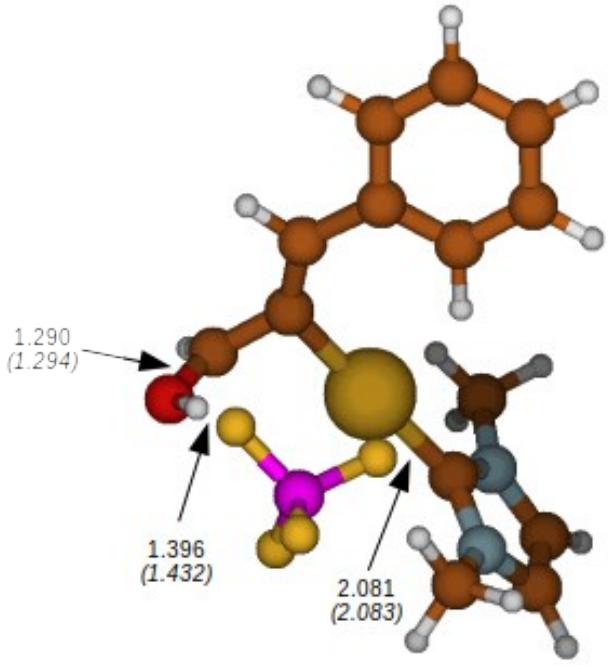
TS2_OTs



PC_OTs

Figure S5. Optimized geometries of stationary points for the intramolecular nucleophilic attack in the 1-phenyl-2-propyn-1-ol assisted by the BF_4^- counterion. The most relevant bond lengths and angles at the BP86/ZORA level are reported (value in parenthesis refer to BP86/ZORA/D3 results)





PC_{BF4}

Figure S6. Energy profiles for the preequilibrium step with OTf^- (blue line), OTs^- (red line) and TFA^- (green line) counterions calculated at the BP86/ZORA//B2PLYP/CPCM level. Energies are reported with respect to the corresponding RC taken as zero reference energy.

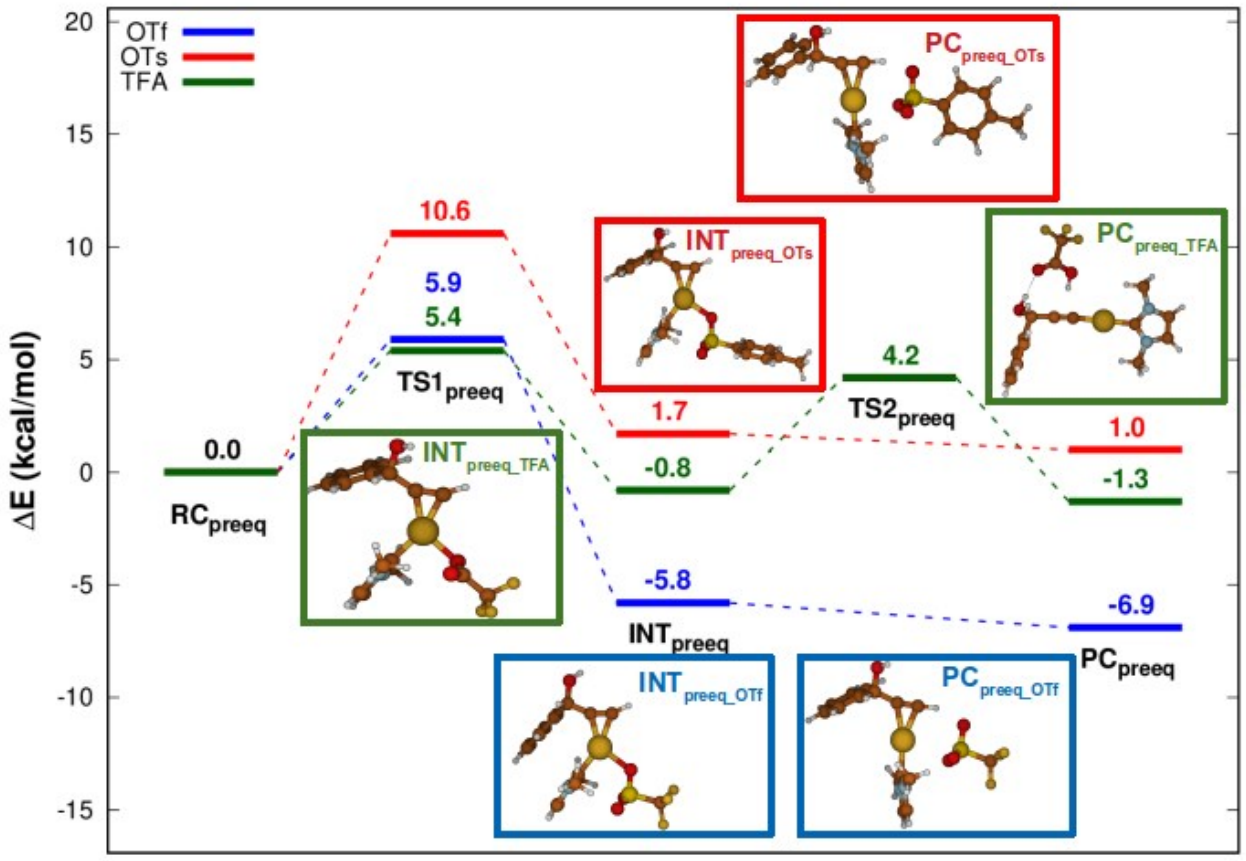


Figure S6 shows that the pre-equilibrium step occurs via formation of a tri-coordinated intermediate species (INT_{preeq_X}) where both the anion and the alkyne moiety are coordinated to the gold center, that is favored for OTf^- with an activation barrier of 5.9 kcal/mol (vs. 10.6 kcal/mol for OTs^-), as expected on the basis of their coordinating ability trend. Surprisingly, the calculated activation barrier for TFA^- is the lowest (5.4 kcal/mol), thus suggesting that coordination ability should not be the only important feature in this step. Indeed, upon de-coordination of the anion, the expected gold-alkyne complex (PC_{preeq_X}) (with the anion remaining in the first coordination sphere, simultaneously interacting with Au and the acidic hydrogen of the terminal alkyne moiety) is obtained in a barrierless and almost thermoneutral process for OTf^- and OTs^-, whereas for TFA^- a stable σ-bonded gold-alkynyl complex is formed through abstraction of the acidic hydrogen of the terminal alkyne by the anion with an energy barrier of 5.0 kcal/mol.

Figure S7. Electronic energy (ΔE, in blue), enthalpy (ΔH_{298}, in red) and Gibbs' free energy (ΔG_{298}, in green) profiles at 298 K for the OTf^--assisted intramolecular nucleophilic attack in the 1-phenyl-2-propyn-1-ol calculated at the BP86/ZORA/D3//BP86/ZORA/D3 level. Energies are reported with respect to RC taken as zero reference energy.

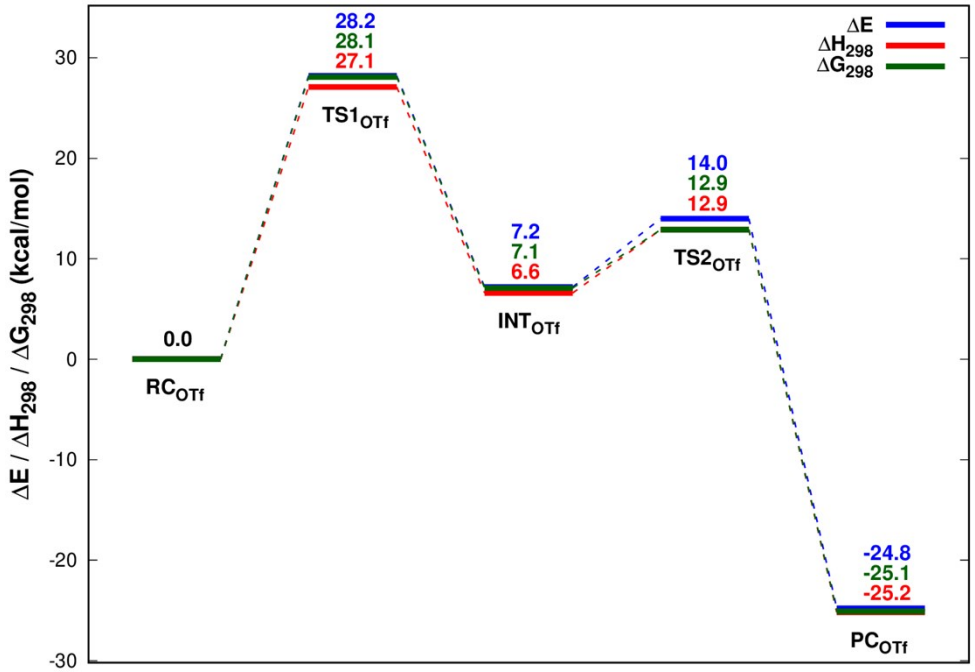


Figure S8. Electronic energy (ΔE, in blue), enthalpy (ΔH_{298}, in red) and Gibbs' free energy (ΔG_{298}, in green) profiles at 298 K for the OTs^--assisted intramolecular nucleophilic attack in the 1-phenyl-2-propyn-1-ol calculated at the BP86/ZORA/D3//BP86/ZORA/D3 level. Energies are reported with respect to RC taken as zero reference energy.

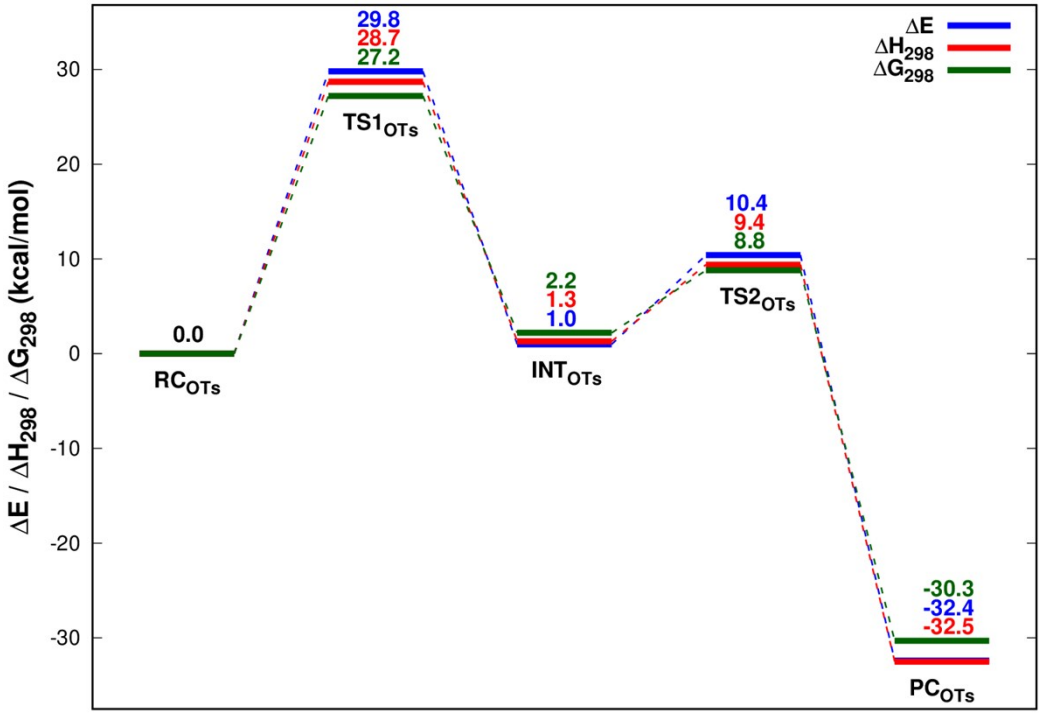
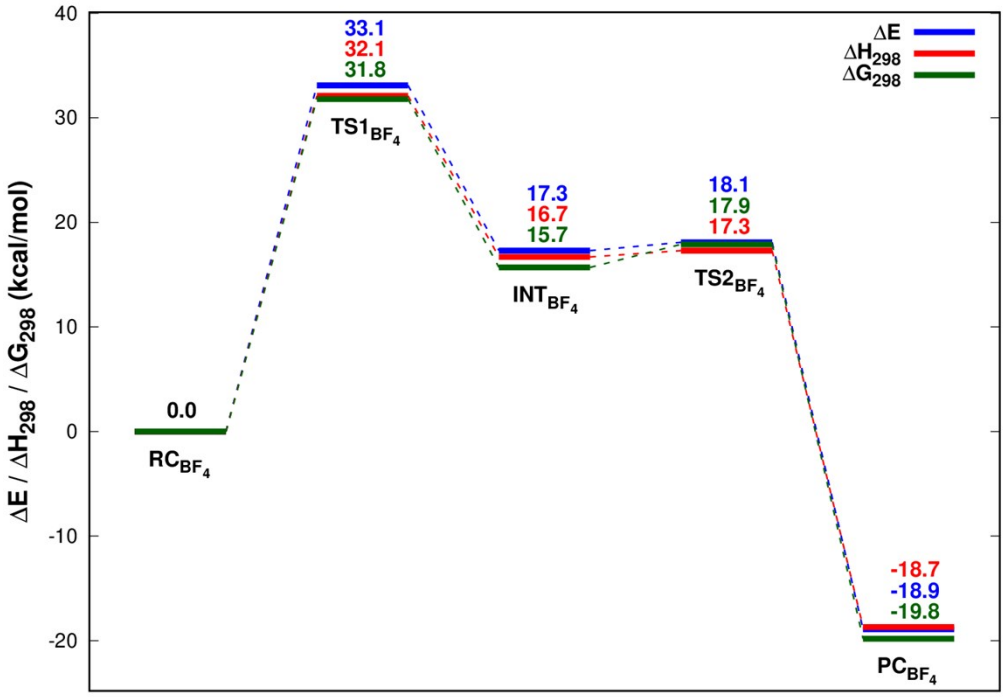


Figure S9. Electronic energy (ΔE, in blue), enthalpy (ΔH_{298}, in red) and Gibbs' free energy (ΔG_{298}, in green) profiles at 298 K for the BF_4^--assisted intramolecular nucleophilic attack in the 1-phenyl-2-propyn-1-ol calculated at the BP86/ZORA/D3//BP86/ZORA/D3 level. Energies are reported with respect to RC taken as zero reference energy.



As a general result, from Figures S7-S9 we observe that electronic energies ΔEs can be considered a very good approximation to both reaction enthalpies ΔHs and Gibbs' free energies ΔGs.

Figure S10. Reaction profiles for the intramolecular nucleophilic attack in the 1-phenyl-2-propyn-1-ol assisted by the OTf^- counterion calculated with different computational protocols. In blue the BP86/ZORA//B2PLYP results, in red the BP86/ZORA/D3//B2PLYP results and in green the BP86/ZORA/D3//DLPNO-CCSD(T) results are shown. Energy are given with respect to the corresponding RC taken as zero reference energy.

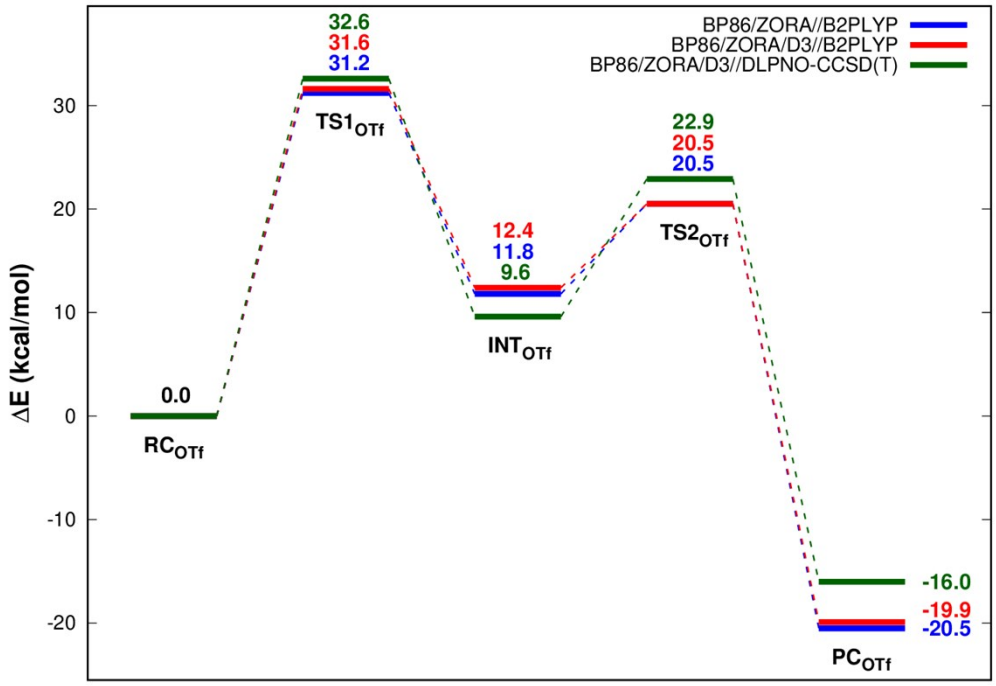


Figure S11. Reaction profiles for the intramolecular nucleophilic attack in the 1-phenyl-2-propyn-1-ol assisted by the OTs^- counterion calculated with different computational protocols. In blue the BP86/ZORA//B2PLYP results, in red the BP86/ZORA/D3//B2PLYP results and in green the BP86/ZORA/D3//DLPNO-CCSD(T) results are shown. Energy are given with respect to the corresponding RC taken as zero reference energy.

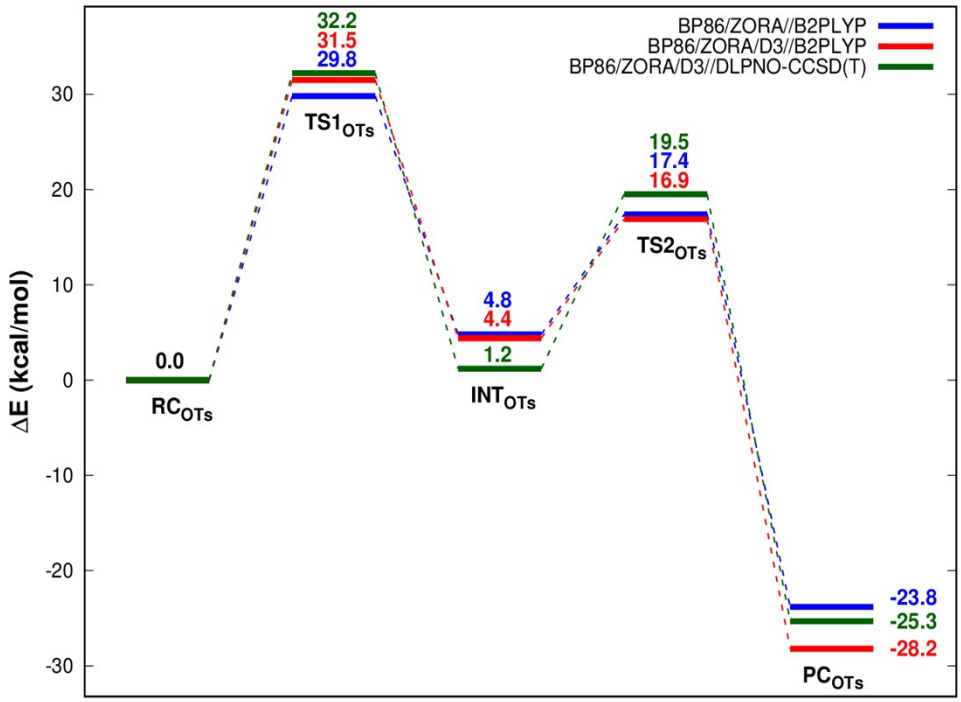
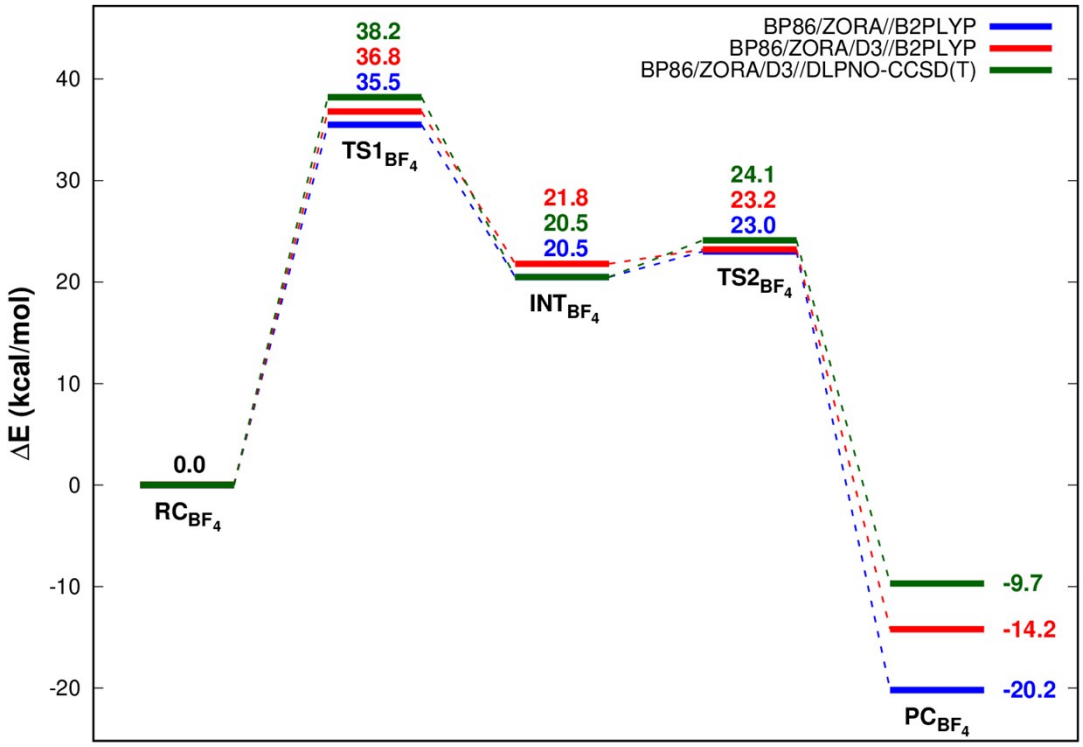


Figure S12. Reaction profiles for the intramolecular nucleophilic attack in the 1-phenyl-2-propyn-1-ol assisted by the BF_4^- counterion calculated with different computational protocols. In blue the BP86/ZORA//B2PLYP results, in red the BP86/ZORA/D3//B2PLYP results and in green the BP86/ZORA/D3//DLPNO-CCSD(T) results are shown. Energy are given with respect to the corresponding RC taken as zero reference energy.



The reaction profiles in Figures S10-S12 highlight that: the BP86/ZORA//B2PLYP protocol, which is computationally less demanding, gives very similar results to those obtained with the BP86/ZORA/D3//B2PLYP setup for all the reaction profiles, indicating that the effect of the dispersion (included in the geometry optimization) on the energies is very small.
These results also allow to compare the performances of the DFT double-hybrid approach (BP86/ZORA/D3//B2PLYP) and the ab-initio one (BP86/ZORA/D3//DLPNO-CCSD(T)), highlighting that overall the reaction profiles are very similar, validating the very good accuracy of a protocol involving energy calculations performed at the B2PLYP level.

Figure S13. Solvation effect on geometries for the intramolecular nucleophilic attack in the 1-phenyl-2-propyn-1-ol assisted by the OTf^- counterion calculated with different computational protocols. In blue the BP86/ZORA/D3//B2PLYP/CPCM results and in red the BP86/ZORA/D3/COSMO//B2PLYP/CPCM results are shown. Energy are given with respect to the corresponding RC taken as zero reference energy.

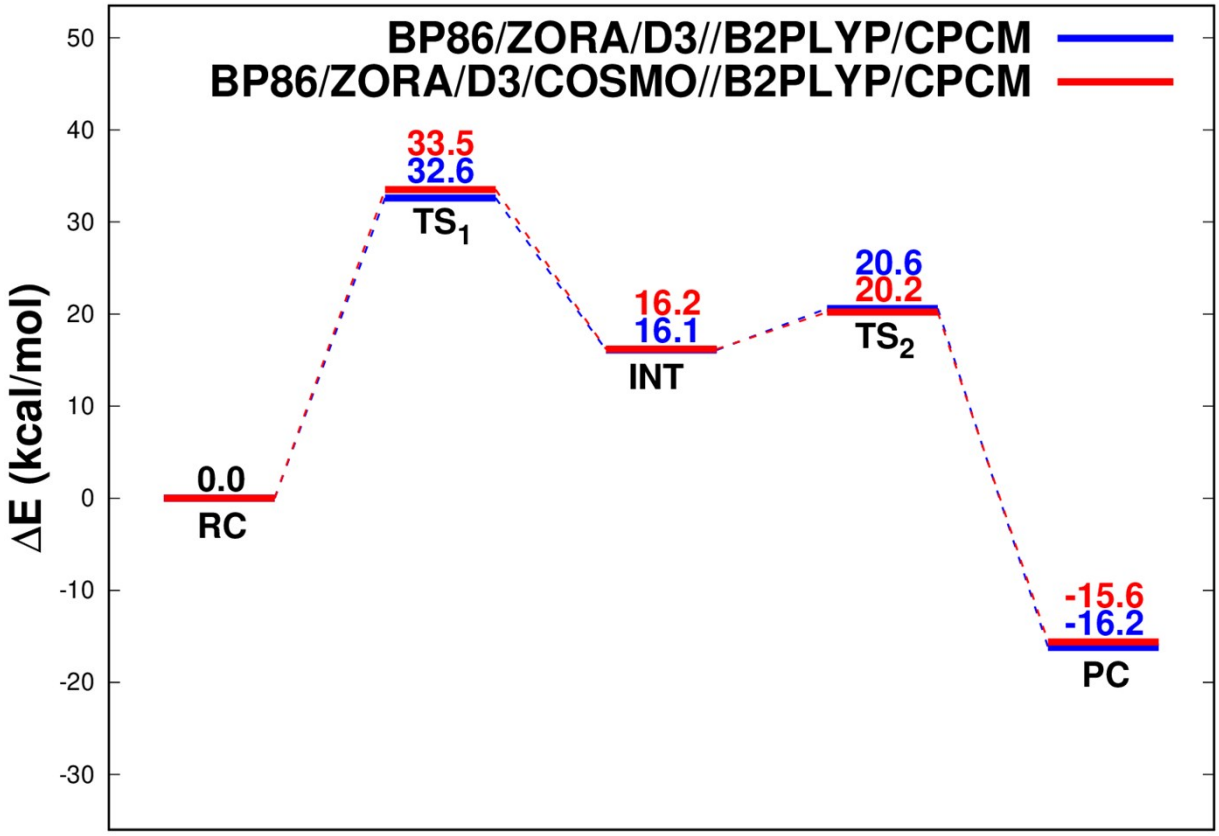


Figure S14. Solvation effect on geometries for the intramolecular nucleophilic attack in the 1-phenyl-2-propyn-1-ol assisted by the OTs^- counterion calculated with different computational protocols. In blue the BP86/ZORA/D3//B2PLYP/CPCM results and in red the BP86/ZORA/D3/COSMO//B2PLYP/CPCM results are shown. Energy are given with respect to the corresponding RC taken as zero reference energy.

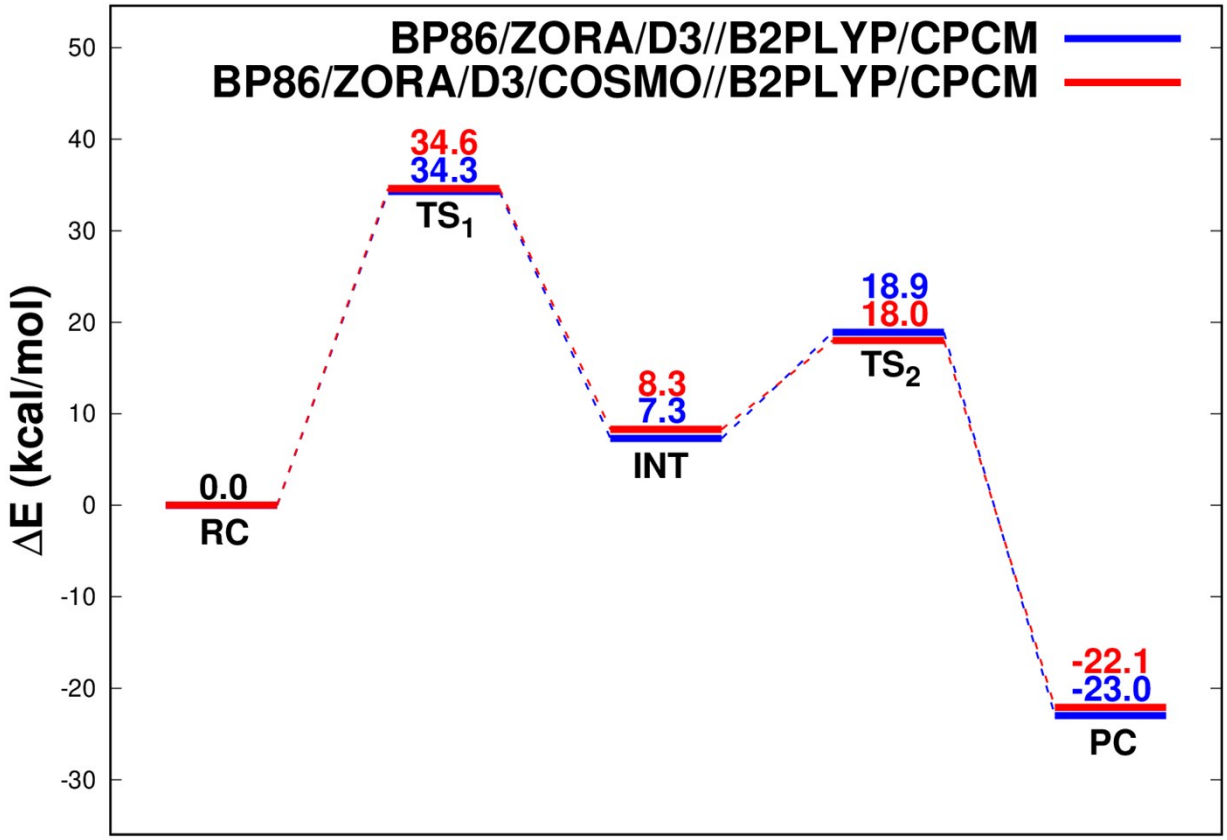


Figure S15. Electronic energy ($\Delta E^{\#}$, in blue), enthalpy ($\Delta H^{\#}_{298}$, in red) and Gibbs' free energy ($\Delta G^{\#}_{298}$, in green) activation barriers at 298 K for the OTf^- - OTs^-- BF_4^- -assisted intramolecular nucleophilic attack in the 1-phenyl-2-propyn-1-ol calculated at the BP86/ZORA/D3/COSMO//BP86/ZORA/D3/COSMO level. Energies are reported with respect to RC taken as zero reference energy.

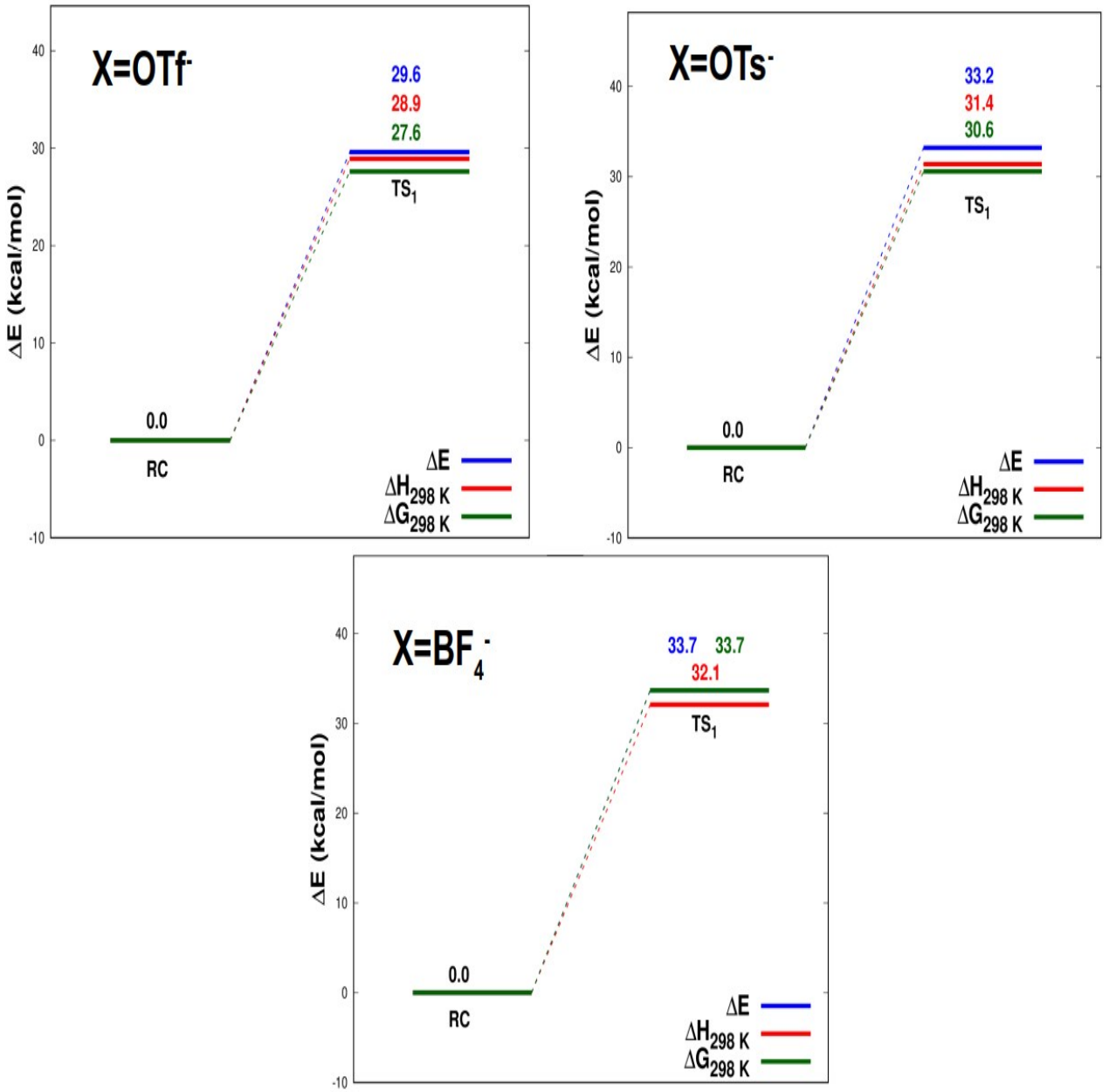


Figure S16. Energy profile for the intramolecular nucleophilic attack in the 1-phenyl-2-propyn-1-ol assisted by the OTf^- counterion where the active catalytic species is a gold-hydroxide complex (NHC-Au-OH). This mechanism has been reported in Ref. 8 for the gold-catalyzed formation of enones. The profile has been calculated at the BP86/ZORA/D3//B2PLYP/CPCM level. Energies are given with respect to RC taken as zero reference energy.

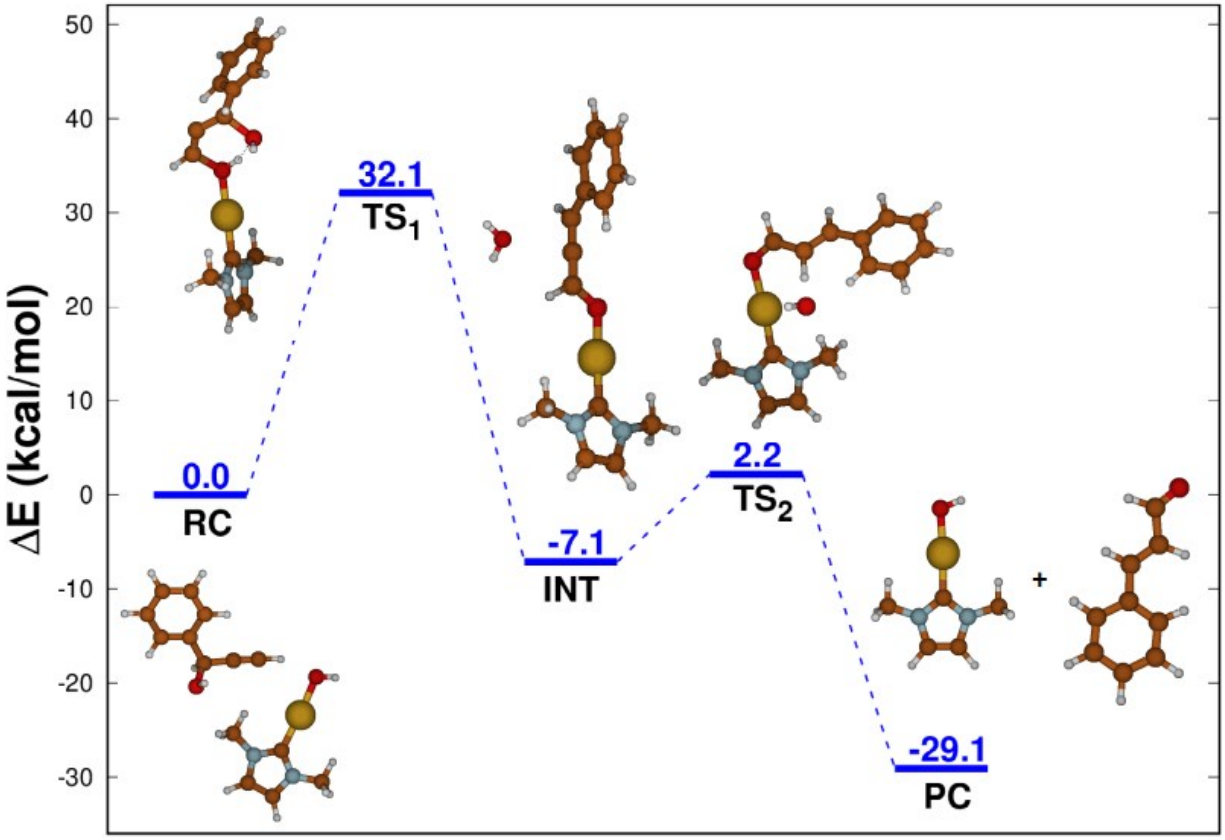
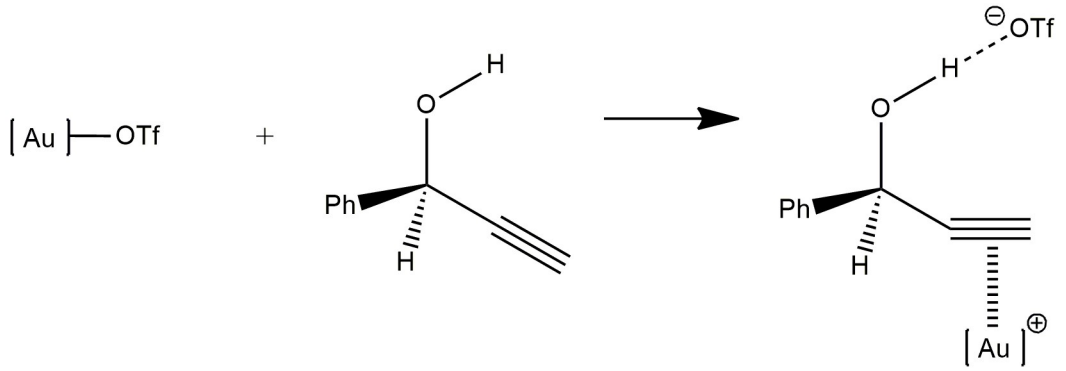
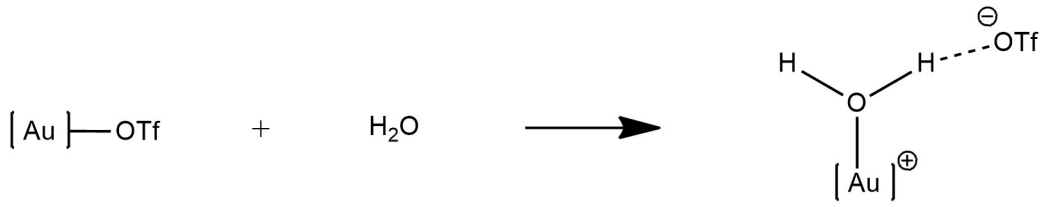


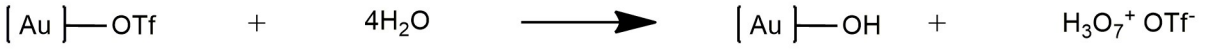
Figure S17. Energetics of the formation of the three active species investigated in this work (i.e. gold-alkyne, gold-water and gold-hydroxide complexes). The calculations have been carried out at the BP86/ZORA/D3//B2PLYP/CPCM level. The mechanism of formation of the gold-hydroxide species is the one suggested as to be more likely to take place in Ref. 8.



E=-11.9 kcal/mol



E=-6.1 kcal/mol



E=-5.1 kcal/mol

Figure S18. Energy profile for the intramolecular nucleophilic attack in the 1-phenyl-2-propyn-1-ol assisted by the OTf^- counterion where the active catalytic species is a gold-water complex ([NHC-Au-OH_2]$^+$). The profile has been calculated at the BP86/ZORA/D3//B2PLYP/CPCM level. Energies are given with respect to RC taken as zero reference energy.

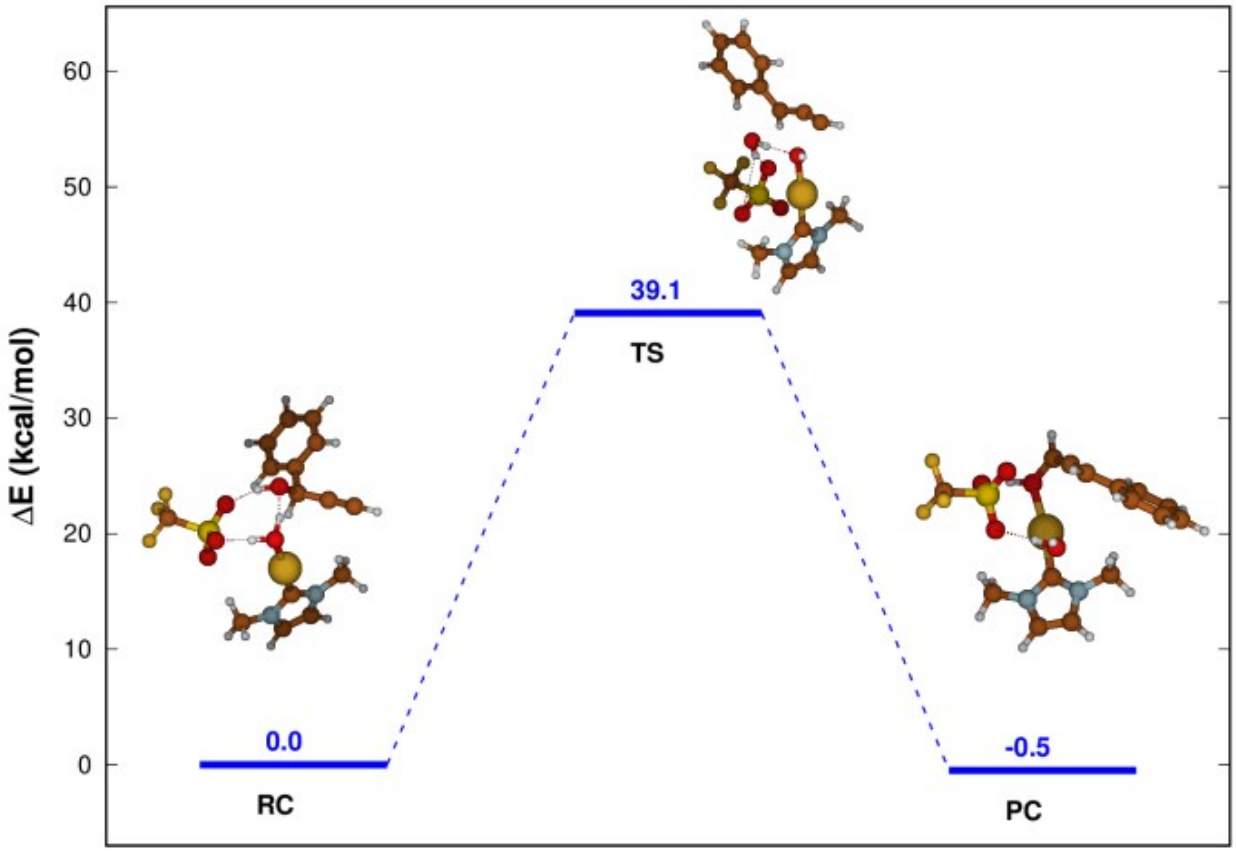
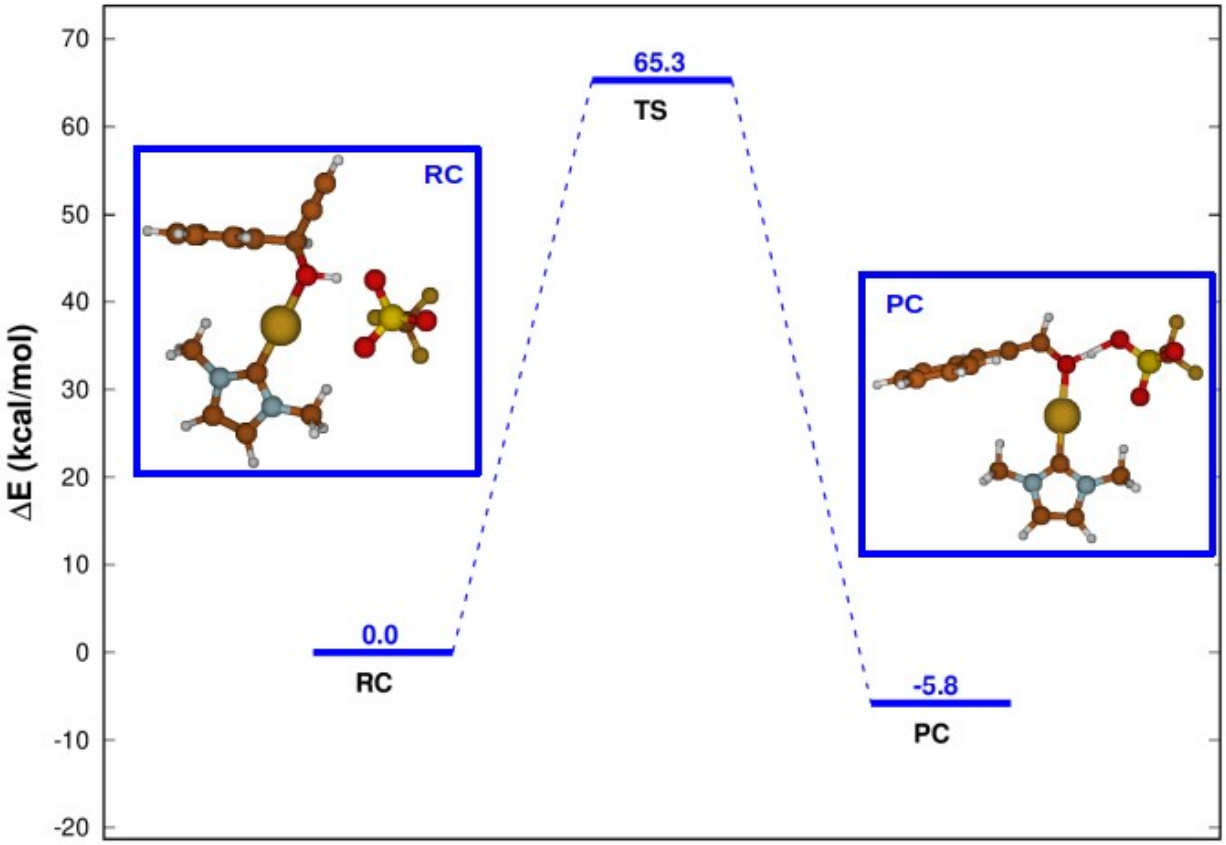


Figure S19. Energy profile for the intramolecular nucleophilic attack in the 1-phenyl-2-propyn-1-ol assisted by the OTf^- counterion where the active catalytic species is a gold-hydroxide complex (RC) formed via coordination of the gold fragment to the propargylic hydroxide group. The profile has been calculated at the BP86/ZORA//B2PLYP level. Energies are given with respect to RC taken as zero reference energy.



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xyz geometries

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RC_OTf (BP86/ZORA)

C	3.395393958	1.570068761	-1.175923512
C	2.610100711	2.441588261	-0.415076854
C	3.184461938	3.591696554	0.131996734
C	4.537853805	3.861722160	-0.077051107
C	5.323446759	2.987415873	-0.830654445
C	4.748302045	1.841047988	-1.383592261
C	1.131213899	2.133926349	-0.185888398
O	0.406524093	3.288473706	0.145920656
C	1.006139524	1.160671361	0.951357278
C	0.892902487	0.599203222	2.051707108
AU	0.600495151	-1.026395155	0.643916276
C	0.298083432	-2.835162130	-0.213580603
N	-0.859658646	-3.331326876	-0.728397674
C	-0.665399747	-4.605466268	-1.219532686
C	0.644718020	-4.919307648	-1.012334188
N	1.219493478	-3.826063068	-0.394729675
C	-2.148899114	-2.629880996	-0.734299350
C	2.625599157	-3.742312263	-0.012022950
H	-1.463994135	-5.174323431	-1.677295889
H	1.206562262	-5.811145152	-1.256837787
H	-1.977039424	-1.550072639	-0.833424376
H	-2.732204096	-2.983237202	-1.589945311
H	-2.691488254	-2.843078605	0.193881064
H	2.787921818	-2.772744235	0.468208904
H	2.870978876	-4.546843507	0.690904244
H	3.262048047	-3.822467616	-0.901031957
H	0.841489661	0.426804529	3.111202548
H	0.717829298	1.642282841	-1.081461838
H	-0.512905621	3.176908133	-0.245741265
H	5.351108774	1.164595036	-1.989810893
H	6.378528265	3.204408352	-0.997213803
H	2.942248888	0.683182736	-1.622887775
H	4.979143347	4.764372163	0.345890106
H	2.557675532	4.277861755	0.698759061
O	-1.938851409	2.883690920	-1.049392923
S	-2.474708949	1.524394831	-1.285506460
O	-1.475199970	0.452737112	-1.063144059
O	-3.319454878	1.369647380	-2.460358642
C	-3.660507808	1.287919136	0.165042192
F	-4.217688827	0.044767211	0.128925530
F	-3.015520541	1.407741690	1.353710582

F	-4.660597041	2.190555324	0.138709512
		42	
	TS1_OTf (BP86/ZORA)		
C	3.653507365	-0.071597651	1.197798834
C	3.357736912	-1.152555121	0.356034724
C	4.402917511	-1.879285116	-0.221694186
C	5.729021591	-1.528130291	0.042698189
C	6.020213203	-0.450146201	0.878277208
C	4.976590328	0.278530596	1.457011674
C	1.916989702	-1.520109741	0.096910874
O	1.806660878	-2.775531536	-0.659865959
C	1.173356082	-0.555335758	-0.809518851
C	0.865525512	-1.182038028	-1.869062965
AU	0.169317169	1.192589844	-0.444671323
C	-0.941036886	2.784027955	0.156715064
N	-2.058137572	2.726504146	0.932941599
C	-2.556282211	3.995205406	1.164328668
C	-1.732920627	4.869555464	0.522841157
N	-0.748937451	4.111741534	-0.087185258
C	-2.672205271	1.495890261	1.443163331
C	0.344718456	4.659323085	-0.882569141
H	-3.443499820	4.167639130	1.759486365
H	-1.763302210	5.948946661	0.452198480
H	-2.032662830	0.636258519	1.211079796
H	-2.788964302	1.572596801	2.529752098
H	-3.653202264	1.352854127	0.976167260
H	0.962533265	3.823620571	-1.225199789
H	-0.053179851	5.201006042	-1.748788719
H	0.952324493	5.337293153	-0.271605508
H	0.445515764	-1.582367566	-2.776956351
H	1.362217857	-1.610689386	1.043071396
H	0.940950698	-3.187318552	-0.324308143
H	5.196155135	1.117335543	2.117663628
H	7.055756264	-0.178813919	1.083202146
H	2.840879727	0.495541728	1.655026904
H	6.537829187	-2.104780254	-0.406268637
H	4.168020479	-2.726993100	-0.861840200
O	-0.493032283	-3.658351223	0.277888801
S	-1.539351591	-2.852185181	0.960952749
O	-1.160931433	-1.439387931	1.160116315
O	-2.197363166	-3.512716965	2.077287642
C	-2.883397810	-2.747965499	-0.362136972
F	-3.925152647	-1.991700760	0.069785692
F	-2.410369003	-2.169550136	-1.503637269
F	-3.358045537	-3.967272819	-0.686521935

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INT_OTf (BP86/ZORA)

C	5.849871	1.335964	0.770151
N	4.716978	0.539828	0.793778
C	3.685182	1.124931	0.115305
N	4.207948	2.305801	-0.331043
C	5.528749	2.450633	0.059402
C	4.629339	-0.755217	1.459344
Au	1.798592	0.397827	-0.166161
C	3.466788	3.282868	-1.120891
H	6.120531	3.319717	-0.196897
H	6.774789	1.048212	1.252754
H	2.446698	2.906032	-1.245456
H	3.440236	4.247494	-0.600193
H	3.934247	3.408186	-2.105032
H	3.629477	-1.159414	1.271882
H	5.383646	-1.439827	1.053461
H	4.781191	-0.638298	2.539200
C	-1.135753	-0.068556	-1.208702
C	-0.060166	-0.326680	-0.444470
H	-1.492276	0.638758	-1.952711
C	-0.861658	-1.468339	0.184430
O	-2.006713	-1.119847	-0.785897
H	-1.232093	-1.248286	1.194585
C	-0.432071	-2.894123	0.057886
C	-0.620095	-3.781184	1.124956
C	-0.219521	-5.114898	1.019584
C	0.365674	-5.573696	-0.160656
C	0.552254	-4.695064	-1.233067
C	0.162148	-3.363014	-1.122880
H	-3.372507	-0.862361	-0.298813
O	-4.363701	-0.794220	0.071526
S	-5.072562	0.537444	-0.344427
H	-0.371188	-5.795978	1.856949
H	0.674916	-6.615381	-0.248001
H	-1.087235	-3.423651	2.044023
H	1.006916	-5.052870	-2.157007
H	0.314402	-2.669810	-1.950004
O	-4.349745	1.209526	-1.406368
O	-6.497101	0.320495	-0.407206
C	-4.782067	1.571805	1.210644
F	-5.318782	2.794078	1.037399
F	-3.458865	1.707213	1.444074
F	-5.352093	0.992194	2.283109

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TS2_OTf (BP86/ZORA)

C	5.647709	1.793536	0.735689
N	4.616271	0.872388	0.815248
C	3.528446	1.284860	0.099200
N	3.909868	2.486378	-0.426730
C	5.201291	2.812098	-0.047738
C	4.677024	-0.374683	1.568569
Au	1.728772	0.352072	-0.120377
C	3.061311	3.320846	-1.271582
H	5.686764	3.727147	-0.361040
H	6.596697	1.650457	1.235762
H	2.102453	2.807771	-1.394892
H	2.895306	4.294487	-0.795608
H	3.529384	3.464576	-2.252669
H	3.717688	-0.886543	1.443639
H	5.484777	-1.009937	1.185570
H	4.845277	-0.166773	2.632120
C	-1.206958	-0.158908	-1.013043
C	-0.094418	-0.501397	-0.331882
H	-1.526631	0.714697	-1.578009
C	-0.658719	-1.707665	0.302976
O	-2.101239	-1.214928	-0.884607
H	-1.299920	-1.549122	1.176361
C	-0.172633	-3.067117	0.150135
C	-0.655715	-4.082850	0.998862
C	-0.219286	-5.394501	0.846545
C	0.700979	-5.706465	-0.158963
C	1.183764	-4.707760	-1.012299
C	0.748931	-3.396140	-0.863222
H	-3.230655	-0.909123	-0.636582
O	-4.423491	-0.698134	-0.379636
S	-4.896270	0.745159	-0.533889
H	-0.596728	-6.176851	1.504100
H	1.039659	-6.735295	-0.282659
H	-1.380604	-3.829349	1.773406
H	1.894400	-4.961468	-1.798508
H	1.104199	-2.604351	-1.522109
O	-3.915675	1.576737	-1.221770
O	-6.293892	0.820128	-0.905895
C	-4.841464	1.331275	1.260087
F	-5.205374	2.628148	1.337495
F	-3.586448	1.213136	1.764260
F	-5.673986	0.606168	2.036710

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PC_OTf (BP86/ZORA)

C	4.334134	-2.725379	-0.392205
N	3.827843	-1.442292	-0.511511
C	2.523562	-1.390682	-0.112630
N	2.227334	-2.670629	0.254039
C	3.323360	-3.498282	0.090452
C	4.584860	-0.299680	-1.008311
Au	1.237021	0.196447	-0.066019
C	0.926033	-3.124390	0.749515
H	3.291546	-4.554491	0.324076
H	5.351874	-2.977357	-0.660031
H	0.213254	-2.296744	0.699605
H	0.557711	-3.944769	0.124078
H	1.018860	-3.463868	1.787489
H	3.908726	0.559342	-1.049607
H	5.422657	-0.076774	-0.336570
H	4.966676	-0.509832	-2.014415
C	-1.489839	0.956011	0.058123
C	-0.234281	1.639505	0.004114
H	-1.616056	0.015214	-0.496977
C	-0.228595	3.004730	0.049600
O	-2.467368	1.314378	0.796282
H	-1.203373	3.505679	-0.002265
C	0.895385	3.925898	0.118503
C	0.629600	5.310297	0.062129
C	1.656412	6.245493	0.158253
C	2.975954	5.817976	0.317335
C	3.258448	4.448052	0.379707
C	2.234418	3.515199	0.275824
H	-3.270250	0.509730	0.790356
O	-4.175046	-0.434496	0.825054
S	-3.750094	-1.882655	0.691561
H	1.428051	7.310010	0.111035
H	3.782838	6.546714	0.392640
H	-0.402271	5.644801	-0.054124
H	4.287829	4.113124	0.509241
H	2.451006	2.445011	0.320656
O	-2.309295	-2.026246	0.457997
O	-4.384404	-2.756187	1.658454
C	-4.532511	-2.334853	-0.964077
F	-4.243081	-3.616795	-1.276809
F	-4.048820	-1.540120	-1.951997
F	-5.871265	-2.194545	-0.925523

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RC_OTf (BP86/ZORA/D3)

C	0.375212835	-3.298519839	-0.636503235

C	1.622910671	-2.891287401	-0.155189027
C	2.563125892	-3.844640997	0.233983356
C	2.251191299	-5.202680168	0.144958406
C	1.003233915	-5.610498790	-0.327761746
C	0.063968689	-4.654083226	-0.721921648
C	1.927708480	-1.406192293	-0.046428676
O	3.301021729	-1.148598358	0.104210966
C	1.208139565	-0.851218806	1.138075807
C	0.816250253	-0.404053946	2.224317291
AU	-0.863464963	-0.109051474	0.861136576
C	-2.630710367	0.289278627	-0.018248601
N	-2.982759924	1.391472394	-0.731890987
C	-4.277127206	1.277726660	-1.195817106
C	-4.750124670	0.072037286	-0.767985411
N	-3.729293357	-0.518434206	-0.048801875
C	-2.109552669	2.546323544	-0.961797264
C	-3.811982400	-1.827816735	0.588319075
H	-4.743890089	2.049202283	-1.793408315
H	-5.706659492	-0.409237640	-0.921070627
H	-1.077438025	2.195152124	-1.084741945
H	-2.435971303	3.052200203	-1.874758170
H	-2.173807255	3.235366329	-0.112861087
H	-2.817185239	-2.078983815	0.968862992
H	-4.526593500	-1.799351718	1.418908365
H	-4.126206579	-2.577780327	-0.145697790
H	0.773713891	-0.087758812	3.249446933
H	1.520191803	-0.886629773	-0.929433708
H	3.419426883	-0.220840747	-0.247527471
H	-0.905219056	-4.967477424	-1.109683493
H	0.765360639	-6.671392055	-0.399238864
H	-0.348423311	-2.545600688	-0.955949868
H	2.989583963	-5.946234254	0.444055122
H	3.536752173	-3.511921985	0.587963593
O	3.196700463	1.309926146	-0.960673956
S	1.969377716	2.054891305	-1.307935194
O	0.733151222	1.240304024	-1.227094486
O	2.060891064	2.939100346	-2.459235241
C	1.783192393	3.235528622	0.150198199
F	0.646331963	3.976484403	0.026222386
F	1.697738507	2.562222348	1.327955667
F	2.824580380	4.084771722	0.230940663

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TS1_OTf (BP86/ZORA/D3)

C	2.068139630	2.840264024	-1.035331666
C	0.980743314	3.362511439	-0.323695423

C	1.022694319	4.680280533	0.134871036
C	2.143145930	5.472797246	-0.125488061
C	3.224586650	4.952846561	-0.835192158
C	3.184322440	3.631223366	-1.290342418
C	-0.214769438	2.488050773	-0.072121869
O	-1.272186680	3.203278757	0.660879280
C	0.072094595	1.325711232	0.855210883
C	-0.604129361	1.524088279	1.910238729
AU	0.879349830	-0.492450720	0.407925926
C	1.548062293	-2.283139216	-0.256551950
N	0.878962314	-3.139987312	-1.074217881
C	1.641897273	-4.263575409	-1.335173429
C	2.820514502	-4.106378061	-0.670812853
N	2.745464251	-2.888467307	-0.017357054
C	-0.477121212	-2.924041607	-1.583533467
C	3.802037382	-2.321320673	0.810699868
H	1.286299199	-5.068118108	-1.964898363
H	3.691900711	-4.744632044	-0.611059784
H	-0.777799683	-1.885720896	-1.401540080
H	-0.492446345	-3.121900282	-2.660379980
H	-1.175839543	-3.595072497	-1.072513391
H	3.451108307	-1.352241847	1.178891399
H	4.012544051	-2.983070235	1.658714969
H	4.712011619	-2.180626508	0.216110015
H	-1.192749300	1.473790332	2.810492030
H	-0.621450229	2.095012779	-1.015381920
H	-2.105851798	2.696470379	0.394263413
H	4.025566530	3.219335313	-1.847293708
H	4.097828741	5.572964869	-1.035311362
H	2.035172817	1.806762507	-1.384693058
H	2.167862706	6.502747491	0.229591926
H	0.170425746	5.077187578	0.681554647
O	-3.244389813	1.604226470	-0.040493077
S	-3.127749232	0.347924078	-0.822559216
O	-1.747512741	0.029472884	-1.239703118
O	-4.166432565	0.136032067	-1.817247162
C	-3.484499053	-0.964994366	0.482819429
F	-3.417080353	-2.208740732	-0.060615759
F	-2.577641508	-0.921840585	1.499914576
F	-4.710626730	-0.809305695	1.018904062

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INT_OTf (BP86/ZORA/D3)

C	-1.576686319	3.214724517	-1.111604707
C	-0.782329513	2.558200957	-0.162342318
C	0.318255685	3.221652537	0.394995118

C	0.620410014	4.525449149	0.007288369
C	-0.175262312	5.176468196	-0.939064952
C	-1.274745411	4.520321766	-1.496424117
C	-1.122176905	1.166485503	0.239786849
O	-2.010512134	1.132464066	1.524269006
C	-0.130286084	0.285660444	0.982350945
C	-0.980635249	0.264650278	2.019901098
AU	1.693436783	-0.354193615	0.438095514
C	3.545662303	-0.920124798	-0.180329831
N	4.260334853	-2.033264290	0.153406908
C	5.487085590	-2.055226593	-0.489875138
C	5.547789036	-0.927817695	-1.250234429
N	4.357954966	-0.248605219	-1.047817817
C	3.780249053	-3.061913482	1.066967854
C	4.003305077	1.017525201	-1.678355463
H	6.200837861	-2.856977413	-0.354962474
H	6.324426118	-0.558493475	-1.906648780
H	2.777509897	-2.770324564	1.394857114
H	3.731462742	-4.029383536	0.553911419
H	4.444445716	-3.136672000	1.935912567
H	3.022577146	1.316783284	-1.294174398
H	4.745943855	1.783704626	-1.427582635
H	3.948762184	0.896210663	-2.766426862
H	-1.091321447	-0.174257459	3.007785064
H	-1.705473300	0.651924686	-0.531291176
H	-3.291186296	0.611067491	1.360117183
H	-1.897485888	5.026930085	-2.233209643
H	0.062114274	6.196124031	-1.242260560
H	-2.435846710	2.695232079	-1.536261774
H	1.477637904	5.037938611	0.443876990
H	0.932407727	2.699848598	1.128176752
O	-4.304502069	0.211127610	1.311520192
S	-4.771651648	-0.119242387	-0.131766357
O	-4.028118300	0.636044374	-1.126079154
O	-6.211296158	-0.197012278	-0.172469759
C	-4.145961369	-1.889429191	-0.300794292
F	-4.443025070	-2.356427783	-1.528072006
F	-2.804268044	-1.921512984	-0.136819304
F	-4.711784755	-2.689771668	0.620271929

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TS2_OTf (BP86/ZORA/D3)

C	5.425283	1.735607	0.820781
N	4.434847	0.773627	0.707316
C	3.341353	1.264800	0.055631
N	3.674772	2.554962	-0.235629

C	4.945134	2.860365	0.223358
C	4.528106	-0.583763	1.228453
Au	1.592550	0.318668	-0.360046
C	2.799192	3.484444	-0.940697
H	5.392468	3.836272	0.089513
H	6.370730	1.542796	1.309994
H	1.841802	2.980617	-1.106728
H	2.639028	4.382167	-0.333162
H	3.239830	3.762282	-1.905195
H	3.619643	-1.115807	0.928366
H	5.406904	-1.087972	0.810327
H	4.596946	-0.566597	2.322532
C	-1.173023	-0.352225	-1.630026
C	-0.182877	-0.557604	-0.747847
H	-1.396379	0.398801	-2.381836
C	-0.833644	-1.639643	0.012272
O	-2.106285	-1.388252	-1.429714
H	-1.573652	-1.340599	0.760607
C	-0.325772	-2.988357	0.144954
C	-0.925423	-3.875779	1.058295
C	-0.451380	-5.176582	1.184599
C	0.624673	-5.601048	0.399611
C	1.225751	-4.727977	-0.514394
C	0.751906	-3.429275	-0.646683
H	-3.125637	-0.995223	-1.159078
O	-4.326082	-0.587730	-0.750671
S	-4.472966	0.913886	-0.617053
H	-0.917105	-5.863133	1.890194
H	0.995444	-6.621245	0.497404
H	-1.767195	-3.531128	1.659242
H	2.059552	-5.071073	-1.125853
H	1.196397	-2.730770	-1.354736
O	-3.442085	1.646283	-1.346739
O	-5.851880	1.352471	-0.703561
C	-4.011980	1.161521	1.193386
F	-4.048234	2.469011	1.521510
F	-2.747886	0.707086	1.435227
F	-4.850522	0.491706	2.013088

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PC_OTf (BP86/ZORA/D3)

C	1.872800	4.472989	0.300956
N	2.122676	3.125775	0.499738
C	1.091966	2.362660	0.034329
N	0.193649	3.260603	-0.456009
C	0.655083	4.555782	-0.302800

C	3.322102	2.585949	1.126035
Au	0.914901	0.338567	0.076318
C	-1.087022	2.907938	-1.068748
H	0.083359	5.414776	-0.628040
H	2.567499	5.244589	0.604798
H	-1.255279	1.832228	-0.967857
H	-1.896361	3.442374	-0.560002
H	-1.077309	3.175025	-2.131370
H	3.194542	1.502466	1.212953
H	4.203384	2.804535	0.511481
H	3.451761	3.018508	2.124615
C	-0.791789	-1.895464	0.085394
C	0.616180	-1.699148	0.121675
H	-1.438301	-1.241459	0.684623
C	1.473532	-2.756211	0.122328
O	-1.377668	-2.734802	-0.681613
H	1.039096	-3.756026	0.240462
C	2.925331	-2.751006	0.033844
C	3.607903	-3.977721	0.154735
C	4.994209	-4.043398	0.046784
C	5.730715	-2.881637	-0.189233
C	5.068276	-1.655162	-0.317158
C	3.686452	-1.589764	-0.202126
H	-2.459249	-2.495750	-0.682558
O	-3.738395	-2.045599	-0.671212
S	-3.912616	-0.564554	-0.908119
H	5.501882	-5.002339	0.144709
H	6.815995	-2.928529	-0.273300
H	3.031375	-4.886411	0.331743
H	5.640502	-0.747390	-0.508012
H	3.165602	-0.633411	-0.299456
O	-2.635102	0.118774	-1.136012
O	-5.033578	-0.238046	-1.765626
C	-4.429043	0.026823	0.803566
F	-4.590075	1.369557	0.801413
F	-3.470814	-0.274172	1.723706
F	-5.581466	-0.542633	1.198517

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RC_OTf (BP86/ZORA/D3/COSMO)

C	3.210687654	1.180788938	-1.046125514
C	2.525868251	2.275251741	-0.509665592
C	3.233860750	3.406217934	-0.100369471
C	4.623901371	3.439721693	-0.229971228
C	5.309251436	2.345076641	-0.759611699
C	4.598898864	1.213269236	-1.169579284

C	1.015976296	2.196844443	-0.345857755
O	0.439860441	3.474904608	-0.202503118
C	0.711857878	1.385359654	0.868870644
C	0.453678267	0.932053095	1.991585943
AU	0.439362090	-0.787327565	0.636113945
C	0.362861133	-2.586993305	-0.259361938
N	-0.697432643	-3.158161528	-0.889983590
C	-0.345226143	-4.382563982	-1.418545187
C	0.969780416	-4.582932177	-1.114469633
N	1.385470057	-3.474221966	-0.405023303
C	-2.035967062	-2.570380729	-0.967718618
C	2.739443382	-3.274905986	0.101862278
H	-1.048720959	-4.996620814	-1.964322958
H	1.634561276	-5.403599428	-1.346500349
H	-1.945814308	-1.480150784	-1.008161026
H	-2.522911463	-2.930102615	-1.877934273
H	-2.623923869	-2.867552187	-0.092809701
H	2.777825437	-2.294482078	0.585119920
H	2.982721686	-4.054267206	0.831291373
H	3.453566709	-3.306753893	-0.727370208
H	0.247405560	0.820371671	3.040268274
H	0.586064032	1.661874046	-1.208027292
H	-0.542071999	3.349412919	-0.335563565
H	5.127428507	0.361091423	-1.596065091
H	6.393864920	2.374990890	-0.859508138
H	2.650676638	0.302856878	-1.373451469
H	5.173333757	4.326617481	0.084708969
H	2.691757985	4.257323938	0.306674733
O	-2.169765762	2.943218840	-0.582305206
S	-2.672424377	1.627990213	-1.036146063
O	-1.619059627	0.617721071	-1.237261350
O	-3.704974074	1.680773300	-2.067195543
C	-3.597667771	1.007941665	0.476827958
F	-4.153362696	-0.204803411	0.230414381
F	-2.770047737	0.872144919	1.540405268
F	-4.584449539	1.859859010	0.820259590

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TS1_OTf (BP86/ZORA/D3/COSMO)

C	3.477600442	0.058878703	1.101780226
C	3.264563519	-1.156716857	0.438869145
C	4.358622735	-1.937117094	0.058562739
C	5.656668862	-1.505976090	0.344420401
C	5.867709423	-0.295164076	1.002835203
C	4.772367878	0.487613651	1.382547051
C	1.855912224	-1.594762100	0.144510676

O	1.835384240	-2.870105048	-0.602216397
C	1.134426550	-0.677781645	-0.819885527
C	0.967674139	-1.362628418	-1.878306995
AU	0.160239906	1.068587265	-0.428948133
C	-0.893352407	2.674488336	0.212696662
N	-1.834366042	2.659072273	1.194710005
C	-2.340799475	3.928351414	1.405879139
C	-1.702256994	4.758116355	0.534129059
N	-0.818896234	3.973134437	-0.185965931
C	-2.250918605	1.468393527	1.934973796
C	0.061984438	4.467364327	-1.238419940
H	-3.103400937	4.128425398	2.146343425
H	-1.799948089	5.822000307	0.365005598
H	-1.758198197	0.589352738	1.506556989
H	-1.967077314	1.570168338	2.988023781
H	-3.336351370	1.350478486	1.855476469
H	0.646550213	3.621966124	-1.612470974
H	-0.532280141	4.892770420	-2.054075657
H	0.735408323	5.230364383	-0.833859115
H	0.672568954	-1.805854586	-2.815171155
H	1.270507830	-1.703060248	1.068140111
H	0.927118239	-3.258739598	-0.393813874
H	4.930101772	1.435452345	1.896502855
H	6.881014022	0.041391159	1.219489688
H	2.622927728	0.673830489	1.388823001
H	6.505081697	-2.121729950	0.046875169
H	4.187917002	-2.880992708	-0.453851349
O	-0.636671515	-3.689516611	-0.117814827
S	-1.623712866	-2.893135015	0.654452663
O	-1.091104014	-1.638168362	1.203092204
O	-2.467529637	-3.679978318	1.549069316
C	-2.818028828	-2.314513287	-0.675536264
F	-3.760297553	-1.503008777	-0.139731491
F	-2.179942024	-1.618872545	-1.648374458
F	-3.441573079	-3.361893324	-1.254111365

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INT_OTf (BP86/ZORA/D3/COSMO)

C	-1.787566597	-3.325173769	0.731274357
C	-0.933330289	-2.601413228	-0.112789300
C	0.109931715	-3.258546980	-0.778488154
C	0.294626190	-4.627979614	-0.603171222
C	-0.562077437	-5.347045104	0.235565435
C	-1.602171975	-4.695684937	0.902912805
C	-1.166790589	-1.153048912	-0.300413790
O	-2.063971827	-0.887769138	-1.620705805

C	-0.144963240	-0.227688404	-0.923362305
C	-0.962521391	0.016604322	-1.951044149
AU	1.693165041	0.282484789	-0.285729817
C	3.554224707	0.758730825	0.382798066
N	4.292284193	1.869499306	0.103690828
C	5.520375527	1.824910569	0.740631163
C	5.555386825	0.656497351	1.439492858
N	4.347821668	0.020819414	1.209086782
C	3.843077250	2.959884974	-0.754848696
C	3.963172217	-1.264088906	1.782604134
H	6.252499322	2.615354553	0.643586680
H	6.323845936	0.230966441	2.070711525
H	2.828129603	2.726355617	-1.089730699
H	3.836219220	3.900011803	-0.192922670
H	4.504232795	3.052173625	-1.623348954
H	2.979795656	-1.528020213	1.381420220
H	4.692638045	-2.032086364	1.503648826
H	3.904345918	-1.186990194	2.873799026
H	-1.041089977	0.607288319	-2.857398232
H	-1.761873111	-0.716380459	0.508274767
H	-3.036150941	-0.373336670	-1.372240596
H	-2.269130003	-5.256632425	1.556543414
H	-0.417180846	-6.418736858	0.370370081
H	-2.599205928	-2.805440170	1.240688627
H	1.106084578	-5.138580107	-1.120850198
H	0.772044121	-2.684937441	-1.426239603
O	-4.189831398	0.218703915	-1.142159120
S	-4.598619611	0.424812867	0.298450042
O	-3.905994552	-0.468215072	1.224587192
O	-6.032524315	0.598857565	0.443339362
C	-3.860790868	2.114165520	0.654035741
F	-4.146685009	2.491120904	1.915296956
F	-2.515188015	2.070319606	0.513274477
F	-4.346284961	3.040937713	-0.194593008

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TS2_OTf (BP86/ZORA/D3/COSMO)

C	-5.319925829	-1.633126076	1.083368078
N	-4.347844461	-0.669344702	0.874886884
C	-3.264836107	-1.195791605	0.237561815
N	-3.580898398	-2.508052964	0.052619597
C	-4.834701202	-2.794646948	0.563879004
C	-4.462060039	0.726816146	1.279555765
AU	-1.546858401	-0.257178381	-0.310013166
C	-2.708248256	-3.483264585	-0.592938201
H	-5.266424314	-3.785225266	0.514906278

H	-6.257354368	-1.413686801	1.576500690
H	-1.777528117	-2.975556514	-0.863253871
H	-2.490273069	-4.304369098	0.098018934
H	-3.187674514	-3.875991812	-1.495949514
H	-3.531837125	1.230752379	1.000170257
H	-5.306059030	1.199623462	0.765413026
H	-4.604368990	0.792736942	2.363529301
C	1.091507513	0.389369032	-1.818371942
C	0.198424606	0.600177981	-0.850333599
H	1.214620728	-0.302763777	-2.644677786
C	0.967474335	1.631742817	-0.117598812
O	2.119840682	1.371705774	-1.612435839
H	1.685623958	1.268318657	0.623645665
C	0.579088978	3.015448623	0.035084245
C	1.285186905	3.836979025	0.934798690
C	0.929216836	5.171900655	1.086874565
C	-0.132755624	5.694039091	0.342120856
C	-0.840513477	4.884958284	-0.555086931
C	-0.487468077	3.551110762	-0.711582329
H	3.017280275	0.905239593	-1.287108358
O	4.203131338	0.340236934	-0.677640879
S	4.238379301	-1.148913702	-0.501655028
H	1.474478007	5.808094624	1.782268908
H	-0.412051269	6.740486753	0.461405439
H	2.111770810	3.415130102	1.506448466
H	-1.664973794	5.303528923	-1.130303799
H	-1.022989895	2.901810848	-1.402902267
O	3.228153256	-1.854363032	-1.285793548
O	5.590926075	-1.689045675	-0.483576133
C	3.655531554	-1.338271650	1.274795948
F	3.669868059	-2.634563673	1.644585460
F	2.385971378	-0.876935979	1.418157573
F	4.446790705	-0.643282133	2.120214411

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PC_OTf (BP86/ZORA/D3/COSMO)

C	1.337605660	-4.761116042	-0.064827644
N	1.813230245	-3.481576970	-0.295362350
C	0.846561709	-2.552095844	-0.056079317
N	-0.242555997	-3.274951383	0.325123954
C	0.039240883	-4.628918476	0.325388782
C	3.169996611	-3.167149263	-0.726400826
AU	0.947813458	-0.529794359	-0.229697598
C	-1.537200658	-2.701861820	0.688667518
H	-0.698146559	-5.372256501	0.597606045
H	1.952497623	-5.640899534	-0.198587604

H	-1.481027823	-1.613051924	0.603587782
H	-2.312803146	-3.081651803	0.015329788
H	-1.783011561	-2.967394376	1.722101286
H	3.216995856	-2.094009267	-0.931992075
H	3.886738874	-3.423261562	0.061876590
H	3.409477659	-3.722703274	-1.639081623
C	-0.480086742	1.900689969	-0.422035802
C	0.883907280	1.521200673	-0.400758959
H	-1.225757263	1.260603659	-0.907279008
C	1.854756599	2.483858882	-0.385139470
O	-0.931936239	2.934583626	0.199604743
H	1.542652727	3.515780574	-0.585015602
C	3.278743544	2.335200651	-0.158816695
C	4.080030884	3.496068782	-0.176963112
C	5.442650487	3.430587069	0.096882683
C	6.035712789	2.200851879	0.391200445
C	5.255974824	1.037582837	0.408861959
C	3.897922357	1.102504806	0.131486110
H	-1.995623849	2.883228037	0.231647094
O	-3.403837471	2.632470444	0.350082591
S	-3.766459922	1.321522846	0.987017800
H	6.044145226	4.338600959	0.083288765
H	7.102684419	2.145494840	0.603979773
H	3.612195296	4.456055854	-0.397496765
H	5.718753443	0.078228961	0.638373280
H	3.285094639	0.197361340	0.139844433
O	-2.614930666	0.436769571	1.178114796
O	-4.714394348	1.443682508	2.084080603
C	-4.745680709	0.493404638	-0.383690849
F	-5.141586501	-0.737088612	0.009357503
F	-3.983963950	0.353492900	-1.496042143
F	-5.838388180	1.211729695	-0.705420915

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RC_OTs (BP86/ZORA)

N	-0.527275528	-4.657594054	-0.292688524
C	-0.681558599	-3.310127590	-0.125236396
N	-1.871558958	-3.015033062	-0.714383453
C	-2.446733946	-4.153205750	-1.242069386
C	-1.604739624	-5.190036694	-0.973640049
AU	0.610461859	-2.050607100	0.791631654
C	1.916873255	-1.076983328	2.238868977
C	2.161499880	-0.473324940	1.184549823
C	2.627011813	0.472793668	0.115430952
O	2.531109333	1.781427262	0.595931457
C	-2.460042518	-1.674734170	-0.816480532

C	0.608136164	-5.436583114	0.189251040
C	4.061487768	0.102038571	-0.274844537
C	4.314826154	-1.082874553	-0.974163027
C	5.617018321	-1.419552689	-1.341992853
C	6.677547496	-0.572310561	-1.009686509
C	6.424877270	0.610648142	-0.314076225
C	5.120578803	0.950024332	0.053463390
O	0.297993460	2.568841938	-0.515467205
S	-0.934484339	1.736795409	-0.391829847
C	-2.137680771	2.803680889	0.426278080
O	-0.731085415	0.596010233	0.547044554
O	-1.529287643	1.349882945	-1.678769381
H	-3.395920573	-4.129755836	-1.761166369
H	-1.682240646	-6.244158791	-1.205518282
H	-1.887565683	-0.974177877	-0.194693139
H	-2.413137723	-1.322744694	-1.852542541
H	-3.501764548	-1.718309896	-0.480306603
H	1.330046083	-4.741121707	0.628476393
H	0.279457244	-6.153895809	0.950808226
H	1.074278282	-5.973129180	-0.645300963
H	1.922100507	-1.388779395	3.266702902
H	1.975288475	0.327049702	-0.763855833
H	1.650469008	2.144804473	0.247181180
H	5.804556462	-2.339374669	-1.896267814
H	7.695857014	-0.831456966	-1.299441157
H	3.486740623	-1.742702227	-1.240905499
H	7.247330883	1.279311620	-0.058979729
H	4.906189291	1.878250450	0.579383116
C	-3.404448485	2.988417397	-0.127716262
C	-4.340138615	3.787087165	0.531197315
C	-4.031765724	4.415200038	1.745169690
C	-2.751067074	4.218795746	2.283014501
C	-1.808821951	3.423162655	1.634333207
H	-3.639892614	2.508144860	-1.076304871
H	-5.329418755	3.926629940	0.090765433
C	-5.039079013	5.298517724	2.437833951
H	-2.487810715	4.698774458	3.227386614
H	-0.817220213	3.281437593	2.062490237
H	-4.790411398	5.435118580	3.497832677
H	-5.072656117	6.296894955	1.975485860
H	-6.051916949	4.878371551	2.374635358

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TS1_OTs (BP86/ZORA)

N	2.298814838	3.881197201	0.329078879
C	1.319447410	2.948561693	0.152654201

N	0.162802477	3.585235563	0.482896299
C	0.416144448	4.890095313	0.860547291
C	1.761263360	5.080692103	0.761118153
AU	1.468281167	1.004362220	-0.413581044
C	1.012112822	-1.236491241	-2.042921332
C	1.348992513	-0.996424615	-0.842078418
C	1.066933456	-2.245465175	-0.030346763
O	0.413349500	-3.098271215	-1.035832701
C	-1.166185914	2.961840168	0.491121714
C	3.717232845	3.648567723	0.082857091
C	2.287262298	-2.912653208	0.553446952
C	2.985049856	-2.287646606	1.596315415
C	4.104321308	-2.895914069	2.160065858
C	4.540054503	-4.137940130	1.687910930
C	3.847153164	-4.762855105	0.651463946
C	2.725561799	-4.153880059	0.082665189
O	-1.994639439	-2.088282620	-0.995840525
S	-2.262421383	-0.755660056	-0.362468073
C	-4.004404206	-0.837449576	0.092708093
O	-2.140225685	0.368164950	-1.313226069
O	-1.514430948	-0.566845126	0.900458863
H	-0.372584777	5.567542003	1.160396377
H	2.368785464	5.955695186	0.951284687
H	-1.199617318	2.121958508	-0.214181550
H	-1.394708398	2.581596885	1.493126661
H	-1.906355836	3.713730665	0.198590969
H	3.834606265	2.611192299	-0.245398079
H	4.081176517	4.324702135	-0.699975836
H	4.291070325	3.808792418	1.003334558
H	0.658610998	-1.213823734	-3.060599083
H	0.341312301	-1.990158718	0.759437571
H	-0.562715264	-2.788423555	-1.015928938
H	4.636657222	-2.403279723	2.974002962
H	5.414741002	-4.615106081	2.129827870
H	2.645144525	-1.319845853	1.968693034
H	4.177919624	-5.733460070	0.281189751
H	2.172673719	-4.639576230	-0.718619836
C	-4.376687543	-1.353423665	1.335150296
C	-5.726834930	-1.438043881	1.673163547
C	-6.726171177	-1.014142503	0.785776456
C	-6.329716349	-0.491008553	-0.453139488
C	-4.982607927	-0.400695230	-0.802391941
H	-3.604468433	-1.671747036	2.034037039
H	-6.010542365	-1.837010558	2.648880454
C	-8.185825746	-1.138353005	1.143935666

H	-7.089272219	-0.142997721	-1.155838770
H	-4.678643650	0.018638191	-1.760456122
H	-8.781873355	-0.339164700	0.684220616
H	-8.597237518	-2.096447560	0.790491775
H	-8.337549990	-1.098839010	2.230278180

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INT_OTs (BP86/ZORA)

C	-5.627039	-0.636771	-0.965404
C	-4.560289	-0.521613	-0.073024
C	-3.397101	-1.273091	-0.253408
C	-3.307354	-2.139235	-1.341573
C	-4.364450	-2.274527	-2.253502
C	-5.521591	-1.510318	-2.046299
S	-4.680391	0.618230	1.306770
O	-6.081413	0.904227	1.534224
C	-4.270472	-3.239174	-3.407815
H	-3.236517	-3.341942	-3.761354
O	-4.042639	1.958722	0.719427
O	-3.832107	0.115202	2.376905
H	-4.615054	-4.241006	-3.109079
H	-4.893839	-2.917219	-4.251441
O	-1.413840	1.998604	0.908996
C	-0.468013	1.643080	-0.238304
C	0.220011	0.651231	0.707860
C	-0.692355	1.011250	1.631400
C	0.259005	2.838348	-0.767791
C	1.077586	3.609555	0.070360
C	1.753720	4.717996	-0.432015
C	1.633395	5.064123	-1.782439
C	0.826052	4.299884	-2.624584
C	0.137544	3.195764	-2.115708
Au	1.791024	-0.597883	0.558391
C	3.390414	-1.859224	0.418340
N	4.460788	-1.769912	-0.426843
C	5.350232	-2.812243	-0.224762
C	4.832855	-3.578484	0.773346
N	3.640453	-2.984690	1.152420
C	4.638509	-0.708469	-1.411359
C	2.761653	-3.488563	2.201883
H	5.208346	-4.480961	1.237838
H	6.262400	-2.919828	-0.797169
H	1.888789	-2.829589	2.249524
H	2.438695	-4.509764	1.966485
H	3.280281	-3.480182	3.168180
H	3.799167	-0.013516	-1.306947

H	5.579755	-0.176877	-1.227154
H	4.644762	-1.127258	-2.425052
H	-1.005531	0.764426	2.642853
H	-1.076742	1.167542	-1.019404
H	-3.024760	1.939713	0.811909
H	0.723139	4.567312	-3.676357
H	2.166167	5.930917	-2.173940
H	-0.505431	2.605701	-2.770889
H	2.380743	5.316580	0.229182
H	1.175257	3.328261	1.118813
H	-2.573609	-1.180870	0.454150
H	-2.396699	-2.723323	-1.483378
H	-6.356364	-1.600410	-2.743086
H	-6.529223	-0.049892	-0.801670

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TS2_OTs (BP86/ZORA)

C	-6.097615	-1.120267	-0.757437
C	-4.844140	-1.254292	-0.158214
C	-3.792197	-1.861837	-0.845601
C	-4.000604	-2.328796	-2.142407
C	-5.249383	-2.203925	-2.767826
C	-6.290370	-1.592743	-2.054106
S	-4.584745	-0.630044	1.505281
O	-5.871774	-0.614115	2.173094
C	-5.476823	-2.744449	-4.156519
H	-4.558746	-2.707864	-4.756845
O	-4.167534	0.874296	1.264879
O	-3.463105	-1.364421	2.078691
H	-5.801486	-3.795596	-4.118786
H	-6.256935	-2.180586	-4.683545
O	-1.676860	1.310018	1.007120
C	-0.342407	1.596831	-0.393340
C	0.315051	0.566877	0.425604
C	-0.748954	0.351613	1.247838
C	0.139864	2.949542	-0.623628
C	1.164300	3.497592	0.172695
C	1.602483	4.799014	-0.046023
C	1.018489	5.575029	-1.053284
C	-0.007188	5.047656	-1.844190
C	-0.445240	3.745046	-1.628605
Au	2.172279	-0.218252	0.292658
C	4.027728	-1.055271	0.171951
N	5.010416	-0.806419	-0.746076
C	6.130721	-1.585915	-0.508253
C	5.852402	-2.345588	0.585234

N	4.569686	-2.010334	0.986498
C	4.885280	0.152357	-1.836940
C	3.881881	-2.595817	2.131720
H	6.450648	-3.084146	1.102777
H	7.017555	-1.536331	-1.126589
H	2.892438	-2.132616	2.199491
H	3.770471	-3.678126	1.994500
H	4.443328	-2.397235	3.052623
H	3.897365	0.617342	-1.758493
H	5.661363	0.923127	-1.755750
H	4.974210	-0.358301	-2.803607
H	-0.977113	-0.419768	1.986455
H	-1.093865	1.259150	-1.115007
H	-3.123049	0.989373	1.154375
H	-0.463938	5.656884	-2.623752
H	1.358504	6.597880	-1.217169
H	-1.250296	3.327126	-2.234585
H	2.394664	5.219482	0.573407
H	1.595858	2.879282	0.959442
H	-2.824568	-1.974689	-0.358932
H	-3.177263	-2.805073	-2.677435
H	-7.271311	-1.487754	-2.520412
H	-6.910860	-0.657211	-0.200987

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PC_OTs (BP86/ZORA)

C	-6.508003	-1.737312	-0.150672
C	-5.176511	-1.596565	-0.548320
C	-4.858459	-0.954340	-1.744999
C	-5.883267	-0.444909	-2.541799
C	-7.226875	-0.567469	-2.163116
C	-7.519586	-1.221392	-0.956626
S	-3.870437	-2.229306	0.504899
O	-4.378771	-3.402297	1.189123
C	-8.331076	-0.038108	-3.041807
H	-7.982119	0.793115	-3.667268
O	-3.706164	-1.096337	1.595398
O	-2.654479	-2.315600	-0.298150
H	-8.704748	-0.823335	-3.716704
H	-9.183794	0.312263	-2.446212
O	-1.988962	0.718246	1.087358
C	0.003064	2.513296	0.173826
C	0.245909	1.177664	0.321584
C	-0.934071	0.339701	0.537347
C	0.932504	3.622581	-0.009195
C	2.325188	3.521754	0.184231

C	3.153314	4.625399	0.013863
C	2.616464	5.863271	-0.358718
C	1.238601	5.986896	-0.547152
C	0.409150	4.882412	-0.367970
Au	1.992503	0.106326	0.204739
C	3.656224	-1.080801	0.071792
N	4.796874	-0.874989	-0.649837
C	5.680533	-1.931260	-0.503245
C	5.083073	-2.825903	0.329858
N	3.852290	-2.291975	0.670638
C	5.043489	0.299678	-1.478508
C	2.882392	-2.945523	1.545158
H	5.425655	-3.782819	0.701592
H	6.643249	-1.958918	-0.996770
H	2.020376	-2.279166	1.647145
H	2.557635	-3.895939	1.105778
H	3.326480	-3.125888	2.531163
H	4.163111	0.946526	-1.414072
H	5.925958	0.840689	-1.116307
H	5.198937	-0.000522	-2.521622
H	-0.874236	-0.715848	0.207928
H	-1.050875	2.819760	0.166373
H	-3.006711	-0.362805	1.315376
H	0.809281	6.948106	-0.829919
H	3.268881	6.726159	-0.492545
H	-0.668177	4.983068	-0.508109
H	4.226835	4.528598	0.179744
H	2.743454	2.558201	0.484720
H	-3.816303	-0.865496	-2.046777
H	-5.632794	0.057812	-3.477255
H	-8.559143	-1.329105	-0.643097
H	-6.741254	-2.252646	0.779628

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RC_OTs (BP86/ZORA/D3)

N	-0.240275654	3.829970776	-0.034639878
C	0.235836015	2.689923903	-0.616943273
N	0.831687655	3.108712598	-1.767172502
C	0.729859225	4.480646851	-1.897825421
C	0.055759151	4.937588417	-0.806121440
AU	0.038357381	0.824202128	0.125208203
C	0.059316802	-0.923823906	1.436774070
C	-0.664783600	-1.270387317	0.495391013
C	-1.471873083	-1.988519141	-0.537178418
O	-1.003139378	-3.307995790	-0.639847060
C	1.511860187	2.248510811	-2.739183306

C	-0.972828303	3.874249327	1.224994956
C	-2.939420397	-1.931581919	-0.138264910
C	-3.601005668	-0.699467489	-0.130022013
C	-4.943017211	-0.625237163	0.236019528
C	-5.632738501	-1.786132141	0.596990975
C	-4.972454054	-3.014741613	0.585980929
C	-3.626627015	-3.090644666	0.219506971
O	1.195794755	-3.066828596	-2.137520386
S	1.777019126	-1.700285683	-2.205167904
C	2.601612261	-1.471690588	-0.616591173
O	0.711455128	-0.650897929	-2.215384790
O	2.800197652	-1.502542089	-3.230505028
H	1.137487095	5.007209822	-2.750371815
H	-0.238254061	5.938821393	-0.521173037
H	1.237786013	1.198346219	-2.560780557
H	1.199668462	2.539781676	-3.747259072
H	2.596694520	2.375242976	-2.644695808
H	-1.088717846	2.844100294	1.576774858
H	-0.413297376	4.457032091	1.965724906
H	-1.959616497	4.324223554	1.067603961
H	0.671336686	-0.917106704	2.319016078
H	-1.327167311	-1.443252827	-1.484540665
H	-0.181705355	-3.274686463	-1.223312784
H	-5.455417869	0.336704656	0.233848180
H	-6.683289180	-1.731187750	0.881108087
H	-3.057963570	0.204570136	-0.413515297
H	-5.507784037	-3.923132112	0.861878028
H	-3.099716919	-4.041987949	0.195535625
C	3.132833053	-0.219879674	-0.290545415
C	3.689112276	-0.003847437	0.966184948
C	3.740705914	-1.032743497	1.920456366
C	3.226745854	-2.285101514	1.566462869
C	2.658513704	-2.507459295	0.310060779
H	3.110982175	0.580992992	-1.026923858
H	4.093698406	0.978958026	1.214085659
C	4.357435826	-0.794194051	3.274173965
H	3.264291572	-3.102157231	2.288699162
H	2.236349826	-3.475146928	0.046884317
H	4.192632005	-1.646908183	3.943758793
H	5.443104690	-0.639929845	3.190872813
H	3.941165177	0.103225949	3.753116819

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TS1_OTs (BP86/ZORA/D3)

N	2.416902562	-3.311457925	-0.681086117
C	1.359813465	-2.533091739	-0.314214788

N	0.259035694	-3.278233817	-0.602649358
C	0.621514026	-4.497887968	-1.141928973
C	1.983465264	-4.523633770	-1.189768040
AU	1.345482522	-0.647815822	0.414959975
C	0.723977408	1.519118507	2.200438837
C	1.083444629	1.287174303	1.003779213
C	0.729322189	2.519108505	0.205806661
O	-0.004012178	3.313897032	1.208566833
C	-1.120729498	-2.820620441	-0.414287967
C	3.811524250	-2.914024042	-0.544165821
C	1.919062177	3.258759111	-0.337337511
C	2.772078418	2.610439266	-1.239629091
C	3.868638440	3.280530263	-1.774127478
C	4.126147398	4.605474766	-1.408831072
C	3.279411079	5.250536805	-0.508508632
C	2.178324925	4.580389415	0.030211487
O	-2.246003492	1.976835889	1.069438746
S	-2.244522882	0.572191879	0.551924791
C	-3.944066002	0.293767418	0.048934936
O	-1.957851469	-0.428821853	1.598361645
O	-1.432863135	0.417548557	-0.677996690
H	-0.110628812	-5.237137136	-1.437887990
H	2.667528544	-5.289743531	-1.529074926
H	-1.190170074	-2.195541514	0.483750520
H	-1.432512344	-2.208346803	-1.267105632
H	-1.766874613	-3.697775624	-0.314652699
H	3.827411704	-1.914510567	-0.098195225
H	4.342338398	-3.617211441	0.108079003
H	4.294368096	-2.885698314	-1.527946362
H	0.342892865	1.462974332	3.206179936
H	0.039136888	2.230490125	-0.602366881
H	-0.935866522	2.898962454	1.174977850
H	4.527160713	2.769888099	-2.476565697
H	4.986089153	5.129740420	-1.824764504
H	2.573111201	1.573220390	-1.514292226
H	3.474786574	6.283170824	-0.219912871
H	1.509237907	5.073331021	0.731819171
C	-4.330905218	0.550280866	-1.265998844
C	-5.658937437	0.358554972	-1.643380318
C	-6.616637586	-0.087226400	-0.723179427
C	-6.203020196	-0.346831952	0.591131606
C	-4.878682901	-0.160326950	0.980344759
H	-3.584213768	0.887047154	-1.983055910
H	-5.958201256	0.556259293	-2.673934138
C	-8.057489775	-0.259360162	-1.127126674

H	-6.931278009	-0.705260807	1.320457581
H	-4.555691381	-0.374621871	1.997726812
H	-8.527366067	-1.094472592	-0.591715109
H	-8.639155756	0.645748655	-0.895104251
H	-8.152346164	-0.443046180	-2.204674962

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INT_OTs (BP86/ZORA/D3)

C	-3.081280	-0.896995	-1.107910
C	-3.183812	-1.180356	0.254317
C	-2.361375	-2.138172	0.843885
C	-1.429724	-2.812404	0.059278
C	-1.294211	-2.535373	-1.306236
C	-2.130773	-1.564483	-1.873820
S	-4.426700	-0.371872	1.257864
O	-5.721459	-0.911564	0.896547
C	-0.295466	-3.276598	-2.152329
H	0.528318	-3.672328	-1.546475
O	-4.411729	1.123887	0.721556
O	-3.968541	-0.416960	2.637948
H	-0.769536	-4.126399	-2.665420
H	0.130606	-2.623986	-2.924635
O	-2.196881	2.321500	1.325843
C	-1.422928	2.130887	0.005823
C	-0.576809	1.080755	0.713444
C	-1.315720	1.303195	1.813466
C	-0.807278	3.396964	-0.480976
C	0.264205	3.978887	0.209600
C	0.837521	5.159886	-0.252060
C	0.355543	5.767053	-1.416167
C	-0.706354	5.190167	-2.112833
C	-1.286337	4.010435	-1.643215
Au	0.843718	-0.166110	0.050644
C	2.210680	-1.483082	-0.669796
N	2.800527	-1.491723	-1.900816
C	3.614509	-2.600846	-2.063502
C	3.542272	-3.309811	-0.903784
N	2.683480	-2.613968	-0.067685
C	2.574642	-0.465363	-2.909251
C	2.316152	-3.023542	1.281004
H	4.022700	-4.232918	-0.607962
H	4.168271	-2.788807	-2.973651
H	1.568455	-2.312507	1.647279
H	1.888738	-4.032984	1.264965
H	3.193842	-3.005954	1.937744
H	1.886832	0.270387	-2.479644

H	3.520026	0.023246	-3.172055
H	2.126451	-0.908131	-3.806782
H	-1.449161	0.933150	2.825984
H	-2.136695	1.721324	-0.721068
H	-3.576655	1.629173	1.061041
H	-1.086707	5.660759	-3.019140
H	0.809149	6.689350	-1.778666
H	-2.122304	3.559665	-2.179914
H	1.667810	5.609640	0.292114
H	0.641009	3.486427	1.105261
H	-2.445813	-2.330550	1.911338
H	-0.783282	-3.559980	0.519989
H	-2.035864	-1.328464	-2.934348
H	-3.736126	-0.152768	-1.557824

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TS2_OTs (BP86/ZORA/D3)

C	-4.471847	0.109388	-0.580470
C	-3.885449	-0.647737	0.439477
C	-2.767908	-1.436863	0.184256
C	-2.215795	-1.447078	-1.095976
C	-2.762640	-0.676072	-2.125585
C	-3.906653	0.092807	-1.851018
S	-4.535365	-0.542042	2.107934
O	-5.959242	-0.812986	2.068853
C	-2.146548	-0.675241	-3.498913
H	-1.086303	-0.953247	-3.454606
O	-4.376624	0.995305	2.430028
O	-3.658941	-1.336389	2.957035
H	-2.652215	-1.396685	-4.158071
H	-2.226316	0.311745	-3.972263
O	-1.938412	1.691775	2.221083
C	-1.200218	1.540684	0.397354
C	-0.360384	0.591157	1.141710
C	-1.039643	0.670660	2.313650
C	-0.720164	2.718867	-0.295433
C	0.580571	3.207301	-0.070343
C	1.034912	4.325597	-0.758937
C	0.193691	4.976256	-1.668398
C	-1.104947	4.507599	-1.890868
C	-1.559926	3.385139	-1.207642
Au	1.142647	-0.497140	0.362903
C	2.626852	-1.609115	-0.465388
N	3.260565	-1.398123	-1.657232
C	4.215356	-2.372805	-1.899470
C	4.185066	-3.220276	-0.835075

N	3.211994	-2.740335	0.026726
C	2.959404	-0.284738	-2.547015
C	2.848830	-3.352116	1.298442
H	4.763824	-4.109221	-0.622214
H	4.825565	-2.381180	-2.792819
H	2.035982	-2.759183	1.729864
H	2.507609	-4.381540	1.138941
H	3.707278	-3.348100	1.980287
H	2.185266	0.321887	-2.065368
H	3.856592	0.324467	-2.707691
H	2.589058	-0.656795	-3.509643
H	-1.023578	0.066258	3.222266
H	-2.182753	1.191564	0.070477
H	-3.355451	1.273728	2.416316
H	-1.756275	5.021327	-2.597074
H	0.550027	5.857497	-2.201820
H	-2.567611	3.001860	-1.370259
H	2.042282	4.703003	-0.585156
H	1.209952	2.686218	0.650263
H	-2.317182	-1.999007	0.998002
H	-1.316234	-2.034345	-1.282038
H	-4.350978	0.695204	-2.644659
H	-5.349039	0.717428	-0.365496

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PC_OTs (BP86/ZORA/D3)

C	-3.384262	-1.796734	-0.610926
C	-3.260448	-0.831459	0.391389
C	-2.883637	0.473407	0.076073
C	-2.633098	0.805529	-1.255689
C	-2.736029	-0.146142	-2.274852
C	-3.114616	-1.452466	-1.930826
S	-3.475389	-1.365792	2.087730
O	-4.489737	-2.399282	2.104444
C	-2.471277	0.214472	-3.711721
H	-2.168208	1.263398	-3.812896
O	-4.048606	-0.103926	2.831213
O	-2.141181	-1.671456	2.604355
H	-1.680926	-0.419908	-4.138738
H	-3.367815	0.063893	-4.329117
O	-2.172099	1.570788	3.077759
C	0.573632	2.839130	2.253671
C	0.049076	1.596990	2.223042
C	-1.005350	1.114718	3.080815
C	1.557678	3.389494	1.320692
C	2.461003	2.586471	0.598816

C	3.337505	3.148728	-0.325022
C	3.347519	4.529709	-0.539977
C	2.481234	5.344167	0.192840
C	1.606631	4.781389	1.119406
Au	0.265096	0.145720	0.778199
C	0.330149	-1.161215	-0.777123
N	0.651819	-0.849955	-2.065842
C	0.514869	-1.951804	-2.893335
C	0.103691	-2.981168	-2.102171
N	-0.002344	-2.479605	-0.816545
C	1.036779	0.483294	-2.509079
C	-0.391170	-3.263713	0.351325
H	-0.119662	-4.012273	-2.340826
H	0.720077	-1.911359	-3.954625
H	-0.722705	-2.583494	1.141834
H	-1.222066	-3.923336	0.081176
H	0.457373	-3.862792	0.702722
H	1.185005	1.106482	-1.621177
H	1.968588	0.431577	-3.083196
H	0.244135	0.919244	-3.127826
H	-0.788154	0.208041	3.679348
H	0.227877	3.535641	3.026376
H	-3.276649	0.565531	3.073093
H	2.490385	6.423771	0.043840
H	4.040145	4.969688	-1.256919
H	0.928891	5.421040	1.686199
H	4.036595	2.508997	-0.864434
H	2.479870	1.513231	0.794446
H	-2.796499	1.230575	0.853213
H	-2.344764	1.828306	-1.499267
H	-3.215206	-2.206078	-2.712713
H	-3.708442	-2.802026	-0.347673

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RC_OTs (BP86/ZORA/D3/COSMO)

N	-1.298193858	-3.539002007	0.464467861
C	-1.176619722	-2.355039369	-0.199432036
N	-1.888383340	-2.518027558	-1.346902034
C	-2.444300216	-3.781867935	-1.398703279
C	-2.075604127	-4.425345935	-0.255473297
AU	-0.148541493	-0.743015395	0.438736766
C	0.659572507	0.905968849	1.617985904
C	1.395422085	0.852117208	0.625120629
C	2.353607738	1.123958697	-0.485139729
O	2.536829961	2.515552905	-0.585988806
C	-2.048077007	-1.513060037	-2.398104578

C	-0.693865492	-3.835408113	1.759245358
C	3.671700275	0.404809350	-0.230131482
C	3.685861358	-0.985059571	-0.071361994
C	4.889269489	-1.656371065	0.135553533
C	6.089664511	-0.941023201	0.186355894
C	6.075181482	0.444716719	0.027358647
C	4.869053361	1.118911123	-0.180335997
O	0.337598217	3.456948592	-1.737514005
S	-0.793432544	2.495646850	-1.874473490
C	-1.595074450	2.479382006	-0.267042922
O	-0.320849273	1.101922458	-2.075376488
O	-1.813312229	2.922914522	-2.840814706
H	-3.042238796	-4.112291270	-2.237297630
H	-2.293885196	-5.423315654	0.099842603
H	-1.443381702	-0.630460939	-2.158636731
H	-1.712612532	-1.933309190	-3.351749897
H	-3.104075857	-1.231824313	-2.476385048
H	-0.070571370	-2.982327195	2.042941746
H	-1.474548158	-3.986322390	2.512501294
H	-0.074492380	-4.734918790	1.681144279
H	0.173944526	1.189181007	2.533619608
H	1.894147069	0.723682389	-1.404631606
H	1.714391024	2.890130907	-1.032110528
H	4.893138967	-2.739444330	0.255211984
H	7.031808735	-1.464334992	0.347433833
H	2.747937320	-1.543044304	-0.110032699
H	7.007172486	1.008510696	0.063182865
H	4.847024497	2.198235005	-0.311586299
C	-2.548055970	1.493901941	0.007903533
C	-3.124656413	1.420089662	1.271448230
C	-2.772099254	2.329955265	2.281495382
C	-1.831205356	3.320846354	1.978893127
C	-1.241124832	3.398295717	0.715639450
H	-2.832182108	0.785786322	-0.768052145
H	-3.858621130	0.640979110	1.481696225
C	-3.409128400	2.249359646	3.643064585
H	-1.545726198	4.040846445	2.747088174
H	-0.490197802	4.153779608	0.493547721
H	-2.894996431	2.896931234	4.362955203
H	-4.462183635	2.563906245	3.601807795
H	-3.395047801	1.221383595	4.030233988

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TS1_OTs (BP86/ZORA/D3/COSMO)

N	2.335184228	3.657757341	0.538096780
C	1.316928661	2.811278639	0.226165474

N	0.181183951	3.492649830	0.533566019
C	0.484863470	4.746726019	1.031099555
C	1.843624386	4.853258872	1.032670868
AU	1.384904589	0.910513844	-0.460465984
C	0.851897083	-1.432587739	-2.119991855
C	1.205300011	-1.053635695	-0.958373417
C	1.009061738	-2.252137253	-0.059943727
O	0.349362734	-3.196251060	-0.984452878
C	-1.173092307	2.951368507	0.406785705
C	3.749675749	3.344629224	0.371049966
C	2.297575537	-2.805672516	0.483225197
C	3.075045864	-2.006663612	1.332063978
C	4.271263828	-2.491895560	1.853667041
C	4.704327177	-3.782138342	1.530780788
C	3.932418164	-4.577908464	0.684944030
C	2.732297713	-4.092126098	0.157967259
O	-2.080090797	-2.222797458	-0.907050454
S	-2.312543246	-0.836675702	-0.375195851
C	-4.046120523	-0.843032102	0.076997785
O	-2.160524919	0.201101954	-1.411127135
O	-1.553472646	-0.577596777	0.863782221
H	-0.281169462	5.447845002	1.333759809
H	2.492386863	5.665340193	1.331837442
H	-1.154954076	2.068974036	-0.241604889
H	-1.547979627	2.653751638	1.391815340
H	-1.824887805	3.716617712	-0.025507712
H	3.822711528	2.338268009	-0.051435891
H	4.215318944	4.064244424	-0.310844114
H	4.256454790	3.373951174	1.341692878
H	0.504377167	-1.530576838	-3.135252002
H	0.311879083	-1.995112593	0.751747332
H	-0.627241494	-2.901637137	-0.953866122
H	4.870237924	-1.863571949	2.512593219
H	5.641637240	-4.161498399	1.936721172
H	2.740292001	-0.996684490	1.574829003
H	4.263981216	-5.584034751	0.428945973
H	2.125770665	-4.707869765	-0.502356604
C	-4.425104603	-1.097963347	1.394287241
C	-5.779154161	-1.131908823	1.725796953
C	-6.768390615	-0.916817660	0.757044970
C	-6.362853084	-0.653508964	-0.559944101
C	-5.014061315	-0.614950139	-0.903267564
H	-3.657898791	-1.257145919	2.149973298
H	-6.073509056	-1.325657832	2.758173638
C	-8.229519005	-0.989283705	1.112505758

H	-7.116843642	-0.470489646	-1.326751679
H	-4.704366373	-0.398308057	-1.924372798
H	-8.820863284	-0.282741609	0.516455528
H	-8.627242114	-1.996240531	0.915494228
H	-8.393611060	-0.772097515	2.175087492

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INT_OTs (BP86/ZORA/D3/COSMO)

C	1.529033301	1.784677250	-1.849133823
C	1.781934269	2.345744380	-0.596104127
C	0.754103148	2.909770715	0.156640997
C	-0.539037134	2.913375624	-0.358411130
C	-0.823952537	2.351595804	-1.608787793
C	0.227847717	1.780356657	-2.339757945
S	3.450971678	2.427246733	0.022608705
O	4.190679570	3.384803055	-0.783201479
C	-2.217455894	2.382644034	-2.171714414
H	-2.966486204	2.517761463	-1.383187906
O	4.063220430	1.013114655	-0.319305722
O	3.383521528	2.614627154	1.465301053
H	-2.329139359	3.212999731	-2.884220969
H	-2.445739724	1.456595386	-2.712881744
O	2.983947586	-0.857187981	1.005002661
C	1.943077393	-1.346493814	-0.041238770
C	0.859689395	-0.731496811	0.830105025
C	1.824481140	-0.328445388	1.672201629
C	2.054902846	-2.814284744	-0.257629601
C	1.454587431	-3.719475947	0.626608794
C	1.611606135	-5.091121920	0.438083955
C	2.366109873	-5.569945371	-0.637092468
C	2.960780177	-4.672869171	-1.526921871
C	2.802925386	-3.300054253	-1.337489902
AU	-1.095676885	-0.401090280	0.532298648
C	-3.041463920	0.055250483	0.162693103
N	-3.825426113	-0.379223075	-0.864619362
C	-5.064364139	0.238998248	-0.847072996
C	-5.063573558	1.082669832	0.221748090
N	-3.822239344	0.957155192	0.823950716
C	-3.390676506	-1.349355330	-1.862288805
C	-3.395721745	1.687189474	2.011668622
H	-5.827409196	1.749102502	0.599342549
H	-5.827851890	0.030800014	-1.584484784
H	-2.337301609	1.462925518	2.176391390
H	-3.525384048	2.763737526	1.855459335
H	-3.978532896	1.369819291	2.883433610
H	-2.356385213	-1.621027083	-1.629578578

H	-4.024423096	-2.242077731	-1.825288615
H	-3.437669414	-0.906479586	-2.863609078
H	1.961867809	0.254954291	2.578141473
H	2.149251554	-0.784143717	-0.961646644
H	3.673826248	0.261797597	0.306925170
H	3.548597789	-5.042568271	-2.366623060
H	2.488679302	-6.643021931	-0.782533990
H	3.269767302	-2.595144295	-2.026768185
H	1.144519712	-5.791571734	1.129908464
H	0.865376360	-3.332203071	1.457033481
H	0.970571741	3.326178167	1.137709326
H	-1.345864477	3.352613701	0.227811427
H	0.024443612	1.328576928	-3.310829379
H	2.342689945	1.354448186	-2.430549195

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TS2_OTs (BP86/ZORA/D3/COSMO)

C	3.591409923	-0.208284168	-1.939218907
C	3.182047847	0.921692713	-1.221539799
C	1.915407592	1.462841257	-1.420293361
C	1.044652578	0.856574128	-2.326337411
C	1.419473309	-0.289774532	-3.035157141
C	2.711082452	-0.806659069	-2.834564160
S	4.281698676	1.623719292	0.010133231
O	5.549186037	1.915372836	-0.661940651
C	0.463710778	-0.969526437	-3.977714630
H	-0.348972557	-0.296757876	-4.275570628
O	4.470210492	0.485323859	1.003747384
O	3.566428781	2.756774122	0.605330068
H	0.975984033	-1.313006318	-4.885365346
H	0.013011926	-1.855473375	-3.505387732
O	2.421161309	-0.463064446	1.980802431
C	1.252128089	-1.190776845	0.621313350
C	0.410035946	-0.097975448	1.147332637
C	1.313334430	0.424938329	1.984792014
C	1.008988193	-2.604653253	0.778025710
C	0.012363018	-3.081899773	1.650556005
C	-0.190319687	-4.448974562	1.787823726
C	0.602247246	-5.348963133	1.065124853
C	1.597048594	-4.885320047	0.198129807
C	1.798940557	-3.518147363	0.052763641
AU	-1.424569857	0.397407648	0.467627417
C	-3.241438545	0.940689137	-0.267669792
N	-3.715344613	0.737683159	-1.529441979
C	-4.980789753	1.278279593	-1.680856191
C	-5.311804857	1.834630166	-0.482819769

N	-4.239419358	1.618259277	0.365692722
C	-2.969675788	0.057949190	-2.581218313
C	-4.181443675	2.057082593	1.755686014
H	-6.204260744	2.357250506	-0.166105534
H	-5.527244602	1.222734723	-2.612639468
H	-3.218500272	1.740096643	2.167372180
H	-4.261312504	3.148214177	1.808291608
H	-4.995250026	1.598619896	2.327872744
H	-2.023657192	-0.281985426	-2.148708708
H	-3.536839834	-0.802965146	-2.950629794
H	-2.768592654	0.749195556	-3.407072750
H	1.377302630	1.317182166	2.601705494
H	1.928630580	-0.931712553	-0.198068133
H	3.340690560	0.013144123	1.572453794
H	2.209953137	-5.592467091	-0.358655922
H	0.443226468	-6.420939557	1.179923198
H	2.569368457	-3.135446564	-0.616745244
H	-0.961700316	-4.823067589	2.459429023
H	-0.588899195	-2.362289404	2.204432758
H	1.613508690	2.335788552	-0.846725293
H	0.051418318	1.281345646	-2.472930616
H	3.028611646	-1.689366857	-3.390870127
H	4.589614523	-0.615417671	-1.784648919

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PC_OTs (BP86/ZORA/D3/COSMO)

C	-3.346453114	-0.671840616	-1.013653675
C	-2.631575035	0.524435374	-1.123338083
C	-1.431607440	0.572323097	-1.831513889
C	-0.951422162	-0.591408390	-2.432886643
C	-1.642572013	-1.802924710	-2.329117661
C	-2.846796427	-1.823967430	-1.609089029
S	-3.256408546	1.936665961	-0.225888727
O	-4.699665772	1.969123364	-0.385892216
C	-1.131334290	-3.052641636	-2.991408324
H	-0.101344412	-2.926670291	-3.344733760
O	-2.662106455	3.184441846	-0.965209919
O	-2.712550081	1.863790876	1.129616497
H	-1.166986244	-3.906935566	-2.302012459
H	-1.751703226	-3.316587096	-3.859906591
O	-0.230507143	3.362284741	-0.463755597
C	2.542093508	2.162304704	-0.063877830
C	1.331553921	1.817783489	0.428485173
C	0.220647319	2.726314932	0.522579808
C	3.657117201	1.268415694	-0.363718256
C	3.790588897	-0.014078189	0.201449737

C	4.837284724	-0.852593848	-0.169687529
C	5.787147157	-0.426172524	-1.103661135
C	5.686051993	0.855001070	-1.652006526
C	4.640330711	1.695516425	-1.277265397
AU	0.500610109	-0.036048826	0.767215186
C	-0.371275721	-1.866478691	0.937661809
N	0.093702548	-3.035919952	0.415218278
C	-0.785775609	-4.076080785	0.663221349
C	-1.827495636	-3.544508936	1.361895114
N	-1.554810501	-2.196911306	1.520311694
C	1.351288917	-3.166452689	-0.309361168
C	-2.413719800	-1.256794114	2.232920650
H	-2.728345546	-4.000811116	1.749189910
H	-0.599272871	-5.086574968	0.325676842
H	-2.173377795	-0.241280584	1.906271059
H	-3.459167241	-1.471238624	1.991638834
H	-2.259364481	-1.347854110	3.314069606
H	1.774179642	-2.164669567	-0.433141711
H	2.049979466	-3.793448778	0.255399854
H	1.171018910	-3.610920317	-1.293294887
H	-0.332761107	2.769633155	1.478519237
H	2.724705646	3.218068065	-0.296953924
H	-1.658083754	3.363901012	-0.659359185
H	6.427471698	1.201566951	-2.371860537
H	6.610113741	-1.080986576	-1.388374194
H	4.561633719	2.693734506	-1.709610277
H	4.927195596	-1.838958072	0.285479287
H	3.068218309	-0.333585053	0.954996510
H	-0.875692628	1.503005455	-1.921558143
H	-0.013531211	-0.551613650	-2.986665451
H	-3.404751256	-2.756409654	-1.521132378
H	-4.291171763	-0.691393772	-0.473414463

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RC_BF4 (BP86/ZORA)

N	-2.739435	-0.989402	0.424742
C	-1.813966	-0.319848	1.169651
N	-1.973142	-0.783784	2.436907
C	-2.975475	-1.731105	2.482820
C	-3.456978	-1.865781	1.215506
Au	-0.455807	1.023245	0.496760
C	0.648187	2.830299	0.066536
C	1.283648	1.981101	-0.575058
C	2.275490	1.245139	-1.417179
O	3.474161	1.026518	-0.718220
C	-1.191697	-0.364935	3.603154

C	-2.916327	-0.843727	-1.016508
C	1.668028	0.016777	-2.094525
C	1.504444	-1.187164	-1.396876
C	0.970900	-2.300304	-2.049085
C	0.593053	-2.222466	-3.392176
C	0.753020	-1.022937	-4.088262
C	1.291806	0.090065	-3.439980
H	-4.232768	-2.505993	0.816758
H	-3.254583	-2.230095	3.401459
H	-2.293905	-0.008764	-1.351645
H	-2.596838	-1.757492	-1.530730
H	-3.968580	-0.636328	-1.242388
H	-0.379867	0.289707	3.273386
H	-1.846250	0.152628	4.314322
H	-0.743478	-1.247984	4.069419
H	0.358213	3.754945	0.531616
H	2.525813	1.965327	-2.216377
H	0.474756	-0.957032	-5.140201
H	0.189404	-3.099011	-3.899732
H	1.432387	1.022068	-3.990725
H	0.861680	-3.236828	-1.502043
H	1.802689	-1.269779	-0.351274
H	3.322183	0.483827	0.102169
B	2.221111	-0.575904	2.485777
F	2.732656	-1.107242	3.658707
F	1.209969	-1.420643	1.942524
F	1.660483	0.715743	2.712303
F	3.261040	-0.444492	1.496408

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TS1_BF4 (BP86/ZORA)

N	3.857559	-0.835506	-0.326855
C	2.720199	-0.087163	-0.397308
N	2.987656	0.870226	-1.328807
C	4.269176	0.722707	-1.826455
C	4.819019	-0.351997	-1.196770
Au	0.967796	-0.298603	0.608593
C	-1.203508	0.753326	1.966159
C	-0.913237	-0.363558	1.421596
C	-2.209585	-1.134980	1.320629
O	-3.178594	-0.085086	1.754860
C	2.057339	1.922540	-1.750392
C	4.037885	-1.985753	0.552063
C	-2.564112	-1.774751	0.005750
C	-2.397524	-1.093141	-1.208899
C	-2.774554	-1.701828	-2.404790

C	-3.313417	-2.991327	-2.403526
C	-3.478783	-3.674625	-1.198063
C	-3.105296	-3.066868	0.001106
H	5.796766	-0.805320	-1.293911
H	4.677489	1.385583	-2.578138
H	3.114989	-2.118391	1.124880
H	4.233818	-2.887107	-0.040635
H	4.873295	-1.807572	1.239379
H	1.096954	1.793537	-1.239814
H	2.472884	2.904525	-1.497334
H	1.897809	1.857667	-2.832446
H	-1.300908	1.822641	2.141529
H	-2.250633	-1.890859	2.115947
H	-3.901427	-4.679263	-1.189615
H	-3.607025	-3.461577	-3.342152
H	-3.239926	-3.597681	0.944942
H	-2.651029	-1.162503	-3.343691
H	-1.989295	-0.081563	-1.217137
H	-3.294741	0.553506	0.993077
B	-2.180450	2.838649	-0.331608
F	-2.661216	3.852914	-1.134952
F	-1.116777	2.134250	-0.971070
F	-1.716465	3.339755	0.918551
F	-3.237983	1.878523	-0.062440

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INT_BF4 (BP86/ZORA)

N	4.358907	-0.400560	0.018350
C	3.255387	0.294191	-0.385593
N	3.708011	1.079458	-1.406472
C	5.058931	0.878190	-1.631692
C	5.470098	-0.057264	-0.733215
Au	1.352545	0.199183	0.346848
C	-1.488345	1.045735	1.316732
C	-0.552428	0.143040	1.011919
C	-1.520891	-0.983754	1.335086
O	-2.580652	0.153269	1.707617
C	2.874111	2.010783	-2.161246
C	4.362204	-1.378633	1.100586
C	-2.010613	-1.936965	0.304350
C	-2.203992	-1.539419	-1.027726
C	-2.656231	-2.460245	-1.968704
C	-2.903012	-3.785088	-1.597293
C	-2.710529	-4.188519	-0.275027
C	-2.272045	-3.264854	0.673103
H	6.444186	-0.499182	-0.568920

H	5.606296	1.407849	-2.400489
H	3.351273	-1.416329	1.518336
H	4.637721	-2.368097	0.716405
H	5.070819	-1.075777	1.880613
H	1.850165	1.927620	-1.783678
H	3.233322	3.037390	-2.022820
H	2.893190	1.753481	-3.226730
H	-1.672927	2.113185	1.366300
H	-1.343377	-1.482630	2.296068
H	-2.908730	-5.218903	0.019205
H	-3.253408	-4.502445	-2.339550
H	-2.127816	-3.573425	1.709773
H	-2.823032	-2.140910	-2.996850
H	-2.028388	-0.503379	-1.314637
H	-3.485984	0.256468	1.038550
B	-4.442532	1.781309	-0.488992
F	-5.719196	1.995156	-0.934232
F	-3.519053	1.545770	-1.499825
F	-3.988622	2.725837	0.426837
F	-4.502837	0.443834	0.326412

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TS2_BF4 (BP86/ZORA)

N	-4.241468	-0.513369	0.319167
C	-3.102113	0.228065	0.441605
N	-3.445165	1.236968	1.294459
C	-4.766251	1.126219	1.691984
C	-5.269461	0.021218	1.077600
Au	-1.278226	-0.058168	-0.425551
C	1.355707	0.657800	-1.864602
C	0.580408	-0.217134	-1.222269
C	1.538355	-1.343518	-1.173597
O	2.616627	0.015534	-2.088096
C	-2.537476	2.297172	1.728360
C	-4.355889	-1.711862	-0.504037
C	2.169625	-1.885315	0.006814
C	2.202702	-1.164074	1.218961
C	2.825801	-1.714713	2.331503
C	3.412615	-2.981963	2.252973
C	3.391732	-3.704875	1.054623
C	2.781676	-3.156158	-0.065412
H	-6.256294	-0.421271	1.116275
H	-5.231303	1.831729	2.368147
H	-3.393026	-1.867267	-1.000631
H	-4.591172	-2.581024	0.121908
H	-5.140532	-1.578154	-1.258196

H	-1.552620	2.101538	1.292715
H	-2.902622	3.271135	1.382128
H	-2.459531	2.299269	2.821663
H	1.248615	1.676718	-2.224053
H	1.544537	-2.018820	-2.037470
H	3.859575	-4.687089	0.999315
H	3.902340	-3.406341	3.129802
H	2.767397	-3.702121	-1.009656
H	2.872278	-1.147199	3.259774
H	1.785172	-0.159121	1.257704
H	3.302424	0.396381	-1.392269
B	3.723813	2.236240	0.228836
F	4.850750	2.831791	0.756138
F	2.768332	1.932388	1.215869
F	3.147641	2.969421	-0.814819
F	4.152821	0.918976	-0.370606

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PC_BF4 (BP86/ZORA)

N	3.484829	-0.613572	-0.398379
C	2.370199	0.173476	-0.423820
N	2.701773	1.221801	-1.225808
C	3.999628	1.096021	-1.684806
C	4.494872	-0.061207	-1.165785
Au	0.584673	-0.149181	0.516039
C	-1.093100	0.372168	2.513953
C	-1.269995	-0.473353	1.402786
C	-2.340333	-1.200218	1.026002
O	-1.574558	1.558646	2.669912
C	1.821256	2.349510	-1.545050
C	3.596129	-1.870391	0.333548
C	-2.541921	-1.993009	-0.185826
C	-1.737835	-1.872169	-1.333150
C	-1.991307	-2.640024	-2.464135
C	-3.056161	-3.547468	-2.478528
C	-3.872730	-3.670843	-1.353413
C	-3.620772	-2.896791	-0.222579
H	5.463237	-0.530813	-1.278504
H	4.455720	1.830706	-2.335437
H	2.645226	-2.045275	0.846467
H	3.794266	-2.695690	-0.360665
H	4.405261	-1.807334	1.070865
H	0.809345	2.134656	-1.188469
H	2.187184	3.257934	-1.053931
H	1.800677	2.494823	-2.630631
H	-0.436136	0.064114	3.339537

H	-3.181966	-1.240523	1.726966
H	-4.711798	-4.366433	-1.358973
H	-3.253722	-4.145421	-3.368105
H	-4.266214	-2.988290	0.652470
H	-1.365572	-2.522157	-3.348936
H	-0.924486	-1.143049	-1.336707
H	-2.100440	1.906448	1.818280
B	-1.795522	2.999355	-0.346460
F	-2.461642	4.015508	-0.994063
F	-1.444679	1.947086	-1.213805
F	-0.660927	3.442697	0.353831
F	-2.724804	2.423888	0.681885

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RC_BF4 (BP68/ZORA/D3)

N	1.441976	-2.376105	-0.680748
C	1.586037	-1.128851	-0.153622
N	2.740869	-0.648850	-0.681110
C	3.307744	-1.577100	-1.531752
C	2.488712	-2.666489	-1.535181
Au	0.268085	-0.175659	1.033197
C	-0.813480	0.843606	2.615398
C	-1.649115	0.751145	1.706297
C	-2.814034	0.808188	0.779003
O	-2.992746	2.104681	0.271715
C	3.305357	0.673833	-0.414480
C	0.332257	-3.275800	-0.390843
C	-2.724316	-0.305334	-0.263924
C	-1.959148	-0.134774	-1.423184
C	-1.886558	-1.162727	-2.363169
C	-2.573630	-2.360640	-2.155862
C	-3.327925	-2.536344	-0.994127
C	-3.401193	-1.509521	-0.051675
H	2.556399	-3.603890	-2.070551
H	4.228703	-1.381692	-2.064298
H	-0.396894	-2.729813	0.214982
H	-0.148216	-3.584318	-1.324008
H	0.692583	-4.153027	0.159094
H	2.595654	1.243314	0.191187
H	4.263026	0.562640	0.106763
H	3.439016	1.204743	-1.361587
H	-0.319194	1.114812	3.529658
H	-3.695450	0.603216	1.410227
H	-3.873766	-3.465011	-0.829266
H	-2.531606	-3.153080	-2.903484
H	-4.000909	-1.640779	0.850425

H	-1.292632	-1.016589	-3.264717
H	-1.421599	0.794366	-1.602833
H	-2.173415	2.411597	-0.201645
B	0.527559	2.770249	-1.050501
F	1.215412	3.807379	-1.656955
F	0.760916	1.540857	-1.729206
F	0.920602	2.627529	0.311642
F	-0.892514	3.023110	-1.079137

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TS1_BF4 (BP68/ZORA/D3)

N	3.699074	0.799568	0.410423
C	2.595408	0.000894	0.404419
N	2.843023	-0.945415	1.350751
C	4.081075	-0.743606	1.933164
C	4.621970	0.358332	1.342910
Au	0.902672	0.167665	-0.691259
C	-1.339163	-0.844506	-2.063823
C	-0.944786	0.256962	-1.557244
C	-2.172184	1.118913	-1.407833
O	-3.239740	0.138412	-1.768394
C	1.937647	-2.045165	1.690562
C	3.871569	1.967283	-0.444182
C	-2.384577	1.782115	-0.078010
C	-2.102720	1.110798	1.119365
C	-2.333916	1.742444	2.338822
C	-2.841373	3.043724	2.376039
C	-3.122697	3.715259	1.185771
C	-2.893834	3.084584	-0.037186
H	5.567219	0.858379	1.506216
H	4.466685	-1.391863	2.708670
H	2.997319	2.031851	-1.099216
H	3.939614	2.875432	0.165881
H	4.778385	1.858628	-1.049934
H	0.963196	-1.878250	1.219610
H	2.356255	-2.993217	1.334313
H	1.807479	-2.083561	2.777081
H	-1.519776	-1.906495	-2.203431
H	-2.204252	1.870557	-2.206726
H	-3.521193	4.729114	1.208507
H	-3.020241	3.533082	3.333244
H	-3.114926	3.605134	-0.969876
H	-2.121139	1.211955	3.266310
H	-1.720543	0.090280	1.096913
H	-3.354254	-0.467514	-0.980099
B	-2.282307	-2.708313	0.401368

F	-2.752057	-3.640997	1.303346
F	-1.142089	-2.022980	0.924850
F	-1.927040	-3.310499	-0.836314
F	-3.305414	-1.713014	0.142368

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INT_BF4 (BP68/ZORA/D3)

N	4.289504	0.415114	-0.053538
C	3.126860	-0.206071	0.295037
N	3.453779	-0.938802	1.398030
C	4.788538	-0.778271	1.728353
C	5.317365	0.077888	0.811536
Au	1.294281	-0.088882	-0.577635
C	-1.505043	-0.913141	-1.666675
C	-0.577960	-0.022569	-1.312618
C	-1.570464	1.112685	-1.449973
O	-2.648843	-0.011813	-1.885888
C	2.511389	-1.780135	2.128864
C	4.419074	1.320986	-1.187439
C	-2.000462	1.913348	-0.282148
C	-1.996058	1.363491	1.007924
C	-2.405816	2.135335	2.089877
C	-2.805147	3.460800	1.898451
C	-2.806379	4.015231	0.617275
C	-2.409843	3.240368	-0.470762
H	6.320452	0.468594	0.703894
H	5.242439	-1.278602	2.573386
H	3.446882	1.363221	-1.688396
H	4.698103	2.323001	-0.841242
H	5.176777	0.945927	-1.885064
H	1.532541	-1.681356	1.648855
H	2.833650	-2.826949	2.091868
H	2.443380	-1.448975	3.171231
H	-1.674140	-1.974382	-1.805330
H	-1.474196	1.717913	-2.358972
H	-3.122215	5.046778	0.466115
H	-3.123004	4.061773	2.750252
H	-2.414557	3.663404	-1.476208
H	-2.422750	1.697965	3.087182
H	-1.709130	0.323248	1.148476
H	-3.418635	-0.195215	-1.111526
B	-4.020609	-1.866779	0.448817
F	-5.155383	-2.178670	1.151284
F	-2.894845	-1.692429	1.253006
F	-3.759957	-2.719889	-0.622394
F	-4.287259	-0.485661	-0.200406

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TS2_BF4 (BP68/ZORA/D3)

N	-4.011463	0.362664	-0.293055
C	-2.763526	-0.184989	-0.318962
N	-2.818547	-1.115165	-1.314631
C	-4.074317	-1.146425	-1.894868
C	-4.829138	-0.213223	-1.251644
Au	-1.113364	0.210692	0.790201
C	1.508696	-0.556837	2.150584
C	0.704243	0.379908	1.652593
C	1.772957	1.406350	1.485113
O	2.836159	0.053742	2.086246
C	-1.699471	-1.970900	-1.710962
C	-4.417175	1.416537	0.626683
C	2.197462	1.974350	0.214610
C	1.877902	1.350449	-1.004277
C	2.287960	1.925335	-2.200645
C	3.011135	3.121384	-2.194389
C	3.336265	3.747171	-0.987135
C	2.934846	3.172882	0.213267
H	-5.859483	0.084749	-1.392964
H	-4.321658	-1.819535	-2.704929
H	-3.558874	1.644412	1.266238
H	-4.708704	2.314450	0.069188
H	-5.256460	1.076535	1.244532
H	-0.813403	-1.690577	-1.131871
H	-1.944028	-3.020284	-1.512339
H	-1.489796	-1.835141	-2.777500
H	1.453843	-1.580923	2.500298
H	1.941647	2.068058	2.341365
H	3.904203	4.676462	-0.987166
H	3.330890	3.566579	-3.136469
H	3.185145	3.647743	1.162585
H	2.055620	1.432402	-3.143359
H	1.347301	0.400523	-0.996603
H	3.254953	-0.351089	1.213481
B	2.857244	-2.192162	-0.471860
F	3.638053	-2.834652	-1.407716
F	1.632681	-1.751829	-1.026128
F	2.631644	-2.947851	0.679976
F	3.606577	-0.960723	-0.036898

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PC_BF4 (BP68/ZORA/D3)

N	3.025368	1.752587	0.037361
C	2.171783	0.731965	0.336719

N	2.721103	0.127540	1.424160
C	3.900403	0.750090	1.789489
C	4.093286	1.777999	0.916819
Au	0.448462	0.243051	-0.622227
C	-0.932815	-1.020680	-2.520293
C	-1.388120	-0.151261	-1.521793
C	-2.592380	0.343992	-1.198039
O	-0.953251	-2.314153	-2.483879
C	2.164358	-1.046976	2.097267
C	2.830457	2.691556	-1.059492
C	-2.904377	1.201463	-0.054185
C	-2.183283	1.125215	1.149939
C	-2.489742	1.972237	2.210008
C	-3.526409	2.902953	2.093819
C	-4.270690	2.965473	0.914331
C	-3.968777	2.113727	-0.146357
H	4.882701	2.514684	0.851540
H	4.492292	0.415077	2.630796
H	1.891139	2.428624	-1.556265
H	2.766643	3.714791	-0.671878
H	3.659328	2.616046	-1.772829
H	1.110998	-1.154456	1.824854
H	2.698476	-1.948964	1.780282
H	2.257571	-0.913100	3.179809
H	-0.439490	-0.623501	-3.417381
H	-3.434487	0.120347	-1.861711
H	-5.091953	3.675814	0.823001
H	-3.766776	3.562067	2.927621
H	-4.551861	2.161768	-1.066988
H	-1.932561	1.890638	3.142995
H	-1.421814	0.352918	1.262405
H	-1.317103	-2.665948	-1.568460
B	-0.640110	-3.047831	0.741699
F	-0.665955	-4.198468	1.498083
F	-0.879766	-1.897470	1.525396
F	0.566039	-2.897080	0.028232
F	-1.721695	-3.120549	-0.272449

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RC_OTf_preeq

N	3.561632	2.776968	0.583059
C	3.371548	1.615627	-0.106536
N	4.395020	1.569716	-1.007353
C	5.208444	2.682171	-0.879277
C	4.684409	3.442049	0.120026
Au	1.949276	0.278588	0.112161

O	0.441040	-1.109733	0.354529
S	0.278270	-2.259197	-0.648073
O	1.215702	-2.188688	-1.760276
C	4.607533	0.491811	-1.971732
C	2.695483	3.258298	1.655031
O	-1.127543	-2.519823	-0.907236
C	0.857814	-3.721022	0.397673
F	2.146027	-3.549625	0.775184
F	0.771748	-4.856310	-0.323189
F	0.102228	-3.852202	1.504618
C	-3.489213	-0.392714	0.067446
C	-4.341429	0.400431	0.396011
C	-5.343003	1.393603	0.783747
O	-4.912633	2.737924	0.444400
C	-6.739438	1.115570	0.231666
C	-7.822236	1.824561	0.770827
C	-9.109271	1.640307	0.270146
C	-9.330084	0.744022	-0.779901
C	-8.257582	0.033763	-1.319302
C	-6.967876	0.216225	-0.813803
H	6.078864	2.837795	-1.502904
H	5.009553	4.387389	0.533956
H	3.775334	-0.214214	-1.886203
H	4.634967	0.902711	-2.987375
H	5.549730	-0.025026	-1.755034
H	1.897181	2.523772	1.798067
H	3.269108	3.362725	2.583380
H	2.257660	4.224718	1.379191
H	-2.727783	-1.097090	-0.219118
H	-5.405054	1.417507	1.882938
H	-4.801458	2.756983	-0.523505
H	-9.943820	2.194267	0.700513
H	-10.336981	0.597142	-1.170983
H	-7.647795	2.530982	1.583625
H	-8.423577	-0.671436	-2.133930
H	-6.130338	-0.350178	-1.221326

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TS1_OTf_preeq

F	-5.288747	1.688238	-0.908974
C	-4.606960	2.608001	-0.193614
F	-4.240032	3.608667	-1.023011
S	-3.098197	1.831869	0.630027
O	-3.637000	0.754525	1.458267
O	-2.434625	2.936818	1.328865
AU	-0.595986	-0.033463	0.007155

C	1.272974	1.848521	-0.533646
C	2.477658	1.458651	-1.279680
O	3.209582	2.639960	-1.681610
C	-0.301928	-1.920724	0.568037
N	0.426260	-2.909498	-0.026497
C	0.352924	-4.082651	0.707336
C	-0.435618	-3.821588	1.784348
N	-0.834027	-2.499934	1.682912
C	1.161118	-2.761836	-1.275529
C	-1.691552	-1.812873	2.649758
C	0.312687	2.340711	0.035482
C	3.442959	0.579484	-0.502698
C	3.543357	0.648742	0.889616
C	4.481608	-0.131869	1.565517
C	5.327602	-0.985656	0.854812
C	5.233432	-1.056309	-0.536999
C	4.293900	-0.275964	-1.211608
O	-2.333793	1.358782	-0.579604
H	0.854350	-4.990926	0.400527
H	-0.749258	-4.458074	2.601178
H	1.045149	-1.726129	-1.607709
H	2.224213	-2.975753	-1.115923
H	0.753465	-3.437662	-2.037000
H	-1.086584	-1.390899	3.461460
H	-2.238781	-1.007256	2.145482
H	-2.406556	-2.532741	3.061472
H	-0.505124	2.851697	0.527993
H	2.158823	0.904598	-2.182178
H	2.572485	3.251116	-2.095109
H	5.896677	-1.714721	-1.098072
H	6.061557	-1.593168	1.384244
H	4.227976	-0.319790	-2.299972
H	4.553864	-0.071287	2.651322
H	2.880311	1.314025	1.442317
F	-5.430802	3.114308	0.747911

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INT_OTf_preeq

F	-5.174996	-0.388656	1.350817
C	-4.369371	0.493433	0.721038
F	-4.957238	0.854290	-0.440295
S	-2.688710	-0.291932	0.404827
O	-2.152932	-0.579963	1.734218
O	-1.999173	0.849191	-0.298198
Au	0.285488	0.734941	-0.521896
C	1.959930	1.934194	-0.792128

C	3.381637	1.538259	-0.981351
O	4.252711	2.660954	-0.805723
C	0.280527	-1.317503	-0.347432
N	-0.078599	-2.250230	-1.265800
C	-0.033603	-3.519691	-0.718195
C	0.383024	-3.373114	0.571018
N	0.575959	-2.020064	0.774131
C	-0.633151	-1.924772	-2.573612
C	0.920755	-1.398585	2.047030
C	0.975776	2.726287	-0.689843
C	3.783193	0.440782	-0.014061
C	4.190003	0.753177	1.285632
C	4.526660	-0.267888	2.173955
C	4.447378	-1.603602	1.773584
C	4.031468	-1.916428	0.478868
C	3.704119	-0.895155	-0.412414
O	-2.969406	-1.435311	-0.461800
H	-0.309459	-4.401741	-1.279453
H	0.549534	-4.103790	1.350407
H	-0.174147	-0.995566	-2.925094
H	-0.410880	-2.735757	-3.274196
H	-1.715498	-1.780890	-2.472810
H	1.590151	-0.554503	1.856126
H	0.001203	-1.048233	2.529396
H	1.437149	-2.131773	2.672117
H	0.524639	3.704391	-0.653162
H	3.472471	1.135005	-2.007062
H	3.884833	3.402046	-1.317534
H	3.966323	-2.955627	0.158895
H	4.713508	-2.398782	2.469400
H	3.379479	-1.137668	-1.424292
H	4.852014	-0.019889	3.183742
H	4.253215	1.796714	1.588450
F	-4.248516	1.591357	1.497972

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TS2_OTf_preeq

F	-5.426644	0.887032	1.052955
C	-4.408950	1.609227	0.528994
F	-4.844403	2.172396	-0.622942
S	-2.902672	0.516924	0.220956
O	-2.566323	0.007080	1.557770
O	-1.917987	1.475498	-0.336111
Au	0.502060	-0.118563	-0.497158
C	2.016789	1.419736	-0.979157
C	3.458596	1.155556	-1.231825

O	4.086024	2.344857	-1.735951
C	-0.358488	-1.900577	-0.076614
N	-1.056776	-2.701815	-0.923824
C	-1.635660	-3.745237	-0.233561
C	-1.278097	-3.600286	1.073990
N	-0.490849	-2.471336	1.149804
C	-1.332627	-2.383613	-2.322721
C	-0.037814	-1.858447	2.396317
C	0.920984	1.986173	-0.849067
C	4.193970	0.730422	0.027414
C	4.260169	1.590531	1.129653
C	4.955012	1.205923	2.274459
C	5.583395	-0.041486	2.328944
C	5.518151	-0.901322	1.232305
C	4.826979	-0.513637	0.082483
O	-3.385669	-0.484707	-0.739171
H	-2.254666	-4.487254	-0.719353
H	-1.524030	-4.193612	1.944270
H	-0.470738	-1.854414	-2.740363
H	-1.498413	-3.313578	-2.875808
H	-2.219103	-1.737778	-2.363426
H	0.917830	-1.355918	2.219040
H	-0.788390	-1.125308	2.717200
H	0.092158	-2.640120	3.151335
H	0.043465	2.606683	-0.761403
H	3.529677	0.335835	-1.966882
H	3.605105	2.623972	-2.535992
H	6.010996	-1.872681	1.267091
H	6.125785	-0.340486	3.225766
H	4.782934	-1.182135	-0.778453
H	5.006653	1.880760	3.128581
H	3.771303	2.563363	1.085172
F	-4.113772	2.607096	1.396296

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PC_OTf_preeq

C	5.047340	0.413342	0.091603
C	4.139931	1.474102	0.041184
C	4.013640	2.330505	1.141203
C	4.790886	2.123973	2.278858
C	5.693781	1.057944	2.329224
C	5.820609	0.201813	1.235170
C	3.308878	1.706990	-1.209080
O	3.631109	3.007195	-1.725724
C	1.850281	1.620995	-0.936412
C	0.650068	1.902544	-0.798390

Au	0.763126	-0.240748	-0.397539
C	0.139755	-2.100597	0.080602
N	-0.404274	-3.023755	-0.754743
C	-0.914810	-4.084379	-0.035586
C	-0.673957	-3.820482	1.280674
N	-0.022022	-2.606145	1.331173
C	-0.592039	-2.821243	-2.190302
C	0.279063	-1.869578	2.557933
O	-2.247275	1.939113	-0.288375
S	-2.593556	0.541793	0.037869
O	-2.470609	-0.402050	-1.087240
C	-4.452931	0.620931	0.341216
F	-4.743975	1.457239	1.363303
F	-4.936642	-0.607299	0.654840
F	-5.106033	1.057605	-0.759661
O	-2.054414	0.054760	1.319409
H	-1.403440	-4.924406	-0.510605
H	-0.913177	-4.386851	2.170637
H	0.314007	-2.374865	-2.611344
H	-0.777908	-3.790292	-2.663303
H	-1.440381	-2.142477	-2.341668
H	1.241735	-1.361768	2.445241
H	-0.511425	-1.127658	2.725038
H	0.331862	-2.576858	3.391108
H	-0.393806	2.222967	-0.685447
H	3.563978	0.923285	-1.943402
H	3.060150	3.175516	-2.497080
H	6.526695	-0.627690	1.266979
H	6.299699	0.897992	3.220965
H	5.153279	-0.249548	-0.768425
H	4.691368	2.795684	3.131257
H	3.309054	3.160704	1.100118

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RC_OTs_preeq

N	1.742896	4.023830	-1.861961
C	1.309462	3.016258	-1.049854
N	2.432213	2.566060	-0.420334
C	3.544704	3.273467	-0.838813
C	3.112115	4.193971	-1.743124
Au	-0.503489	2.282715	-0.838492
C	2.551966	-1.569406	-1.830562
C	1.676489	-2.054189	-1.148460
C	0.603065	-2.674951	-0.344627
C	1.157675	-3.876145	0.415108
C	1.270847	-5.119576	-0.216441

C	1.796927	-6.211240	0.473496
C	2.217777	-6.071817	1.798952
C	2.102449	-4.834206	2.433461
C	1.572079	-3.742094	1.742983
C	2.460418	1.442177	0.516456
C	0.881472	4.811370	-2.736483
O	-0.482352	-3.088012	-1.171900
O	-2.394133	1.496525	-0.604521
S	-2.445349	0.021328	-0.139708
O	-1.598197	-0.198232	1.034673
C	-4.155920	-0.124566	0.361041
C	-4.537507	0.306384	1.632151
C	-5.870272	0.188059	2.021318
C	-6.832861	-0.359141	1.161411
C	-6.421579	-0.785931	-0.109833
C	-5.093113	-0.674424	-0.514527
C	-8.267416	-0.511909	1.597388
O	-2.240293	-0.888129	-1.277072
H	-8.961378	-0.216893	0.799006
H	-8.490722	-1.559387	1.850086
H	-8.484287	0.096581	2.483800
H	3.653470	4.948031	-2.298985
H	4.537096	3.067536	-0.459976
H	-0.141089	4.438547	-2.623204
H	0.920573	5.869755	-2.452449
H	1.198956	4.696670	-3.779659
H	1.470566	1.347862	0.973429
H	2.694576	0.509990	-0.013466
H	3.209988	1.639904	1.289878
H	3.317932	-1.175147	-2.462931
H	0.254313	-1.931866	0.394269
H	-1.094433	-2.318330	-1.259278
H	2.415985	-4.719847	3.471493
H	2.627250	-6.927139	2.336821
H	1.468668	-2.778836	2.245299
H	1.877288	-7.178029	-0.024383
H	0.929231	-5.225416	-1.245086
H	-4.772633	-1.018385	-1.496265
H	-7.152979	-1.218039	-0.794623
H	-6.168371	0.523187	3.015866
H	-3.791564	0.717600	2.310367

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TS1_OTs_preeq

N	0.550458	3.276176	0.471952
C	0.882960	2.203734	-0.303686

N	1.887195	2.656682	-1.110481
C	2.170722	3.986714	-0.844809
C	1.333922	4.372487	0.156268
Au	-0.013480	0.420312	-0.287842
C	0.165685	-2.036103	0.059953
C	1.304573	-1.738038	0.387097
C	2.677035	-1.598417	0.899828
C	3.718224	-1.352089	-0.178428
C	3.643047	-1.991779	-1.420226
C	4.645520	-1.800090	-2.370752
C	5.731498	-0.967905	-2.087401
C	5.811649	-0.328184	-0.848955
C	4.807427	-0.520695	0.101159
C	2.510868	1.873040	-2.169292
C	-0.501147	3.260839	1.489321
O	3.070550	-2.803377	1.597935
O	-2.041514	-0.502480	-0.572882
S	-3.174973	0.532799	-0.674154
O	-3.108241	1.498503	0.434862
C	-4.613283	-0.505032	-0.375857
C	-5.003674	-0.794835	0.933003
C	-6.100595	-1.624683	1.156693
C	-6.826232	-2.173633	0.089107
C	-6.418665	-1.863982	-1.215818
C	-5.322399	-1.035175	-1.453961
C	-8.030919	-3.045098	0.339571
O	-3.298919	1.083420	-2.022103
H	-8.948399	-2.439733	0.400918
H	-8.174135	-3.773448	-0.468922
H	-7.938774	-3.594335	1.285467
H	1.227237	5.323594	0.660872
H	2.927365	4.537934	-1.387128
H	-0.111301	2.858737	2.432835
H	-0.848257	4.287107	1.646879
H	-1.337118	2.641765	1.136689
H	2.347968	0.813190	-1.952400
H	2.062772	2.116940	-3.140588
H	3.586345	2.078876	-2.194098
H	-0.821649	-2.367978	-0.202369
H	2.695060	-0.741912	1.596618
H	2.360621	-3.018052	2.230189
H	6.659510	0.317429	-0.619885
H	6.515711	-0.821249	-2.830126
H	4.872970	-0.027995	1.072301
H	4.580310	-2.303073	-3.335432

H	2.794456	-2.639653	-1.639634
H	-5.013539	-0.786452	-2.468140
H	-6.970229	-2.277319	-2.062134
H	-6.402291	-1.849022	2.181463
H	-4.451646	-0.360452	1.765200

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INT_OTs_preeq

N	0.432139	2.707080	1.176690
C	0.673465	1.713939	0.280451
N	0.935896	2.353730	-0.889227
C	0.833191	3.723739	-0.734151
C	0.513712	3.947178	0.570012
Au	0.580038	-0.335711	0.590792
C	1.144001	-2.330029	0.949867
C	2.199654	-1.625332	0.950844
C	3.665307	-1.405799	1.089624
C	4.315145	-0.982392	-0.217158
C	4.282190	-1.832587	-1.328938
C	4.895246	-1.452156	-2.521100
C	5.542298	-0.216415	-2.615515
C	5.576283	0.634592	-1.510664
C	4.966653	0.249423	-0.314160
C	1.135407	1.670558	-2.163912
C	-0.037081	2.481781	2.539588
O	4.315052	-2.611527	1.534118
O	-1.664931	-0.495847	0.386108
S	-2.471378	0.657419	-0.204777
O	-2.620558	1.766099	0.749351
C	-4.095880	-0.089139	-0.396482
C	-5.034085	0.013562	0.630497
C	-6.287032	-0.580356	0.480112
C	-6.624951	-1.277541	-0.687701
C	-5.665153	-1.366483	-1.706889
C	-4.409632	-0.777971	-1.569656
C	-7.992577	-1.888730	-0.859646
O	-2.005041	1.020621	-1.551115
H	-8.654274	-1.217974	-1.428987
H	-7.941452	-2.837528	-1.409835
H	-8.471847	-2.078248	0.109040
H	0.333604	4.868334	1.107516
H	0.989312	4.412830	-1.553146
H	0.450317	1.586593	2.938917
H	0.223095	3.347705	3.157103
H	-1.123357	2.328684	2.518723
H	1.800129	0.813924	-2.012375

H	0.162589	1.327358	-2.536748
H	1.595951	2.367293	-2.871199
H	0.615737	-3.266640	1.032080
H	3.817684	-0.595356	1.824303
H	3.822280	-2.938688	2.307917
H	6.084426	1.596689	-1.575507
H	6.021586	0.079332	-3.548730
H	5.001384	0.910752	0.552763
H	4.868718	-2.120898	-3.381409
H	3.778474	-2.795824	-1.252433
H	-3.672624	-0.836923	-2.368999
H	-5.906991	-1.902882	-2.626206
H	-7.018890	-0.497071	1.285469
H	-4.779831	0.566893	1.533080

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TS2_OTs_preeq

N	0.012574	3.236357	0.419357
C	0.446358	2.177287	-0.312912
N	0.361895	2.576282	-1.608677
C	-0.136303	3.859918	-1.686817
C	-0.360070	4.274643	-0.407635
Au	0.877404	0.318137	0.346973
C	0.713016	-1.745566	1.031231
C	1.932910	-1.529755	0.976990
C	3.405799	-1.687219	1.082743
C	4.097941	-1.669458	-0.268799
C	3.696568	-2.545731	-1.283597
C	4.363515	-2.551083	-2.507021
C	5.432139	-1.677676	-2.728046
C	5.833665	-0.801190	-1.719568
C	5.168835	-0.800282	-0.491713
C	0.578639	1.689692	-2.750412
C	-0.265393	3.181324	1.851479
O	3.719028	-2.937502	1.722141
O	-1.921197	-0.591108	0.959552
S	-2.548404	0.248210	-0.105388
O	-2.719703	1.655928	0.308176
C	-4.212816	-0.424813	-0.287324
C	-5.256971	0.080833	0.488438
C	-6.531790	-0.474796	0.381836
C	-6.790991	-1.536552	-0.495725
C	-5.728599	-2.028143	-1.267862
C	-4.450258	-1.480214	-1.170043
C	-8.178321	-2.112811	-0.630284
O	-1.896521	0.070431	-1.424914

H	-8.730420	-1.627385	-1.449937
H	-8.146356	-3.187750	-0.851862
H	-8.762647	-1.969081	0.287695
H	-0.759764	5.204019	-0.025233
H	-0.294618	4.362634	-2.631292
H	0.473715	2.531924	2.330420
H	-0.198752	4.190750	2.270142
H	-1.270276	2.762026	1.991145
H	1.512363	1.136433	-2.608737
H	-0.265313	0.989806	-2.807112
H	0.645227	2.295959	-3.658950
H	-0.338455	-1.995056	1.107574
H	3.793309	-0.842638	1.678105
H	3.253617	-2.960069	2.577886
H	6.667881	-0.119817	-1.885490
H	5.951333	-1.682153	-3.686370
H	5.486514	-0.120191	0.299910
H	4.047868	-3.237243	-3.292664
H	2.861463	-3.224295	-1.110928
H	-3.631599	-1.857316	-1.781542
H	-5.906145	-2.853621	-1.960048
H	-7.343304	-0.074466	0.992691
H	-5.063076	0.912817	1.163879

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PC_OTs_preeq

N	-0.016353	2.646636	-1.204230
C	0.180080	2.101072	0.024373
N	-0.412920	2.957032	0.896799
C	-0.983381	4.017703	0.222644
C	-0.733334	3.821526	-1.104003
Au	0.914987	0.263055	0.424543
C	1.010227	-1.890555	0.755229
C	2.181773	-1.500563	0.882351
C	3.643468	-1.463898	1.141639
O	4.082870	-2.739720	1.638947
C	-0.577845	2.679228	2.323140
C	0.317390	1.968018	-2.455745
C	4.449571	-1.144274	-0.105486
C	5.329819	-0.059640	-0.110022
C	6.090938	0.226038	-1.245561
C	5.978060	-0.578382	-2.379659
C	5.101607	-1.667454	-2.376529
C	4.337357	-1.948019	-1.245843
O	-1.834350	-2.217681	0.334328
S	-2.302222	-0.831409	0.073833

O	-1.751168	-0.248150	-1.175154
O	-2.148913	0.069219	1.244411
C	-4.079208	-0.972338	-0.197843
H	-1.512770	4.811133	0.732998
H	-1.004124	4.411019	-1.969675
H	0.390515	2.407865	2.755615
H	-0.959213	3.579496	2.814248
H	-1.281811	1.844569	2.434624
H	1.344992	1.594952	-2.403488
H	-0.374259	1.127143	-2.591870
H	0.227221	2.683027	-3.279094
H	-0.015537	-2.285735	0.645894
H	3.835764	-0.672696	1.887059
H	3.512656	-2.978416	2.392107
H	6.775856	1.073802	-1.240699
H	6.573208	-0.359379	-3.266166
H	5.423120	0.564115	0.780216
H	5.012437	-2.298810	-3.260425
H	3.651253	-2.794691	-1.242470
C	-4.820691	0.172069	-0.509725
C	-6.194009	0.074970	-0.711202
C	-6.858590	-1.158549	-0.608353
C	-6.098274	-2.290956	-0.297549
C	-4.718541	-2.205314	-0.092785
H	-4.316441	1.134063	-0.594041
H	-6.765195	0.973276	-0.954204
C	-8.347745	-1.250395	-0.828889
H	-6.592082	-3.260785	-0.213287
H	-4.127578	-3.087241	0.148334
H	-8.706516	-2.279876	-0.707587
H	-8.896523	-0.615776	-0.117784
H	-8.623235	-0.914106	-1.839191

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RC_TFA_preeq

C	-7.155758009	0.284647469	0.413470995
C	-7.040322218	-0.808395138	-0.449735573
C	-8.201138485	-1.480832041	-0.857817072
C	-9.453710313	-1.068981066	-0.407858931
C	-9.562063331	0.022132435	0.459885202
C	-8.411414939	0.696262115	0.868222561
C	-5.690343987	-1.327159450	-0.944432932
O	-5.434285640	-2.663436323	-0.437977315
C	-4.570891651	-0.428347731	-0.667507871
C	-3.626894626	0.287270501	-0.419655794
O	-1.193087439	2.280510628	0.321250477

C	-0.064441434	1.818969345	0.403133468
C	1.096574743	2.791683746	0.827294850
F	2.077021503	2.847820801	-0.127932199
O	0.267965262	0.586196441	0.173377480
AU	2.053635098	-0.389471245	0.250098567
C	3.715819656	-1.442290807	0.291598479
N	3.854184927	-2.791850931	0.137838814
C	5.184228636	-3.163624053	0.234703179
C	5.896131434	-2.025430072	0.453398583
N	4.986323861	-0.982646820	0.485365547
C	2.750708856	-3.718862957	-0.095146065
C	5.339992463	0.418392527	0.697428348
F	1.695165700	2.376085429	1.985569143
F	0.660205440	4.045363456	1.027145108
H	6.958801995	-1.871376442	0.586729088
H	5.507245551	-4.192032844	0.140951318
H	4.419235361	1.008490997	0.665525701
H	5.819391757	0.540305870	1.675716411
H	6.019841556	0.756845853	-0.093116498
H	1.823787404	-3.138267671	-0.128967233
H	2.891991637	-4.238865567	-1.049817750
H	2.695353606	-4.449946224	0.719935071
H	-2.782915699	0.924878429	-0.199538481
H	-5.759058442	-1.478542870	-2.033224295
H	-5.282235120	-2.570798510	0.520040432
H	-10.349113845	-1.597826611	-0.735462760
H	-10.541668788	0.346611203	0.811265700
H	-8.114891376	-2.338803240	-1.525962256
H	-8.488359158	1.551122081	1.540486454
H	-6.255581891	0.818478640	0.718578286

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TS1_TFA_preeq

N	-1.801853649	-2.304217484	-0.662237854
C	-0.729849536	-1.887757281	0.075335306
N	-0.353550565	-2.988422626	0.790156829
C	-1.177620648	-4.064173536	0.507721059
C	-2.085795471	-3.637217666	-0.410886148
AU	0.186991171	-0.109782589	0.093113345
O	2.197178506	0.785415196	-0.372784988
C	3.178004082	0.011014223	-0.071792525
C	4.553752975	0.666099910	-0.453634405
F	4.717790458	1.865602828	0.177337870
C	0.778270884	-3.016938103	1.716796961
C	-2.518928987	-1.473689858	-1.621122749
C	-1.043241370	1.997938030	0.938147784

C	0.074760334	2.311669383	0.553444091
C	-2.381323078	1.857604523	1.535976824
O	-2.715042153	3.045257955	2.291569642
C	-3.492130213	1.652794646	0.520227567
C	-4.571819128	0.825811123	0.845580714
C	-5.635012637	0.668422427	-0.045260782
C	-5.623952475	1.339604522	-1.269639888
C	-4.548231030	2.168694556	-1.597730659
C	-3.487060984	2.325167543	-0.706310273
O	3.180450363	-1.105221237	0.446835242
F	4.631386721	0.899961114	-1.793943250
F	5.606660255	-0.110599068	-0.118060384
H	-1.044177624	-5.032321328	0.972125351
H	-2.892254928	-4.162040889	-0.905690280
H	0.460011270	-2.697353717	2.717040895
H	1.164237127	-4.040397593	1.767860499
H	1.562455634	-2.345069129	1.341083616
H	-2.127484753	-0.455303809	-1.541414496
H	-2.360062416	-1.846918916	-2.640299086
H	-3.590223526	-1.468142662	-1.389569963
H	1.037434705	2.672666178	0.241876067
H	-2.364359239	0.981440493	2.207888231
H	-1.961567677	3.238144419	2.878878369
H	-6.475159977	0.026442447	0.219734805
H	-6.454183172	1.220559886	-1.965800701
H	-4.583243553	0.308724816	1.806151172
H	-4.537270893	2.697314541	-2.550790310
H	-2.646450502	2.970707082	-0.960698120

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INT_TFA_preeq

N	0.111112062	-2.498769377	-0.939512569
C	0.272428607	-1.630256816	0.096192376
N	0.721946740	-2.397627180	1.124930357
C	0.847541715	-3.720139648	0.737005123
C	0.463441589	-3.785683148	-0.567221886
AU	0.046810201	0.436844008	0.059744799
O	2.057876922	0.622762613	-0.912329762
C	3.052844695	0.461028775	-0.122020496
C	4.419356553	0.635816426	-0.880495290
F	4.582116934	1.924411184	-1.292579278
C	1.072808930	-1.868675760	2.443329300
C	-0.303893269	-2.108692522	-2.282605821
C	-1.644187506	1.528731671	0.645654960
C	-0.756436271	2.357234651	0.264867653
C	-2.982910293	1.177663345	1.194269221

O	-3.695585555	2.364968921	1.589447524
C	-3.845037393	0.431139356	0.189700794
C	-4.290771776	-0.863240495	0.466682168
C	-5.093480135	-1.546732238	-0.449961664
C	-5.460032430	-0.933189233	-1.647948977
C	-5.020933998	0.364601837	-1.926582398
C	-4.214985930	1.042618829	-1.014088083
O	3.080018462	0.210245626	1.085335295
F	4.481353022	-0.156529526	-1.988961186
F	5.481191953	0.321825739	-0.105297956
H	1.196004444	-4.491150254	1.411280948
H	0.413793870	-4.623431735	-1.250002287
H	0.181251081	-1.450200572	2.924277707
H	1.464459772	-2.687443252	3.054151328
H	1.833142376	-1.086977098	2.317532145
H	-0.816937065	-1.144818264	-2.217586917
H	0.570063125	-2.006897261	-2.937044355
H	-0.988488238	-2.861732707	-2.687796862
H	-0.415289717	3.364099398	0.079652083
H	-2.829126363	0.517529861	2.066697999
H	-3.089865691	2.898964244	2.133995923
H	-5.439378010	-2.555102608	-0.222544474
H	-6.091337117	-1.461598237	-2.362384492
H	-4.013610751	-1.338678084	1.408749819
H	-5.309404384	0.849262830	-2.859376106
H	-3.873188545	2.055064253	-1.227638356

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TS2_TFA_preeq

N	-1.255360304	-3.128156278	-0.177684301
C	-0.239719159	-2.227952715	-0.053674217
N	0.899869328	-2.968718931	-0.041835722
C	0.599623999	-4.313642805	-0.153213003
C	-0.754980350	-4.417188600	-0.238251674
AU	-0.363955600	-0.218473233	0.050274362
O	3.465790921	2.558134028	0.324773375
C	3.574833591	1.384236984	-0.053539059
C	4.974791658	0.686560973	0.151471417
F	5.816982689	1.383418170	0.947328383
C	2.261697271	-2.437059753	0.101747966
C	-2.672352372	-2.786823799	-0.249094193
C	-0.929358222	1.925869773	0.293494119
C	0.243229520	1.897362945	-0.109039979
C	-2.237829827	2.408185241	0.806146830
O	-2.310676157	3.836676409	0.690974157
C	-3.426891172	1.820230532	0.067125292

C	-4.472786983	1.234304207	0.785340065
C	-5.589145564	0.725277091	0.117641627
C	-5.665686957	0.807474689	-1.273217158
C	-4.623567329	1.397546794	-1.994580916
C	-3.507826650	1.900891518	-1.328288575
O	2.714757514	0.633599258	-0.616316069
F	5.610595848	0.501200534	-1.044316133
F	4.844897076	-0.561756330	0.719637266
H	1.369327439	-5.074052384	-0.168408369
H	-1.395149104	-5.283320373	-0.341569226
H	2.597655809	-2.559692803	1.137798421
H	2.927354963	-2.993504422	-0.565908663
H	2.294874626	-1.370854458	-0.170480809
H	-2.764138021	-1.696577443	-0.230264192
H	-3.103473319	-3.171862506	-1.180419236
H	-3.206936828	-3.212865739	0.608163949
H	1.316174221	1.822277481	-0.397818401
H	-2.308172410	2.103999578	1.866160805
H	-1.516170549	4.215000046	1.110446360
H	-6.403102388	0.275181937	0.685804140
H	-6.539097308	0.417945348	-1.796166527
H	-4.417827848	1.183402910	1.873857219
H	-4.683174581	1.468394004	-3.080463323
H	-2.695813913	2.364616212	-1.888321326

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PC_TFA_preeq

N	4.477400856	0.329375998	0.118325463
C	3.360876674	-0.444481944	-0.019298661
N	3.841450832	-1.720367678	-0.093557671
C	5.222724511	-1.739356599	-0.004088706
C	5.624118829	-0.446134836	0.129611279
AU	1.423866641	0.157909568	-0.089870232
O	-3.580178329	-1.625738192	0.727560978
C	-2.735109534	-2.314279628	0.191868288
C	-2.902873717	-3.866056321	0.087423366
F	-4.052605359	-4.264778965	0.653367941
C	3.004913536	-2.907177283	-0.246047736
C	4.459915899	1.783540189	0.238754688
C	-1.622226510	1.173172136	-0.174847473
C	-0.467532809	0.752511516	-0.152360074
C	-2.989403675	1.723286512	-0.193128273
O	-3.777821710	1.255877318	0.905141728
C	-2.939535272	3.247247143	-0.153302346
C	-2.886298163	3.976984398	-1.344467003
C	-2.810817429	5.370293165	-1.317462619

C	-2.793989168	6.045140687	-0.095204149
C	-2.853720866	5.318429174	1.096308010
C	-2.924224087	3.925207463	1.069423382
O	-1.599805932	-1.945475077	-0.368456718
F	-1.877537274	-4.500803534	0.714689465
F	-2.906183602	-4.261932286	-1.210668078
H	5.795861138	-2.656488193	-0.042205134
H	6.613842966	-0.020363465	0.230749755
H	3.262124393	-3.432868010	-1.173180804
H	3.143444173	-3.578525979	0.609605982
H	1.961410132	-2.579966024	-0.288641471
H	3.415930723	2.110331018	0.202603545
H	4.906415790	2.088510931	1.192625083
H	5.015083330	2.237841892	-0.590539995
H	-1.441651870	-0.938467779	-0.278664599
H	-3.464662783	1.433416788	-1.151077473
H	-3.717195552	0.275854626	0.911048311
H	-2.773794016	5.929769631	-2.252497018
H	-2.741201452	7.133820503	-0.071477926
H	-2.905001119	3.451001820	-2.300566132
H	-2.848766813	5.840491408	2.053645983
H	-2.982261064	3.351371873	1.992770426

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RC (NHC-Au-OH catalyzed) (BP86/ZORA/D3)

N	-3.547993887	-1.346370048	-0.352682638
C	-3.631293644	-2.728697491	-0.296460285
C	-2.410868224	-3.176912469	0.104561204
N	-1.611657509	-2.060573516	0.284091899
C	-2.300266894	-0.912797955	0.004391030
AU	-1.608624749	0.927609723	0.085469778
O	-0.754867455	2.732553907	0.217976870
C	-0.215973704	-2.095536679	0.707886096
C	-4.636970973	-0.462107333	-0.738694169
H	1.064539843	2.024591563	0.288345900
C	1.790398484	1.219694427	0.368084763
C	2.547224689	0.277922460	0.452278665
C	3.428975191	-0.884227037	0.505595433
C	4.900795189	-0.553623103	0.283786633
O	2.988134202	-1.921080016	-0.414376265
H	3.041415805	-1.530422371	-1.306015769
H	3.328570614	-1.363277726	1.492425677
H	-1.312276065	3.404833732	-0.206377775
H	-2.047448864	-4.181526596	0.274645551
H	-4.537317706	-3.265837289	-0.542997548
H	-5.491095193	-0.595656308	-0.064008378

H	-4.266605920	0.565338442	-0.663604822
H	-4.945835689	-0.666865377	-1.770950793
H	0.394931001	-2.645494737	-0.015660883
H	0.149724819	-1.065205078	0.759007364
H	-0.137195897	-2.564851832	1.695611461
C	5.839771913	-1.586134616	0.410117520
C	7.193099168	-1.338156569	0.196561000
C	7.623374698	-0.053077105	-0.146550769
C	6.692766336	0.977351024	-0.272549042
C	5.335362990	0.728830912	-0.056792229
H	5.499014091	-2.589494108	0.666349853
H	7.916131942	-2.147151514	0.298938792
H	8.682595553	0.142084374	-0.312145080
H	7.022058907	1.981679516	-0.537776841
H	4.603157881	1.530832680	-0.144841123

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TS1 (NHC-Au-OH catalyzed) (BP86/ZORA/D3)

N	-3.903472340	-0.277144636	0.873586294
C	-5.149112998	-0.824807017	0.616162103
C	-5.001417165	-1.646658060	-0.458091492
N	-3.669473136	-1.580763801	-0.830942724
C	-2.973735152	-0.734970773	-0.014918603
AU	-1.048094611	-0.309401481	-0.086052182
O	0.930064927	0.107381095	-0.237651396
C	-3.084898765	-2.309386592	-1.950684535
C	-3.613594503	0.664224979	1.947953575
C	1.616786216	1.563298788	-0.093448295
C	2.776657005	1.656958153	0.465942221
C	3.578923846	0.607657147	1.022800927
C	4.695091545	0.092088068	0.150551606
O	2.709743162	-0.775449589	1.347338239
H	3.957417229	0.824851496	2.031480206
H	1.550237684	-0.431393490	0.393050007
H	-5.719691484	-2.263664936	-0.981196715
H	-6.021226777	-0.586950294	1.210322051
H	-3.858822440	0.214643313	2.916862114
H	-2.543769904	0.891505120	1.907994614
H	-4.190593886	1.585614015	1.808502978
H	-2.016322420	-2.074867478	-1.978718596
H	-3.221073607	-3.387582716	-1.808999244
H	-3.554551817	-1.995725784	-2.890054684
H	2.339221753	-0.603868553	2.231929842
C	5.718662706	-0.680930204	0.712268176
C	6.732458429	-1.209483858	-0.085583895
C	6.732136257	-0.973558170	-1.462069366

C	5.713632720	-0.204580432	-2.029662761
C	4.704347520	0.326710347	-1.227989418
H	5.708739243	-0.879311423	1.784688939
H	7.523435539	-1.809078299	0.365560814
H	7.523529398	-1.385052718	-2.088695399
H	5.709115612	-0.014317069	-3.103268255
H	3.909837164	0.938532107	-1.654047248
H	0.926083290	2.248192733	-0.571884260

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INT (NHC-Au-OH catalyzed) (BP86/ZORA/D3)

N	-3.709482090	-0.627888514	1.019884338
C	-5.031351454	-0.246122574	1.182178498
C	-5.208484739	0.880742326	0.441452336
N	-3.990600719	1.161840131	-0.156369960
C	-3.046352723	0.235101746	0.191350317
AU	-1.165203029	0.162674042	-0.367653219
O	0.735973101	0.181369328	-0.992047151
C	1.606240689	-0.776118822	-0.606835132
C	2.897650902	-0.775526655	-0.882542924
C	4.194944499	-0.820121369	-1.103301047
C	5.235506519	-0.257633847	-0.225836685
C	-3.741500817	2.289397537	-1.044288770
C	-3.096239190	-1.789068280	1.649618343
H	1.217601450	-1.629622983	-0.030939536
H	4.574768789	-1.305621455	-2.013216464
H	-6.084262731	1.497609070	0.290814190
H	-5.722679419	-0.800823658	1.802277040
H	-3.621742859	-2.703100417	1.349321761
H	-2.056052837	-1.835599444	1.312105995
H	-3.123166563	-1.686897096	2.740916052
H	-3.953660509	3.231559597	-0.525581905
H	-2.685922297	2.259398763	-1.331903257
H	-4.367306303	2.210454056	-1.941099123
C	6.589777051	-0.398181066	-0.569917666
C	7.595084599	0.122506806	0.244294047
C	7.264591573	0.796180432	1.420794740
C	5.918121132	0.944322893	1.773357681
C	4.916295815	0.425752486	0.960905765
H	6.850247332	-0.924608222	-1.489718561
H	8.640446458	0.002030188	-0.040853217
H	8.047766339	1.205290365	2.058620669
H	5.652249241	1.472714756	2.689456979
H	3.864952919	0.542858927	1.225598973

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H_2O (BP86/ZORA/D3)

O	0.000000000	0.000000000	0.093506374
H	-0.000000000	-0.766363918	-0.503162234
H	0.000000000	0.766363918	-0.503162234

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TS2 (NHC-Au-OH catalyzed) (BP86/ZORA/D3)

N	-3.617600547	0.677337830	-0.087623450
C	-4.118899217	1.781647125	0.579758406
C	-3.044164117	2.532632163	0.948652713
N	-1.915388231	1.877423071	0.493069137
C	-2.253601673	0.724705497	-0.147595355
AU	-1.024562535	-0.576733954	-0.967465604
O	0.163922986	-2.079414384	-1.791870917
C	1.431563259	-2.035680182	-1.651826613
C	2.151660838	-0.932806294	-1.154761106
C	3.262651439	-1.088389020	-0.388457466
C	4.108534223	-0.024860209	0.132351155
C	-0.537031012	2.333157441	0.690723124
C	-4.430925274	-0.381002819	-0.668701792
H	1.961572568	-2.926933081	-2.039696601
O	1.085486296	1.422438978	-1.668482137
H	3.557618393	-2.093732411	-0.054339113
H	-2.986237440	3.469573626	1.485953512
H	-5.179041354	1.938526710	0.726358334
H	-5.095086042	-0.803967362	0.093811989
H	-5.026306257	0.010995001	-1.502050838
H	-3.748547617	-1.154236397	-1.036528442
H	-0.116093569	1.857014022	1.584728196
H	0.060185221	2.063749200	-0.203867868
H	-0.551502493	3.419181427	0.826603120
H	1.648126078	0.209842486	-1.435227693
H	0.894734624	1.444446992	-2.621831532
C	5.214411713	-0.370878631	0.933866786
C	6.059285743	0.606620655	1.451123215
C	5.809730678	1.953015761	1.178050516
C	4.712441926	2.310001285	0.385564755
C	3.863531858	1.339710628	-0.133989422
H	5.403932060	-1.424444909	1.146261819
H	6.910669261	0.320451343	2.068355308
H	6.465557166	2.723115364	1.584190809
H	4.516838329	3.361530249	0.174276881
H	2.999929008	1.621172606	-0.744696773

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cinnemaldehyde (BP86/ZORA/D3)

H	-3.334347975	-1.536669233	0.000167198
C	-3.315029724	-0.415450549	0.000094634

C	-1.975581906	0.164211554	0.000029732
C	-0.885397243	-0.634641861	0.000059662
C	0.514413073	-0.239734740	0.000039377
O	-4.354869687	0.228773142	0.000071378
H	-1.914545274	1.253429133	-0.000046046
H	-1.064428495	-1.715864415	0.000093580
C	1.502903536	-1.242072720	-0.000034469
C	2.855954289	-0.914678200	-0.000081859
C	3.247799022	0.424565055	-0.000036252
C	2.277868243	1.433027887	0.000041927
C	0.927600884	1.107426754	0.000089407
H	1.194876913	-2.288172656	-0.000058014
H	3.606307759	-1.704419457	-0.000151609
H	4.305569816	0.685244582	-0.000059500
H	2.581858258	2.479201493	0.000066296
H	0.183255363	1.902211544	0.000171200

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NHC-Au-OH (BP86/ZORA/D3)

C	-3.311983451	-0.670299869	-0.013914707
N	-1.985395076	-1.071528052	-0.005959473
C	-1.139851689	0.006186903	0.001378408
N	-1.982189971	1.086745766	0.000102947
C	-3.309824270	0.689682587	-0.011334807
C	-1.536124560	-2.455503657	-0.006106185
AU	0.827589115	0.010872556	0.009563607
C	-1.527914016	2.469629768	-0.012041973
H	-4.131782472	-1.376104982	-0.016951867
H	-4.127701063	1.397751695	-0.013905989
H	-0.441639826	-2.443515994	0.021500240
H	-1.921279209	-2.979553083	0.876862572
H	-1.875039077	-2.965234697	-0.916153988
H	-0.442032310	2.461918376	0.126867588
H	-1.768334796	2.942971786	-0.971957854
H	-2.001056842	3.027399583	0.804508046
O	2.807960947	0.126425989	0.014713440
H	3.170542223	-0.775430717	0.045484735

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NHC-Au-OTf (BP86/ZORA/D3)

N	-2.999939047	1.438024734	0.476164668
C	-4.369051897	1.588688777	0.338748766
C	-4.846773445	0.417732285	-0.164173931
N	-3.757235145	-0.423235574	-0.322326510
C	-2.608749962	0.196476298	0.069891659
C	-3.821376644	-1.785196615	-0.837279252
C	-2.091202326	2.467456295	0.976634116

H	-4.879782473	2.503488949	0.607717969
H	-5.853578144	0.114330674	-0.417708524
H	-1.083896374	2.040718011	1.030946213
H	-2.087951722	3.325363031	0.294851851
H	-2.407992670	2.786088226	1.975783899
H	-2.803440165	-2.186589481	-0.840593988
H	-4.457835722	-2.401642550	-0.192254401
H	-4.218624928	-1.782553650	-1.858769679
AU	-0.767540092	-0.467367367	0.081038671
O	1.197634096	-1.098069874	0.127789601
S	2.223509736	-0.047825390	0.582987192
O	3.401981745	-0.680080357	1.135398108
O	1.607668202	1.081051468	1.272992296
C	2.771648273	0.655753983	-1.079880980
F	3.706575852	1.607364728	-0.887533811
F	3.289370765	-0.307429323	-1.866105176
F	1.721453783	1.216842688	-1.729611649

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1-phenyl-2-propyn-1-ol (BP86/ZORA/D3)

C	0.528554826	-1.136988186	0.073496296
C	0.115124745	0.175965592	-0.160280417
C	1.076358285	1.190349824	-0.265641901
C	2.430336956	0.892643952	-0.135834844
C	2.839827242	-0.422987788	0.099410513
C	1.887061180	-1.435101923	0.203875616
C	-1.354425658	0.563803878	-0.304355132
O	-1.705765962	1.645997520	0.584466995
C	-2.275850372	-0.563331546	-0.155469655
C	-3.056939311	-1.472177351	-0.001904132
H	-3.754066670	-2.272241078	0.126820230
H	-1.502039560	0.995651843	-1.307162016
H	-1.585515826	1.313905290	1.492720845
H	3.170270400	1.688262327	-0.219459661
H	3.899527096	-0.655678698	0.200407215
H	0.752117697	2.216540144	-0.437049363
H	2.199168069	-2.462789980	0.388167239
H	-0.218473465	-1.925870889	0.152125799

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[NHC-Au-OH_2]$^+$$OTf^-$ complex (BP86/ZORA/D3)

N	3.544720924	0.897120395	0.732662505
C	2.310086798	0.802293654	0.165312287
N	2.113414632	1.992308335	-0.463872378
C	3.210249710	2.816380635	-0.295003843
C	4.112359651	2.130255030	0.460653088
AU	1.021828160	-0.676660857	0.238238854

O	-0.466927938	-2.170095092	0.289744758
C	0.914265228	2.332610986	-1.235165031
C	4.169090620	-0.148522424	1.533223027
O	-2.045325684	-0.580004534	-1.167503872
S	-2.434435379	0.211246171	0.025535416
C	-4.305747830	0.332566725	-0.111603534
F	-4.650501339	0.977472237	-1.246696744
O	-2.235758774	-0.529768570	1.299263427
O	-1.979701706	1.600503051	0.034181035
F	-4.860632150	-0.898507397	-0.133732762
F	-4.811999593	1.012150870	0.938079405
H	-0.980306492	-1.917329433	-0.533341888
H	5.090058200	2.411130429	0.827936153
H	3.252275033	3.811201979	-0.717430203
H	0.945131654	1.833514004	-2.209964351
H	0.013497506	2.017958858	-0.693893805
H	0.893605114	3.416846485	-1.377064736
H	4.339248935	0.211200590	2.554419613
H	3.486630580	-1.003349327	1.555740349
H	5.121207683	-0.448863820	1.081321195
H	-1.116861125	-1.748476811	0.946960409

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$H_3O_7^+$ OTf^- (BP86/ZORA/D3)

C	2.005193307	0.000529678	0.063803701
S	0.134772100	0.002796049	-0.119624246
O	-0.167147881	1.248988255	-0.846168917
O	-0.343729157	-0.002819687	1.291021178
O	-0.168498753	-1.237113346	-0.856401728
O	-2.902349720	-0.005515767	1.096557808
O	-2.723221583	-1.977930681	-0.483332474
O	-2.726171117	1.976418599	-0.472132265
H	-2.962121241	-0.853358356	0.473693954
H	-2.963462448	0.845279568	0.478030838
H	-1.898116915	-0.005136327	1.351161051
H	-1.757116411	1.845290860	-0.696142897
H	-2.800456464	2.869285646	-0.096748070
H	-1.755060216	-1.841400311	-0.708107837
H	-2.793289490	-2.873249265	-0.112984154
F	2.580853700	0.005785770	-1.150886770
F	2.399252703	1.093121919	0.742646228
F	2.397304854	-1.099214048	0.732192934

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RC ($[NHC\text{-}Au\text{-}OH_2]^+$ catalyzed) (BP86/D3/ZORA)

C	-4.923258412	1.996175928	-0.506311316
C	-3.767025230	1.461116880	0.068056406

C	-3.687086671	1.310761761	1.456962169
C	-4.756498842	1.695808907	2.264331752
C	-5.910754394	2.229638781	1.688502619
C	-5.992232530	2.379216203	0.302446273
C	-2.559259432	1.088153005	-0.770521265
O	-1.629381203	2.201022819	-0.881242519
C	-2.886404578	0.638821103	-2.119036004
C	-3.128309744	0.253788130	-3.238187282
O	0.614566653	1.164673548	-1.813469499
AU	0.249582352	-0.815843011	-1.249574587
C	-0.082433797	-2.641491148	-0.608285314
N	0.694548784	-3.341317905	0.261684735
C	0.129048898	-4.572614271	0.536386753
C	-1.030909480	-4.644358513	-0.173935158
N	-1.145058876	-3.452584280	-0.869686321
C	1.948298455	-2.838913488	0.827665048
C	-2.260100292	-3.102734732	-1.741814679
H	-3.346982763	-0.066513903	-4.234130202
H	-1.202579774	2.259012960	0.023946616
H	-2.032354181	0.256944012	-0.260621654
H	1.190429154	1.479468120	-1.040651719
H	-1.777517896	-5.424245445	-0.236809880
H	0.589983716	-5.279613143	1.212741772
H	2.733064443	-2.852147688	0.063222253
H	1.796142588	-1.816793962	1.195111296
H	2.234753996	-3.488672644	1.659488368
H	-3.201367648	-3.166305694	-1.184522031
H	-2.116863488	-2.074472879	-2.088279002
H	-2.291989132	-3.781046557	-2.602342078
H	-2.773421346	0.916340760	1.902194465
H	-4.686277703	1.581659884	3.345605551
H	-6.746881218	2.530027721	2.319545391
H	-6.891863485	2.796334229	-0.149460426
H	-4.982697612	2.106759698	-1.588709325
H	-0.267548608	1.639269283	-1.632407068
O	1.844609711	1.739947847	0.440820440
S	0.988182135	1.379569356	1.596534838
O	-0.417456889	1.823284883	1.462543113
O	1.158287993	0.019060558	2.105361064
C	1.655457761	2.481195326	2.965139798
F	1.553859321	3.781639955	2.622273753
F	0.957262692	2.281324488	4.103541145
F	2.953800486	2.199335528	3.203997877

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TS1 ([NHC-Au-OH_2]$^+$ catalyzed) (BP86/D3/ZORA)

C	-5.148082913	-1.646474697	0.179688945
C	-4.229449469	-0.603177359	0.388884417
C	-4.623419049	0.728658273	0.158507930
C	-5.913717925	1.009188742	-0.272639944
C	-6.821619623	-0.033852158	-0.476553567
C	-6.437741431	-1.360148051	-0.249616627
C	-2.873580930	-0.848829850	0.832789434
O	-1.868824640	-0.613294129	-1.105056336
C	-2.358163903	-2.059118293	1.223098958
C	-1.584489383	-3.023155246	1.234913441
O	-0.373769756	-2.830714099	-0.500029262
AU	1.288690615	-1.664068473	-0.153100371
C	2.753651634	-0.377151235	0.136704286
N	3.473214874	0.276085651	-0.814557218
C	4.306903061	1.214723283	-0.236056328
C	4.117260332	1.134352255	1.108448918
N	3.173558618	0.146858448	1.319489133
C	3.230487529	0.165484092	-2.246971099
C	2.560521288	-0.140099936	2.609649612
H	-1.094944308	-3.906592211	1.589579272
H	-1.260279375	0.076537951	-0.705276717
H	-2.303707315	0.024790979	1.165726009
H	-0.159888875	-3.687034971	-0.911237054
H	4.546935169	1.703452955	1.920622742
H	4.940137496	1.863115993	-0.825593911
H	2.843945332	-0.835754573	-2.458055492
H	2.484631191	0.914950968	-2.536251804
H	4.169947195	0.322904557	-2.786725208
H	1.853340564	0.663542004	2.846177931
H	2.024904558	-1.090407360	2.527461941
H	3.338104873	-0.213798517	3.377349771
H	-3.899480376	1.529550932	0.306625690
H	-6.214635666	2.039982728	-0.454190942
H	-7.834163373	0.186944964	-0.813221200
H	-7.151301077	-2.167403251	-0.409296699
H	-4.835187132	-2.673857013	0.363817417
H	-1.355490270	-1.462590427	-1.060619762
O	1.014040556	2.108597678	-1.043156992
S	0.344602928	2.173036281	0.255106362
O	-0.633653623	1.076985321	0.487910187
O	1.175142994	2.472741332	1.419400213
C	-0.780694479	3.668560166	0.107024957
F	-1.654314610	3.514381090	-0.918023676
F	-1.502781638	3.844236582	1.240162917
F	-0.066682130	4.791344589	-0.114453074

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INT ([NHC-Au-OH_2]$^+$ catalyzed) (BP86/D3/ZORA)

C	4.002331538	-0.968900672	-0.092323553
C	3.034134038	-1.938865874	0.220669741
C	2.951985812	-3.092847567	-0.573670179
C	3.807227461	-3.269048815	-1.659862866
C	4.759996612	-2.296146851	-1.966865418
C	4.855851537	-1.146382219	-1.175060870
C	2.092149954	-1.757514106	1.326425773
O	-0.515576032	-2.150286979	-1.066345489
C	1.983077338	-0.670506680	2.057576474
C	1.774024732	0.442537742	2.698648972
O	0.843009122	1.405839662	2.204245276
AU	0.422589565	1.218390425	0.122939897
C	-0.216848135	0.966209382	-1.715622844
N	0.379705954	0.330381758	-2.755219311
C	-0.501285515	0.196695869	-3.811585294
C	-1.671578679	0.777290779	-3.425783496
N	-1.478274427	1.248364116	-2.140605387
C	1.697002993	-0.289231568	-2.688534567
C	-2.509891124	1.850712493	-1.298287085
H	2.227900545	0.732856075	3.644785497
H	-0.839956412	-3.057518387	-0.952935915
H	1.389860986	-2.571028576	1.532200648
H	-0.099899954	1.095691360	2.550699552
H	-2.610568985	0.897683527	-3.948287952
H	-0.223409629	-0.294665048	-4.733593114
H	2.320326095	0.282993344	-1.997605880
H	1.593727218	-1.312629288	-2.311864397
H	2.149266217	-0.286457257	-3.684740991
H	-2.864833070	1.110159768	-0.572279232
H	-2.081597697	2.702353691	-0.761011422
H	-3.328885719	2.192520167	-1.937683942
H	2.197544375	-3.843113916	-0.339487245
H	3.729417675	-4.168723866	-2.269752600
H	5.431442268	-2.434713086	-2.813635800
H	5.603211042	-0.387440649	-1.405901259
H	4.070858026	-0.073249941	0.525615459
H	-1.029675512	-1.640421325	-0.395111304
O	-2.086277599	-0.665041411	0.748656095
S	-1.812913366	-0.780083172	2.196482384
O	-1.019008145	-1.930600211	2.602895670
O	-1.435095875	0.518950749	2.832427825
C	-3.518739098	-1.052328779	2.937677854
F	-4.045746461	-2.202076217	2.462638707

F	-3.449602325	-1.134527070	4.280667295
F	-4.349876068	-0.036952460	2.611102035

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RC_acid (BP86/ZORA)

C	-0.671350	3.002722	-0.656794
C	-0.621513	2.628608	0.693046
C	-1.297617	3.394028	1.651177
C	-2.018310	4.522659	1.263001
C	-2.062454	4.895340	-0.082080
C	-1.387858	4.135996	-1.040642
C	0.230712	1.462228	1.151646
O	1.613841	1.845943	1.347066
C	0.188556	0.297068	0.225311
C	0.491042	-0.594610	-0.581116
Au	-1.606731	-0.956327	-0.124922
C	-3.471734	-1.742708	-0.058046
N	-4.565685	-1.342212	-0.763897
C	-5.652800	-2.135477	-0.461254
C	-5.230648	-3.053675	0.453701
N	-3.895495	-2.799875	0.689475
C	-4.602081	-0.231839	-1.716848
C	-3.067154	-3.573765	1.615598
O	3.552720	0.047033	0.994365
S	3.992357	0.437561	-0.483439
C	5.815820	0.860935	-0.184014
F	5.897171	1.880747	0.681929
O	3.951470	-0.734877	-1.321481
O	3.320997	1.669664	-0.880025
F	6.353621	1.214408	-1.356153
F	6.448846	-0.207572	0.309092
H	-5.765586	-3.854626	0.947839
H	-6.625027	-1.985358	-0.912925
H	-2.059764	-3.148508	1.618167
H	-3.490527	-3.519851	2.624498
H	-3.021447	-4.618349	1.288643
H	-3.620334	0.249537	-1.725376
H	-4.834580	-0.609266	-2.718785
H	-5.362083	0.494252	-1.408675
H	1.032376	-1.238200	-1.255956
H	-0.106884	1.127859	2.141723
H	2.843024	0.707687	1.297045
H	-2.540128	5.116255	2.012627
H	-2.619319	5.782024	-0.383217
H	-1.251019	3.112779	2.703970
H	-1.415057	4.429903	-2.089298

H	-0.141754	2.416420	-1.409191
H	1.929356	2.292576	0.527603

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TS_acid (BP86/ZORA)

C	-0.533611	-3.770927	0.121367
C	0.177108	-3.090217	-0.881063
C	0.418698	-3.721500	-2.111775
C	-0.036934	-5.019933	-2.332620
C	-0.734900	-5.694570	-1.329014
C	-0.983236	-5.069955	-0.103504
C	0.734776	-1.728364	-0.644733
O	2.070943	-1.819732	0.177705
C	0.026267	-0.782894	0.288531
C	0.858082	-0.638674	1.254363
Au	-1.740324	0.248271	0.197155
C	-3.479481	1.298802	0.046046
N	-3.657163	2.632008	0.258771
C	-4.978110	2.987546	0.056179
C	-5.642000	1.852234	-0.293100
N	-4.710941	0.829519	-0.295615
C	-2.608445	3.571849	0.652345
C	-5.022019	-0.560769	-0.622004
O	4.612910	-0.639371	0.139500
S	4.734314	0.358196	1.384510
C	4.491702	2.015643	0.499249
F	5.444912	2.196584	-0.416201
O	3.584422	0.188278	2.257077
O	6.085685	0.320885	1.861996
F	4.534821	2.994519	1.409581
F	3.281604	2.021320	-0.105156
H	-6.684104	1.689553	-0.535877
H	-5.330732	4.003702	0.176586
H	-4.104608	-1.148933	-0.527123
H	-5.777305	-0.947016	0.071597
H	-5.395562	-0.629342	-1.649915
H	-1.665558	3.022882	0.729092
H	-2.511220	4.359830	-0.102799
H	-2.851724	4.018544	1.622917
H	1.452811	-0.273879	2.083922
H	1.031090	-1.242454	-1.581732
H	3.686916	-1.002519	0.087233
H	0.152309	-5.505179	-3.289135
H	-1.090832	-6.709429	-1.503063
H	0.964931	-3.194639	-2.895134
H	-1.533958	-5.595815	0.675394

H	-0.740255	-3.278429	1.072144
H	2.133297	-2.736952	0.521008

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PC_acid (BP86/ZORA)

C	0.678624	2.586796	-0.702693
C	-0.370692	2.788910	0.218703
C	-1.090340	4.001492	0.196743
C	-0.759440	4.996360	-0.717109
C	0.286562	4.789776	-1.620408
C	1.003083	3.585831	-1.610697
C	-0.697293	1.804516	1.246122
O	2.037621	0.289437	2.506815
C	-0.091750	0.580591	1.438813
C	0.934870	-0.167998	1.806136
Au	-1.817759	-0.119817	0.424128
C	-3.260176	-1.206213	-0.511465
N	-4.340564	-1.811431	0.055439
C	-5.075811	-2.483747	-0.899946
C	-4.438705	-2.299992	-2.090539
N	-3.329985	-1.518434	-1.835230
C	-4.697384	-1.754634	1.473268
C	-2.371857	-1.096316	-2.857845
O	4.513863	0.239306	1.277470
S	4.378735	-0.055600	-0.284902
C	5.004059	-1.843614	-0.337635
F	6.264359	-1.906855	0.096158
O	2.973077	-0.102496	-0.650717
O	5.335855	0.754726	-0.985426
F	4.932159	-2.277722	-1.603119
F	4.218105	-2.612441	0.443417
H	-4.681386	-2.657205	-3.083135
H	-5.979124	-3.029662	-0.659702
H	-1.615715	-0.464096	-2.384079
H	-1.888346	-1.974416	-3.299959
H	-2.889506	-0.526731	-3.637372
H	-3.907077	-1.219527	2.007266
H	-5.648543	-1.225144	1.598389
H	-4.784491	-2.770640	1.873231
H	1.012613	-1.233811	1.609163
H	-1.448172	2.129502	1.977890
H	3.619980	0.136410	1.715115
H	-1.311808	5.934879	-0.724622
H	0.547826	5.569577	-2.335174
H	-1.900525	4.160131	0.909632
H	1.820982	3.432620	-2.313507

H	1.239820	1.651525	-0.693727
H	1.917110	1.231263	2.735829

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RC_acid (BP86/ZORA/D3)

C	0.265004310	2.302493264	-0.727642678
C	0.102973536	2.256383684	0.664641529
C	-0.702493497	3.200374542	1.306565346
C	-1.340706059	4.192211143	0.560908456
C	-1.167418949	4.247095794	-0.822798977
C	-0.363632601	3.302059907	-1.466587075
C	0.847152219	1.214525772	1.475122905
O	2.267545442	1.474682479	1.521765504
C	0.603920307	-0.147798670	0.937522850
C	0.665612645	-1.279443459	0.440642710
Au	-1.451140538	-0.719943577	0.403011510
C	-3.449751975	-0.637609870	0.151588541
N	-4.148276799	0.348377654	-0.472103423
C	-5.501095044	0.069750615	-0.451744309
C	-5.649238567	-1.120871688	0.194872164
N	-4.383753150	-1.536803758	0.561757989
C	-3.557787853	1.549367884	-1.059917683
C	-4.098926283	-2.782527746	1.271315205
O	3.792545212	-0.655482082	1.180284556
S	3.916794738	-0.590070581	-0.400038299
C	5.797071075	-0.483366757	-0.575454153
F	6.232323812	0.627671375	0.033196584
O	3.496521895	-1.845262651	-0.971442293
O	3.367747326	0.672885788	-0.885013908
F	6.083990232	-0.432774901	-1.880357465
F	6.358357011	-1.560277810	-0.020447321
H	-6.536419004	-1.697747742	0.420816132
H	-6.235717204	0.732631703	-0.889713394
H	-3.038069166	-2.792211214	1.536785745
H	-4.704257957	-2.832850651	2.182200622
H	-4.323162976	-3.640196527	0.627851078
H	-2.472526601	1.501423513	-0.934827774
H	-3.801591365	1.598893482	-2.126241955
H	-3.938105605	2.439093168	-0.548121661
H	1.016514149	-2.225946061	0.064982599
H	0.510267370	1.241124669	2.519574678
H	3.267435788	0.159682407	1.494577138
H	-1.959462552	4.933487695	1.064635536
H	-1.651310605	5.033317646	-1.400909714
H	-0.820771589	3.167809729	2.389633477
H	-0.221536822	3.347393859	-2.545293871

H	0.893765097	1.566512168	-1.230696741
H	2.550069800	1.704204071	0.604620676
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TS_acid (BP86/ZORA/D3)

C	0.706082956	3.359061268	0.713538933
C	-0.014103175	3.015198797	-0.441122974
C	-0.080209772	3.912066982	-1.516969087
C	0.562095232	5.145564032	-1.434680231
C	1.269833038	5.487193198	-0.280854817
C	1.342106948	4.594611710	0.792188334
C	-0.751683180	1.728779024	-0.520436706
O	-2.142280877	1.844245081	0.215078954
C	-0.245741474	0.559010884	0.271974976
C	-1.189302276	0.358115141	1.119108673
Au	1.512704383	-0.458168739	0.131831170
C	3.296926627	-1.407196549	-0.057166855
N	3.520215839	-2.732233467	-0.267609134
C	4.876606316	-2.995824517	-0.336485135
C	5.516842573	-1.806221571	-0.167838350
N	4.535073201	-0.846210727	0.001267856
C	2.476293618	-3.744972161	-0.401857949
C	4.797716309	0.574200623	0.214258514
O	-4.689083179	0.999905551	-0.345474899
S	-4.975708298	-0.218938088	0.643268938
C	-4.450044288	-1.657381127	-0.465840720
F	-5.207186821	-1.703052608	-1.562476815
O	-4.027336787	-0.194096634	1.743924798
O	-6.391805752	-0.316499889	0.839126929
F	-4.563114112	-2.798621381	0.221565609
F	-3.153895269	-1.482002487	-0.824839809
H	6.571719691	-1.565971395	-0.153614400
H	5.265924297	-3.992581072	-0.496844594
H	3.835742853	1.087000797	0.307831496
H	5.378404857	0.713218298	1.132696092
H	5.349116635	0.984044484	-0.638929358
H	1.505852125	-3.247303648	-0.319201687
H	2.554744811	-4.233386954	-1.379138716
H	2.574684292	-4.490567441	0.394528236
H	-1.903229553	-0.070098707	1.812894552
H	-1.019470009	1.462101189	-1.548731171
H	-3.753114136	1.321343421	-0.210623390
H	0.511485807	5.840284011	-2.271432152
H	1.771337841	6.451934680	-0.218275946
H	-0.633892714	3.641452080	-2.416320150
H	1.899298244	4.862786005	1.688497516

H	0.771507324	2.652815523	1.541272655
H	-2.114894245	2.668314821	0.747038163

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PC_acid (BP86/ZORA/D3)

C	0.531439457	2.433538522	-0.458843293
C	-0.376629380	2.794879346	0.554193443
C	-1.027578513	4.039724817	0.489669231
C	-0.757059973	4.912615684	-0.560194886
C	0.153747557	4.548269549	-1.554439197
C	0.798143297	3.305404298	-1.502909850
C	-0.638615130	1.914372891	1.693344386
O	2.203469122	0.314797006	2.722192614
C	-0.031665921	0.705450335	1.934533165
C	0.972533402	-0.095756173	2.229955395
AU	-1.698387215	0.036422770	0.806264043
C	-2.880020193	-1.114431557	-0.359670080
N	-4.153671367	-1.538912444	-0.146248959
C	-4.586066205	-2.319929058	-1.200405760
C	-3.553763274	-2.389127862	-2.088815390
N	-2.517360077	-1.647581779	-1.557798514
C	-4.962034370	-1.208829942	1.025295340
C	-1.217953672	-1.458252088	-2.205260502
O	3.690409459	0.475941228	0.411187253
S	3.101473333	-0.335966009	-0.825002103
C	4.408033803	-1.693019620	-0.987749794
F	5.601406268	-1.150400172	-1.232536242
O	1.859296859	-0.993418469	-0.454724264
O	3.191760664	0.502904223	-1.990921918
F	4.048142914	-2.492715987	-2.000502569
F	4.450524681	-2.399028129	0.154007755
H	-3.471979805	-2.901587392	-3.038363683
H	-5.575182608	-2.757841446	-1.229695120
H	-0.533591416	-0.985773225	-1.494631393
H	-0.811746282	-2.431722757	-2.497360416
H	-1.331358659	-0.821279217	-3.089124072
H	-4.330128114	-0.668937876	1.735979141
H	-5.806857430	-0.576596479	0.731041773
H	-5.330775107	-2.129236171	1.489757829
H	0.953943387	-1.170640084	2.078209112
H	-1.315855157	2.314253264	2.457362832
H	3.223670556	0.243214722	1.267426452
H	-1.255147461	5.879762708	-0.603892005
H	0.363516761	5.233908329	-2.374312339
H	-1.734847737	4.320336926	1.270428517
H	1.510126379	3.018465630	-2.274942785

H	1.012178554	1.458597147	-0.419387989
H	2.166617561	1.265786401 49	2.944925981

RC_GVL (BP86/ZORA)

C	-3.576477	-2.238421	1.001834
C	-2.210568	-1.953254	0.907052
C	-1.597048	-1.179882	1.899034
C	-2.347786	-0.695504	2.971581
C	-3.712903	-0.976743	3.059446
C	-4.326558	-1.750417	2.072823
C	-1.408761	-2.492883	-0.276872
O	-0.104080	-2.939506	0.019138
C	-1.401248	-1.533564	-1.417766
C	-1.406373	-0.952704	-2.513367
Au	-1.107766	0.693521	-1.145341
C	-0.823955	2.522528	-0.325898
N	-1.765992	3.476933	-0.085370
C	-1.183706	4.608338	0.449289
C	0.152238	4.355952	0.545179
N	0.354895	3.076482	0.069514
C	-3.199698	3.333689	-0.336542
C	1.666549	2.429962	-0.021738
O	1.795379	-1.032306	0.568414
C	2.896650	-1.518038	0.802489
O	3.983704	-0.737897	0.930583
C	3.260188	-2.976150	0.996300
H	-1.758194	5.484910	0.719572
H	0.961992	4.972571	0.913185
H	-3.379380	2.335482	-0.745415
H	-3.754107	3.448931	0.601303
H	-3.528879	4.090769	-1.056886
H	1.537252	1.343171	-0.032485
H	2.182777	2.755850	-0.932256
H	2.260024	2.707898	0.854856
H	-1.441866	-0.771990	-3.573821
H	-1.944947	-3.373967	-0.670777
H	-5.387246	-1.988965	2.144745
H	-4.294189	-0.607256	3.903771
H	-4.057370	-2.856176	0.241521
H	-1.861720	-0.106972	3.749608
H	-0.527026	-0.977227	1.852176
H	0.491681	-2.176574	0.242075
C	4.783663	-2.979943	0.846204
C	5.177243	-1.558429	1.270286
H	5.271285	-1.487531	2.364332

C	6.389121	-0.965489	0.589818
H	6.272737	-0.982158	-0.501362
H	6.562830	0.067154	0.914084
H	7.276464	-1.557068	0.851247
H	5.067407	-3.146598	-0.202014
H	5.283315	-3.738893	1.457560
H	2.937277	-3.266567	2.008290
H	2.713972	-3.610730	0.290446

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TS_GVL (BP86/ZORA)

C	1.273489	2.323879	1.237535
C	1.340905	1.747742	-0.036874
C	1.361315	2.574965	-1.168349
C	1.314585	3.959857	-1.022685
C	1.241154	4.530240	0.251552
C	1.221835	3.710759	1.381660
C	1.385497	0.251227	-0.183155
O	2.350763	-0.182677	-1.210574
C	0.131130	-0.432856	-0.713998
C	0.480642	-1.178762	-1.680743
Au	-1.860541	-0.437804	-0.218090
C	-3.811411	-0.353801	0.363312
N	-4.517371	-1.290926	1.054795
C	-5.813950	-0.862996	1.275306
C	-5.921604	0.371376	0.712277
N	-4.688565	0.668031	0.160754
C	-3.991095	-2.578804	1.502810
C	-4.381961	1.912788	-0.541804
O	4.387982	-1.145181	0.179673
C	5.599552	-1.067501	0.021116
O	6.446948	-1.593876	0.917649
C	6.364885	-0.430963	-1.124919
H	-6.541558	-1.463541	1.805684
H	-6.760807	1.052724	0.658953
H	-2.940905	-2.642104	1.203577
H	-4.065577	-2.653616	2.593522
H	-4.554328	-3.395716	1.037629
H	-3.340540	1.871428	-0.873962
H	-5.039855	2.022608	-1.411239
H	-4.516062	2.765618	0.133103
H	0.599069	-1.844909	-2.519902
H	1.636937	-0.212417	0.782141
H	1.178541	4.151971	2.376998
H	1.207280	5.613667	0.362938
H	1.271793	1.685046	2.122163

H	1.338585	4.598977	-1.904998
H	1.429964	2.127869	-2.159639
H	3.175672	-0.533164	-0.747316
C	7.784018	-0.298617	-0.565865
C	7.852279	-1.429580	0.470581
H	8.115619	-2.384517	-0.008880
C	8.723760	-1.181606	1.680036
H	8.428440	-0.256622	2.191585
H	8.661414	-2.014521	2.389727
H	9.769530	-1.082783	1.360144
H	7.911506	0.670838	-0.064915
H	8.567442	-0.394528	-1.325247
H	6.315455	-1.120972	-1.981586
H	5.893179	0.507992	-1.433373

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PC_GVL (BP86/ZORA)

C	0.877607	4.854083	-0.567773
C	0.211074	3.609543	-0.449552
C	-1.191793	3.582862	-0.626879
C	-1.888476	4.745491	-0.918228
C	-1.209045	5.965929	-1.032836
C	0.176562	6.017687	-0.856651
C	1.015431	2.444929	-0.183268
O	2.941565	0.452828	-0.247346
C	0.648209	1.120050	0.003008
C	1.718513	0.208036	0.134966
Au	-1.229555	0.277166	0.163660
C	-3.062274	-0.614185	0.354637
N	-3.775043	-1.275095	-0.601554
C	-4.970721	-1.749731	-0.090607
C	-5.012448	-1.377673	1.217183
N	-3.840684	-0.686222	1.471773
C	-3.341063	-1.462605	-1.983467
C	-3.489521	-0.115907	2.769801
O	4.310890	-1.610960	0.310210
C	5.514450	-1.828516	0.173759
O	6.033820	-2.997877	0.543143
C	6.580606	-0.917878	-0.401019
H	-5.681006	-2.303572	-0.690652
H	-5.765886	-1.545386	1.975858
H	-2.365470	-0.981436	-2.100570
H	-3.251644	-2.531871	-2.207490
H	-4.061597	-1.002692	-2.669620
H	-2.518335	0.378329	2.671312
H	-4.245169	0.617134	3.074858

H	-3.422063	-0.909181	3.523248
H	1.544613	-0.792462	0.549593
H	2.084710	2.673335	-0.094272
H	0.704388	6.966246	-0.945151
H	-1.763456	6.877024	-1.256647
H	1.959394	4.888199	-0.433239
H	-2.968967	4.713037	-1.054346
H	-1.718535	2.631023	-0.524983
H	3.558433	-0.357361	-0.041574
C	7.883846	-1.576227	0.062942
C	7.488773	-3.050490	0.227909
H	7.549792	-3.585331	-0.731310
C	8.194466	-3.820980	1.318725
H	8.084432	-3.318190	2.287914
H	7.801678	-4.840797	1.400544
H	9.264451	-3.885391	1.080889
H	8.198508	-1.165602	1.031919
H	8.711690	-1.453960	-0.643324
H	6.471447	-0.928864	-1.496807
H	6.436161	0.115742	-0.068729

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RC_GVL (BP86/ZORA/D3)

C	-2.079780399	-3.075262974	0.168944147
C	-0.789043104	-2.667404172	0.517830051
C	-0.568320053	-2.031549049	1.742485097
C	-1.637066966	-1.802888961	2.610385565
C	-2.925457352	-2.209136506	2.260731484
C	-3.145738955	-2.848923429	1.038728801
C	0.357137175	-2.856343657	-0.479063530
O	1.642710920	-2.946896584	0.088693468
C	0.296216324	-1.761905996	-1.484669670
C	0.309475724	-0.947014485	-2.418298134
AU	-0.395001967	0.225490232	-0.726206105
C	-1.106035704	1.556004256	0.605497901
N	-2.400574694	1.703852433	0.995528630
C	-2.505657121	2.676168953	1.970373938
C	-1.245342605	3.148634438	2.191276873
N	-0.402605265	2.448907335	1.350628011
C	-3.523244571	0.925259697	0.478871195
C	1.043268499	2.651697571	1.254246617
O	2.452807338	-0.458364086	0.829559575
C	3.632570247	-0.291681260	0.538063426
O	4.178904659	0.934128813	0.549392937
C	4.655997356	-1.332789331	0.141966952
H	-3.451111284	2.943218853	2.423472256

H	-0.884388118	3.909680956	2.870266099
H	-3.128841127	0.182381560	-0.219909915
H	-4.021312921	0.407214579	1.304171845
H	-4.229793862	1.585057229	-0.036094028
H	1.519106063	1.699975933	0.998403436
H	1.267998308	3.403216774	0.489123125
H	1.416249181	2.992849210	2.224178188
H	0.438939995	-0.516700971	-3.395458777
H	0.190533583	-3.793836334	-1.034904091
H	-4.145787642	-3.186756856	0.769910037
H	-3.754574168	-2.049351592	2.949448854
H	-2.252252172	-3.578197227	-0.783519466
H	-1.458370401	-1.318233541	3.569513867
H	0.437182611	-1.726346656	2.025029472
H	1.899625855	-2.052285115	0.439837219
C	5.776915397	-0.498187130	-0.480712647
C	5.628127559	0.857532432	0.220215745
H	6.142070857	0.855923649	1.192523127
C	6.007133843	2.073824826	-0.588729616
H	5.446517160	2.103475364	-1.531675653
H	5.818810798	2.998208945	-0.031049811
H	7.078234848	2.030893629	-0.825111345
H	5.613001585	-0.376571839	-1.560077485
H	6.775112699	-0.923017654	-0.333952037
H	4.976672621	-1.846383398	1.061604561
H	4.206597314	-2.089858513	-0.509365823

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TS_GVL (BP86/ZORA/D3)

C	2.053685273	-0.325449307	-1.111783441
C	1.789157740	-0.020321347	0.226672537
C	1.668750615	-1.055139792	1.163272907
C	1.808638087	-2.380952961	0.761317699
C	2.059825661	-2.683760261	-0.581423515
C	2.183719838	-1.655400993	-1.516400482
C	1.597870220	1.408984642	0.645872480
O	2.421121032	1.793207113	1.804754889
C	0.225660507	1.767673381	1.195276887
C	0.482085607	2.417347598	2.260539159
AU	-1.513900035	1.053472873	0.408137233
C	-3.071889726	0.113659624	-0.477405561
N	-4.373586043	0.492015962	-0.576061501
C	-5.107846072	-0.454625360	-1.269450744
C	-4.242591970	-1.448179627	-1.612829157
N	-3.001586184	-1.084209500	-1.120363204
C	-4.925516117	1.725655839	-0.023478176

C	-1.783295674	-1.876350254	-1.272346330
O	4.553212138	2.077057883	0.372482193
C	5.115746018	0.994116128	0.246880643
O	5.703472993	0.650050007	-0.905826388
C	5.269742456	-0.106443878	1.276191853
H	-6.167505102	-0.342720421	-1.457247383
H	-4.403415582	-2.368737037	-2.158017877
H	-4.108694459	2.283186918	0.443452744
H	-5.368337217	2.327429517	-0.824452438
H	-5.686712522	1.491080446	0.728650899
H	-0.962299450	-1.343205704	-0.782499506
H	-1.913458425	-2.856170950	-0.800436954
H	-1.551065120	-2.003763488	-2.335127190
H	0.509012204	2.970492976	3.185173049
H	1.813696822	2.080357926	-0.196958142
H	2.387027339	-1.886968513	-2.561267719
H	2.164860028	-3.721802593	-0.894821527
H	2.160396145	0.480867250	-1.837641738
H	1.717347541	-3.183020330	1.492622461
H	1.462312643	-0.812071307	2.205384294
H	3.323896626	2.079484395	1.440567903
C	5.641242179	-1.320927363	0.426333354
C	6.332906227	-0.688789067	-0.788245968
H	7.394975022	-0.492015076	-0.580889038
C	6.163486967	-1.415893673	-2.100217626
H	5.098644727	-1.560698591	-2.321004718
H	6.628813125	-0.863298532	-2.924003280
H	6.642395264	-2.401402835	-2.033382807
H	4.733650076	-1.847437202	0.102480099
H	6.292442668	-2.036846502	0.938132548
H	6.078161506	0.193942550	1.960491146
H	4.355474375	-0.212535085	1.867952519

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PC_GVL (BP86/ZORA/D3)

C	-0.660425454	-4.522888096	-0.235746507
C	-0.915486503	-3.137265430	-0.099672828
C	-2.246413044	-2.720597220	0.130653798
C	-3.269076545	-3.649574215	0.230218340
C	-2.994998117	-5.017139107	0.095089859
C	-1.687710091	-5.451705317	-0.138485338
C	0.207160993	-2.241544159	-0.175215485
O	2.627715881	-0.938154718	0.190250076
C	0.247653251	-0.858741372	-0.098343150
C	1.536326781	-0.284801035	-0.094303346
AU	-1.315654853	0.478020978	-0.031871581

C	-2.838893445	1.830950165	0.014390998
N	-3.342465547	2.486104734	1.097420002
C	-4.379649351	3.327678832	0.732436729
C	-4.532693947	3.197051538	-0.613463809
N	-3.584641558	2.279681030	-1.033555080
C	-2.852227812	2.322941110	2.461863226
C	-3.406379594	1.850280905	-2.416608501
O	4.527730636	0.714391553	-0.013830056
C	5.725144813	0.466492642	0.129301440
O	6.634462708	1.426537790	-0.012866275
C	6.376887865	-0.854315771	0.480689095
H	-4.912261413	3.938298565	1.449443749
H	-5.224527056	3.671904598	-1.296503473
H	-2.038432575	1.591819248	2.440438250
H	-2.477046894	3.279247182	2.843201850
H	-3.657407361	1.957610694	3.109048392
H	-2.593530977	1.118022940	-2.438364468
H	-4.327783837	1.387859538	-2.787803872
H	-3.144239966	2.708292396	-3.045687982
H	1.665807026	0.783611667	-0.305983635
H	1.161602491	-2.754828741	-0.342905941
H	-1.475537684	-6.514388740	-0.244153148
H	-3.804167568	-5.742834348	0.168851900
H	0.362597151	-4.855374396	-0.413595541
H	-4.290661042	-3.317122903	0.409508045
H	-2.456248059	-1.652211886	0.224196620
H	3.454213661	-0.306054268	0.118057399
C	7.844748464	-0.620601366	0.114007316
C	8.000112127	0.898467149	0.260526943
H	8.205554075	1.176479128	1.304393893
C	8.972794619	1.566291386	-0.679700047
H	8.724993922	1.335754946	-1.723403539
H	8.971248859	2.653535952	-0.544685275
H	9.985481771	1.196252135	-0.473110778
H	8.031830003	-0.912525683	-0.927988784
H	8.548350936	-1.164096732	0.752564285
H	6.234807232	-1.016669112	1.560388248
H	5.890956155	-1.684541117	-0.042423376

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RC_water

C	-0.944031	3.291857	-0.343114
C	-1.247063	3.149425	1.018770
C	-2.457289	3.651917	1.507714
C	-3.360405	4.286829	0.650869
C	-3.054999	4.424634	-0.704030

C	-1.844292	3.927444	-1.197124
C	-0.244776	2.510936	1.982520
O	0.925841	3.274430	2.179483
C	0.143139	1.139239	1.546363
C	0.786859	0.140625	1.189514
Au	-1.274260	-0.395665	0.729236
C	-2.884079	-1.411523	0.056363
N	-4.028144	-0.909023	-0.483547
C	-4.874149	-1.933057	-0.872424
C	-4.242193	-3.100768	-0.574421
N	-3.027588	-2.764361	-0.003571
C	-4.326814	0.513545	-0.636920
C	-2.022656	-3.732798	0.432985
O	3.810401	0.675256	-0.160986
S	3.688895	-0.667197	-0.775350
C	5.297748	-1.493276	-0.241253
F	6.366212	-0.826357	-0.732176
O	2.658441	-1.512532	-0.120148
O	3.709288	-0.716545	-2.230052
F	5.350456	-2.767184	-0.695566
F	5.405506	-1.525498	1.108444
H	-4.548683	-4.128137	-0.720826
H	-5.840520	-1.747088	-1.322309
H	-1.219242	-3.190605	0.940376
H	-2.476872	-4.450157	1.125437
H	-1.607147	-4.261289	-0.432594
H	-3.458184	1.090263	-0.304857
H	-4.528677	0.737830	-1.690189
H	-5.196831	0.782692	-0.027237
H	1.557437	-0.577571	0.824295
H	-0.732025	2.427205	2.967322
H	2.932412	2.102803	-0.109074
H	-4.295389	4.685279	1.045513
H	-3.751623	4.929902	-1.373308
H	-2.689471	3.557988	2.570039
H	-1.595884	4.043338	-2.252238
H	0.010505	2.926886	-0.724691
H	1.513691	3.192681	1.366873
O	2.439770	2.971952	-0.032836
H	3.112614	3.652639	-0.193349

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TS_water

C	-0.038446	-2.851069	-1.310571
C	0.544944	-3.476809	-0.200451
C	1.189069	-4.710349	-0.367444

C	1.246854	-5.315253	-1.622773
C	0.663934	-4.686679	-2.724798
C	0.023009	-3.455947	-2.565378
C	0.460344	-2.882343	1.181562
O	-0.777339	-3.263468	1.915847
C	0.408700	-1.380961	1.292099
C	-0.603012	-1.079429	2.004278
Au	1.366710	0.270767	0.537904
C	2.249568	1.886800	-0.320551
N	3.573880	2.103768	-0.563497
C	3.763557	3.315853	-1.203795
C	2.529008	3.867250	-1.365417
N	1.617003	2.983645	-0.819341
C	4.644566	1.183658	-0.198036
C	0.164430	3.182635	-0.826290
O	-3.484497	-0.472423	0.665574
S	-2.756077	0.693633	0.109982
C	-4.154303	1.885044	-0.316657
F	-4.987212	1.344336	-1.232601
O	-1.972364	1.430679	1.119740
O	-2.080784	0.460164	-1.168496
F	-3.649144	3.034433	-0.836162
F	-4.878455	2.205883	0.777822
H	2.227217	4.804576	-1.814079
H	4.744110	3.680533	-1.480117
H	-0.298591	2.548130	-0.062644
H	-0.050874	4.234287	-0.610436
H	-0.247970	2.908251	-1.803593
H	4.192571	0.330758	0.317738
H	5.164818	0.832804	-1.097260
H	5.357749	1.680626	0.470252
H	-1.450879	-0.620478	2.490439
H	1.286009	-3.270396	1.795090
H	-3.176219	-2.118211	0.391190
H	1.749533	-6.275215	-1.740766
H	0.709780	-5.155442	-3.707924
H	1.643966	-5.200418	0.494883
H	-0.435944	-2.962500	-3.421633
H	-0.547020	-1.892498	-1.197369
H	-1.558515	-3.265751	1.266301
O	-2.925900	-3.086916	0.361346
H	-3.704909	-3.562714	0.691086

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INT_water

C	-0.907979	-2.385259	-1.058043

C	-0.304142	-3.163553	-0.059305
C	-0.124478	-4.536281	-0.280177
C	-0.539372	-5.125678	-1.475342
C	-1.145168	-4.344287	-2.460512
C	-1.330853	-2.975217	-2.247210
C	0.144468	-2.558383	1.231333
O	-1.030890	-2.169473	2.157651
C	0.634500	-1.112947	1.334993
C	-0.402905	-0.888169	2.159201
Au	2.082896	0.012185	0.501787
C	3.454211	1.236853	-0.384194
N	4.795676	1.046299	-0.558617
C	5.374546	2.119321	-1.215940
C	4.375262	3.009758	-1.461590
N	3.214013	2.457057	-0.949586
C	5.515220	-0.140467	-0.112303
C	1.900468	3.093794	-1.005088
O	-3.661076	0.743652	1.314897
S	-3.378494	1.513090	-0.009616
C	-5.145549	1.837338	-0.592998
F	-5.800946	0.672277	-0.777884
O	-2.827254	2.813008	0.298877
O	-2.779885	0.661002	-1.018126
F	-5.111455	2.506149	-1.761782
F	-5.819050	2.573414	0.310590
H	4.394071	3.974924	-1.950794
H	6.430211	2.159420	-1.450752
H	1.171190	2.401949	-0.572224
H	1.906583	4.026218	-0.428256
H	1.629384	3.305354	-2.045942
H	4.798234	-0.786749	0.404151
H	5.938227	-0.674794	-0.971726
H	6.319586	0.142153	0.577532
H	-0.824637	-0.089492	2.765973
H	0.744309	-3.270911	1.813770
H	-3.595237	-0.335766	1.246615
H	-0.391192	-6.193659	-1.636245
H	-1.472326	-4.800855	-3.394971
H	0.347154	-5.145697	0.492772
H	-1.806901	-2.361774	-3.011815
H	-1.050166	-1.316837	-0.898014
H	-2.549576	-2.000642	1.603893
O	-3.488461	-1.741012	1.312467
H	-4.097856	-2.128069	1.962097

PC_water

C	0.607788	2.571657	1.974229
C	0.037534	3.330350	0.933950
C	-0.648343	4.511932	1.282997
C	-0.771415	4.912839	2.611058
C	-0.205995	4.141377	3.627955
C	0.483205	2.968407	3.300717
C	0.094891	2.961502	-0.478140
O	-0.534273	1.920416	-3.178600
C	0.667210	1.885782	-1.086279
C	0.523647	1.793110	-2.529381
Au	1.663828	0.262014	-0.314472
C	2.577356	-1.425330	0.401972
N	3.912482	-1.656841	0.570894
C	4.138896	-2.931308	1.062475
C	2.917391	-3.514046	1.206927
N	1.978058	-2.582205	0.802349
C	4.959203	-0.686420	0.272782
C	0.534214	-2.820687	0.785281
O	-3.339349	-0.812761	-1.974062
S	-3.023712	-1.548173	-0.655308
C	-4.710424	-1.505945	0.192511
F	-5.116434	-0.232047	0.373693
O	-2.758730	-2.948285	-0.914228
O	-2.138611	-0.782500	0.206018
F	-4.619934	-2.106623	1.396450
F	-5.633259	-2.151866	-0.545730
H	2.641791	-4.499272	1.559855
H	5.132078	-3.309215	1.267211
H	0.021084	-1.881112	0.560359
H	0.279557	-3.559558	0.017030
H	0.210159	-3.184047	1.766790
H	4.474272	0.225431	-0.090268
H	5.535292	-0.460383	1.178183
H	5.630062	-1.078358	-0.501248
H	1.442320	1.553672	-3.106486
H	-0.386228	3.700217	-1.133027
H	-3.098751	0.290601	-2.003241
H	-1.310874	5.828352	2.853979
H	-0.298108	4.451338	4.668881
H	-1.097017	5.113836	0.491065
H	0.928261	2.362316	4.090331
H	1.154527	1.659285	1.722416
H	-1.914129	1.769008	-2.509594
O	-2.871015	1.585066	-2.161114

H	-3.477185	1.936984	-2.834344

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RC_AuOH

C	1.216983	3.473146	-0.257941
C	0.528485	2.801120	0.760947
C	1.119477	2.671542	2.021333
C	2.387283	3.205322	2.264478
C	3.072963	3.866519	1.244708
C	2.485533	3.996734	-0.017991
C	-0.856460	2.234040	0.505840
O	-0.790140	1.237784	-0.564662
C	-1.813753	3.273089	0.134398
C	-2.612634	4.130332	-0.156456
Au	0.723432	-0.209222	-0.562482
C	2.155353	-1.562282	-0.608315
N	3.468186	-1.385568	-0.276301
C	4.172969	-2.566643	-0.429839
C	3.284126	-3.499633	-0.865826
N	2.055717	-2.872091	-0.970178
C	4.054140	-0.127290	0.173882
C	0.828482	-3.539187	-1.410490
O	-3.048412	0.222391	-0.806387
S	-3.150274	-1.216489	-1.225913
C	-3.538096	-2.068092	0.413710
F	-2.560387	-1.821995	1.327870
O	-4.294502	-1.506910	-2.068516
O	-1.850416	-1.784769	-1.609007
F	-3.615875	-3.407852	0.243890
F	-4.707039	-1.636738	0.929200
H	3.418796	-4.545674	-1.107562
H	5.231407	-2.641459	-0.217989
H	-0.003591	-2.827680	-1.383385
H	0.958697	-3.906226	-2.435104
H	0.611235	-4.380455	-0.742360
H	3.257339	0.621670	0.218014
H	4.493381	-0.253760	1.170347
H	4.827098	0.200907	-0.531113
H	-3.330728	4.877371	-0.419759
H	-1.211767	1.735983	1.422987
H	-1.758698	0.785237	-0.687399
H	2.835990	3.107805	3.253004
H	4.059593	4.289640	1.434256
H	0.583277	2.153731	2.817773
H	3.014637	4.520191	-0.814365
H	0.749630	3.584767	-1.235980

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TS_AuOH

C	-2.588669	4.214417	-0.462238
C	-1.282420	3.773708	-0.795694
C	-0.866283	3.808137	-2.151135
C	-1.729282	4.267809	-3.134768
C	-3.014789	4.700175	-2.788491
C	-3.441434	4.671671	-1.452083
C	-0.372450	3.289893	0.185911
O	-0.872894	0.604988	1.060904
C	-0.614899	3.174266	1.531314
C	-0.752378	2.790731	2.684451
Au	-1.105908	-1.361594	0.849678
C	-1.335368	-3.317130	0.621572
N	-2.495658	-4.044056	0.628819
C	-2.236652	-5.389394	0.440174
C	-0.886535	-5.512021	0.309845
N	-0.351611	-4.242969	0.421735
C	-3.824384	-3.471987	0.804204
C	1.079676	-3.941673	0.346027
O	1.792407	1.250347	0.541075
S	2.818433	0.335453	-0.028003
C	2.710566	0.742184	-1.871021
F	1.469900	0.474886	-2.367655
O	4.193469	0.667514	0.319431
O	2.441415	-1.083026	0.018760
F	3.603231	0.030951	-2.593102
F	2.951868	2.064766	-2.098868
H	-0.270141	-6.386274	0.146203
H	-3.020632	-6.134778	0.411365
H	1.227985	-2.856155	0.325906
H	1.593668	-4.363546	1.217875
H	1.493991	-4.375318	-0.571039
H	-3.705267	-2.391391	0.932374
H	-4.442394	-3.671358	-0.079793
H	-4.305880	-3.897270	1.693196
H	-0.856357	2.519852	3.714354
H	0.632223	2.971311	-0.121671
H	0.110257	0.753261	0.977194
H	-1.407660	4.289670	-4.175089
H	-3.690903	5.061859	-3.563126
H	0.133949	3.458388	-2.405093
H	-4.445057	5.009177	-1.195792
H	-2.906381	4.183227	0.579541

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PC_AuOH

C	3.908966	-2.398672	0.982417
C	4.120021	-2.130404	-0.382558
C	5.439682	-1.964759	-0.837219
C	6.517227	-2.063395	0.042830
C	6.293940	-2.329399	1.394604
C	4.984202	-2.496785	1.859207
C	3.007651	-2.021516	-1.340304
O	-0.442289	-1.320521	-0.509238
C	1.723772	-2.146456	-1.069578
C	0.446856	-2.324003	-0.841746
Au	0.109514	0.598497	0.057573
C	0.564957	2.427505	0.615495
N	1.794178	3.019770	0.618401
C	1.706710	4.319951	1.085201
C	0.397352	4.544224	1.379712
N	-0.288362	3.378307	1.089539
C	3.032869	2.369940	0.201162
C	-1.733618	3.207235	1.250506
O	-2.567830	-2.181298	0.288446
S	-3.561413	-1.175156	0.836939
C	-4.738423	-0.975223	-0.623667
F	-4.072983	-0.527353	-1.715445
O	-4.375201	-1.717827	1.905209
O	-2.970807	0.154937	1.004509
F	-5.702297	-0.078975	-0.319669
F	-5.326048	-2.147116	-0.936448
H	-0.098833	5.423132	1.769676
H	2.571989	4.963744	1.171685
H	-1.988801	2.149770	1.126411
H	-2.026957	3.535444	2.253771
H	-2.264898	3.801701	0.497737
H	2.789530	1.350636	-0.113959
H	3.480002	2.917293	-0.636958
H	3.739285	2.334010	1.038577
H	-0.027455	-3.305741	-0.917422
H	3.304289	-1.809437	-2.375900
H	-1.444537	-1.704835	-0.137714
H	7.534070	-1.936606	-0.329072
H	7.134175	-2.410255	2.083951
H	5.616821	-1.762024	-1.894915
H	4.804221	-2.708969	2.913350
H	2.888430	-2.532552	1.342616