Supporting Information for

Hydrothiolation of alkynes with thiol-catechol derivatives catalysed by CuNPs/TiO_2: exploring the reaction mechanism by DFT calculations

Matías Capurso, Gabriel Radivoy, Fabiana Nador and Viviana Dorn*

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S1. Representative procedure for the synthesis of CuNPs/support catalysts

Anhydrous copper(II) chloride (134 mg, 1 mmol) was added to a suspension of lithium (21 mg, 3 mmol) and 4,4-di-tert-butylbiphenyl (DTBB, 27 mg, 0.1 mmol) in THF (3 mL) at room temperature under a nitrogen atmosphere. The reaction mixture, which was initially brown, rapidly changed to black, indicating that the suspension of copper nanoparticles was formed. This suspension was diluted with THF (3 mL) followed by the addition of 0.8 g of the corresponding support (ZnO, basic Al_2O_3, MgO, C*, Cellulose, MCM41, Zy). The resulting mixture was stirred for 1 h at room temperature, quenched with water and then filtered. The solid was successively washed with EtOH (15 mL) and dried under vacuum.

S2. Study of the TYC reaction with different CuNPs/support catalysts [1]

For this study, thiol **1** (0.2 mmol) and alkyne **2** (0.2 mmol) were added to a reaction tube containing CuNPs/support catalyst (60 mg) in 1,2-DCE (2 mL) under air. The reaction mixture was heated at 80 °C for 48 h. The catalyst was removed by filtration and washed with hexane-AcOEt. Finally, the filtrate was concentrated under vacuum and the reaction crude was analysed by ^{1}H NMR. The results obtained are shown in **Table S1**.

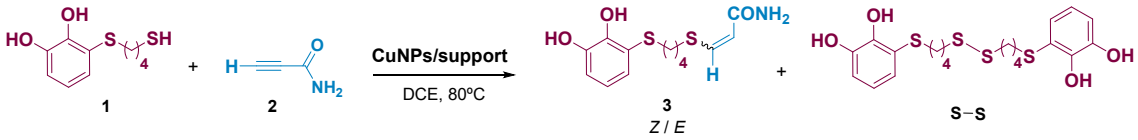


Table S1. TYC reaction with different catalysts

Entry	Catalyst	Conv. *Z* + *E* (%)	Conv. S-S (%)	Selectivity *Z* : *E*
1	$CuNPs/TiO_2$	87	10	86:14
2	$CuNPs/ZnO$[a]	72	-	85:15
3	$CuNPs/Al_2O_3$	68	25	95:5
4	CuNPs/MgO	47	-	88:12

General conditions: alkyne **1** (0.1 mmol), thiol **2** (0.1 mmol), catalyst (30 mg), DCE (1mL) and heating at 80 °C.
[a] other by-products.

S3. General computational procedures

Calculations were performed with ORCA version 4.2.1 [2]. All geometries were optimised in the gas phase using the PBE density functional theory method [3] with D3BJ dispersion correction [4] and the double-ζ def2-SVP basis set for all atoms. [5] For open-shell systems, the unconstrained formalism was adopted. Harmonic frequency calculations were carried out at the same level of theory in order to identify each stationary point as either a minimum (no imaginary frequency) or a transition state (one single imaginary frequency). The transitions states were obtained using scan or NEB [6] keywords followed by the corresponding optTS calculations.

The electronic energies were then improved through single point calculations using the hybrid-GGA functional PBE0 [7], and triple-ζ def2-TZVP basis set [5]. Solvent effects were introduced through the implicit solvation model CPCM [8] for the experimental solvent dichloromethane (DCM) with a dielectric constant of 9.08 as provided for the library of solvents of ORCA 4.2.1.

Electronic energies of structures IN-1, TS-1, IN-2, IN-3, TS-3 and IN-4 were also obtained with B3LYP [9] functional applying the D3BJ dispersion correction as implemented in ORCA 4.2.1, and the 6-311+G* basis set for all atoms. Solvent effects were introduced in the same way as with the aforementioned methodology.

The molecular images presented were obtained with Chemcraft [10], non-relevant hydrogens were removed for clearer viewing.

Example of the ORCA input for geometry optimisation.

```
! UKS OPT PBE D3BJ DEF2-SVP SlowConv PAL4
%scf
MaxIter 999
end
* xyz 0 2
coordinates
*
```

Example of the ORCA input for single point energy calculations.

```
! UKS SP PBE0 D3BJ DEF2-TZVP TightSCF CPCM(CH2Cl2) PAL4
%scf MaxIter 999 end
*xyz 0 2
coordinates
*
```

Example of the ORCA input for NEB-TS calculations.

```
! UKS NEB-TS PBE D3BJ DEF2-SVP PAL4
%NEB NEB_END_XYZFILE "filename.xyz"
END
* xyz 0 2
coordinates
*
```

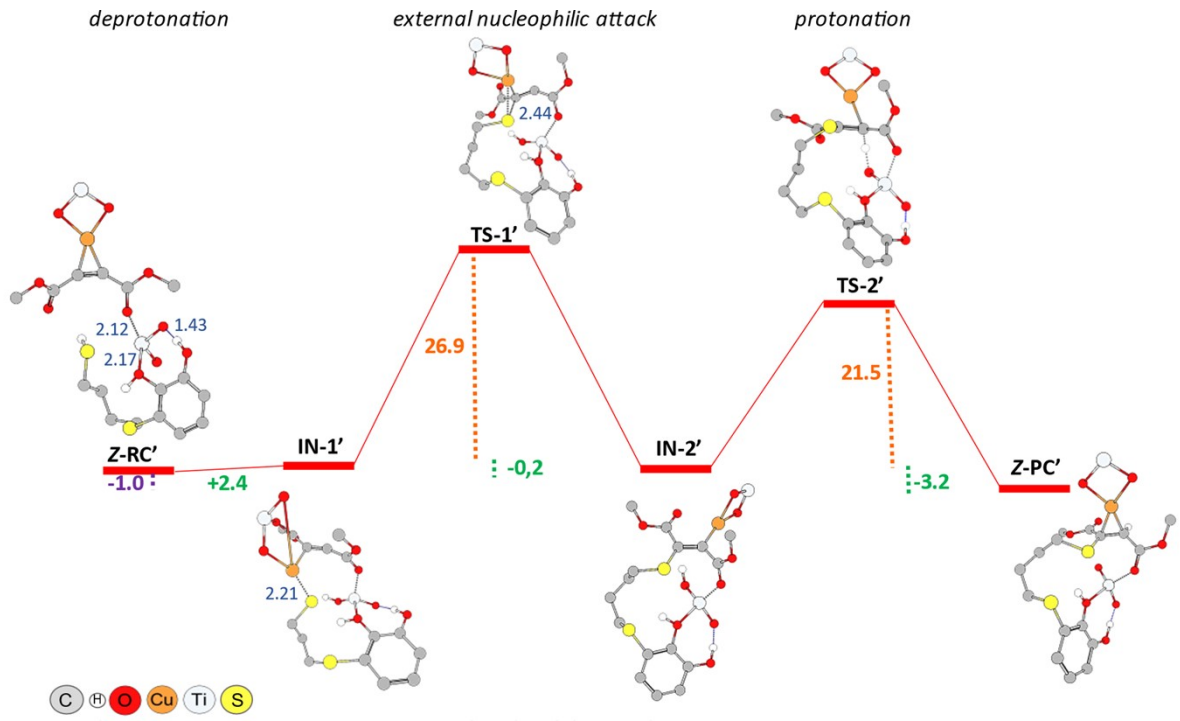


Figure S1. PBE0-D3BJ / Def2-TZVP / CPCM=DCM potential energy profile (kcal/mol) for the thiol deprotonation, nucleophilic addition and protonation steps in the formation of *Z*-vinyl sulphide derived from thiol-catechol 1 and dimethyl acetylenedicarboxylate. Interatomic distances (Å) are detailed in blue.

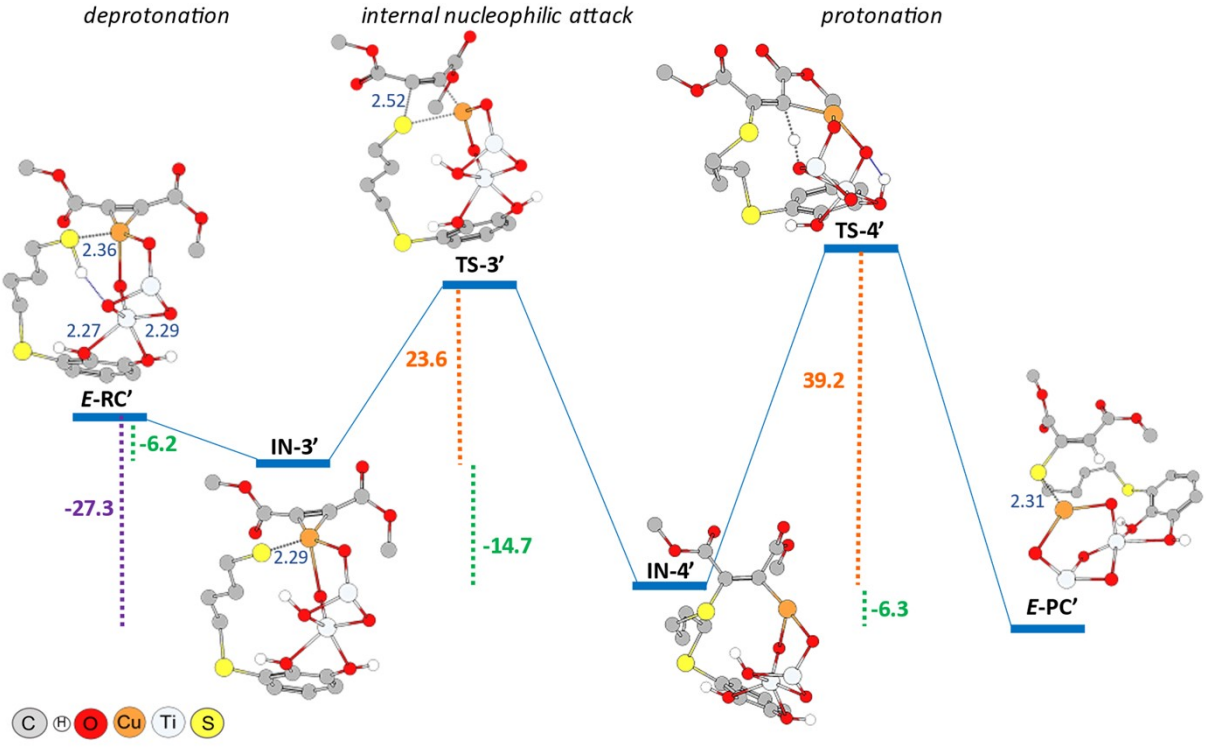
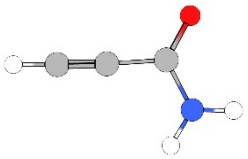


Figure S2. PBE0-D3BJ / Def2-TZVP / CPCM=DCM potential energy profile (kcal/mol) for the thiol deprotonation, nucleophilic addition and protonation steps in the formation of *E*-vinyl sulphide derived from thiol-catechol 1 and dimethyl acetylenedicarboxylate. Interatomic distances (Å) are detailed in blue.

S4. Cartesians coordinates and Energies of Reactive and copper catalysts structures

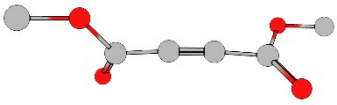
propiolamide
Energy: -245.87096446075Eh
0 1

C	-4.46500	0.31193	-0.00000
C	-3.26445	0.47851	0.00001
H	-5.52819	0.17877	0.00004
C	-1.83008	0.74915	-0.00007
O	-1.38080	1.89015	0.00005
N	-1.05422	-0.37577	-0.00002
H	-1.46464	-1.30138	-0.00006
H	-0.04570	-0.26775	-0.00001



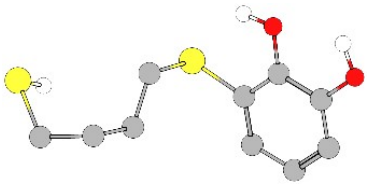
dimethyl acetylenedicarboxylate
Energy: -532.714858164127Eh
0 1

O	-2.72117	0.81405	0.45253
O	2.72117	0.81413	-0.45212
O	-2.53475	-0.80024	-1.14721
O	2.53478	-0.79997	1.14781
C	-4.14398	0.80033	0.26416
C	4.14399	0.80043	-0.26379
C	-2.03615	-0.04890	-0.32924
C	2.03616	-0.04870	0.32979
C	-0.60941	0.03192	-0.07256
C	0.60943	0.03197	0.07303
H	-4.40475	1.06286	-0.78082
H	-4.54998	1.55046	0.96479
H	-4.56037	-0.20297	0.48592
H	4.54997	1.55047	-0.96452
H	4.56037	-0.20290	-0.48544
H	4.40479	1.06308	0.78116



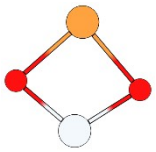
3-((4-mercaptobutyl)thio)benzene-1,2-diol
Energy: -1335.70125443241 Eh
0 1

O	-3.21389	6.72090	1.49179
O	-2.28299	4.98092	-0.37609
C	-2.55512	5.59337	1.89251
C	-2.06609	4.68214	0.93854
C	-2.35692	5.33757	3.24805
C	-1.66931	4.18868	3.65452
C	-1.18156	3.28228	2.71428
C	-1.38834	3.52342	1.34825
H	-0.63853	2.38895	3.02158
H	-2.73983	6.05498	3.97473
H	-1.51257	4.00523	4.71808
S	-0.79272	2.44096	0.06960
C	-2.26228	1.37593	-0.21335
S	-2.29408	-2.07232	-1.16518
C	-3.34162	-1.88978	0.32772
C	-2.63758	0.50996	0.98554
H	-1.99051	0.75890	-1.08228
H	-3.10773	2.01375	-0.51086
C	-3.78608	-0.47042	0.67798
H	-2.92162	1.17249	1.81594
H	-1.74781	-0.04404	1.33044
H	-4.41185	-0.07102	-0.13699
H	-4.44453	-0.55008	1.55985
H	-2.81083	-2.35269	1.17189
H	-4.21699	-2.52028	0.11486
H	-1.78631	4.28464	-0.87939

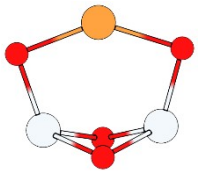


H -3.22489 6.71420 0.51488
H -1.15589 -1.58021 -0.62317

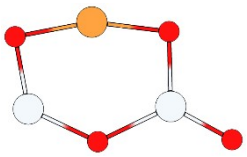
I structure
Energy: -2639.99196595291 Eh
0 2
O 0.78849 -0.532312 -0.71564
Ti 1.414960 0.000611 0.80733
O 0.93981 -1.161681 1.99946
Cu 0.10161 -2.020166 0.41323



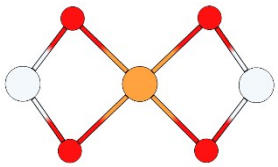
II structure
Energy: -3639.86021355048 Eh
0 2
O 1.45644 0.383663 -0.398256
Ti 0.243412 0.449174 1.009961
Ti 2.274624 -0.991810 0.549571
O 1.57293 -0.252266 2.105486
Cu -0.10795 -2.072845 0.387617
O 1.68951 -2.595846 0.172173
O -1.16317 -0.571536 0.815753



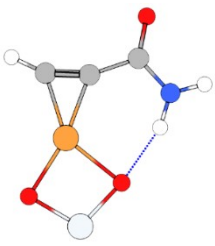
III structure
Energy: -3639.824434684238 Eh
0 2
O 1.219558 0.4410450 -0.2458650
Ti 1.321182 -0.0292400 1.4400820
O 0.766738 -1.636601 2.13123900
Cu 0.437448 -1.198466 -0.6730430
O -0.272310 -2.9125040 -0.5334520
Ti -0.039186 -3.1449780 1.2243030
O -0.532030 -4.570376 1.9432450



IV structure
Energy: -3639.696633224879 Eh
0 2
O 0.912040 -0.3105600 -0.287942
Ti 1.5628390 0.248129 1.203741
O 1.272586 -0.9678420 2.373306
Cu 0.415944 -1.866253 0.798322
O -0.454671 -2.7648830 -0.796867
Ti -0.737083 -3.9821120 0.371285
O -0.086874 -3.437518 1.859376



I-A structure
Energy: -2885.929468406649 Eh
0 2
Ti -0.74246 -0.18530 -1.53635
Cu -0.17987 -0.07933 0.96809
O -0.37885 -1.50520 -0.48992
O -0.63636 1.16945 -0.49769
C 0.22370 0.27259 2.84379
C 0.28649 -0.96460 2.62255
H 0.27426 1.18362 3.42081
C 0.48593 -2.41296 2.88463
O 0.79044 -2.79411 4.01105
N 0.30152 -3.19763 1.79788
H 0.05163 -2.78681 0.88928
H 0.43200 -4.19751 1.90439

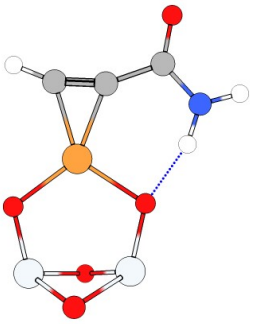


II-A structure

Energy: -3885.771815656656 Eh

0 2

O	-2.211500	-0.085360	-1.99249
Ti	-0.962200	1.264010	-1.78983
Ti	-0.778290	-1.236460	-1.98973
O	0.290630	0.143890	-2.56335
Cu	-0.21286	-0.158370	0.83401
O	-0.366070	-1.742040	-0.39655
O	-0.608080	1.504280	-0.14818
C	0.206640	0.240510	2.73528
C	0.278870	-1.009630	2.56141
H	0.237530	1.207610	3.23502
C	0.501910	-2.448490	2.89479
O	0.822120	-2.775530	4.03456
N	0.315550	-3.278140	1.83932
H	0.049890	-2.889260	0.91192
H	0.462200	-4.276700	1.98845

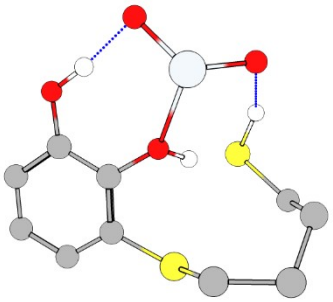


S-T structure

Energy: -2335.44193262496 Eh

0 2

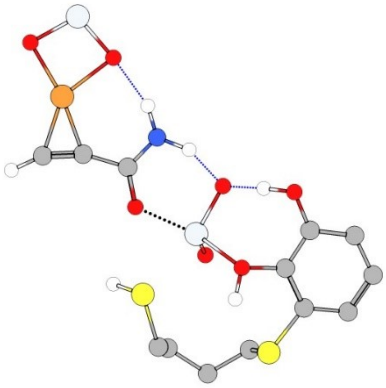
Ti	0.410659	-1.086057	0.816404
O	0.615307	0.567203	0.841883
O	-0.324026	-1.642751	2.207606
O	2.298898	-1.801080	1.038479
C	3.525988	-1.589099	0.410209
C	4.394836	-2.694387	0.241851
C	5.648218	-2.511906	-0.367458
H	6.315461	-3.376363	-0.489576
C	6.014811	-1.230741	-0.811420
H	6.994536	-1.078668	-1.288188
C	5.145807	-0.148025	-0.664560
H	5.418108	0.858924	-1.011883
C	3.878341	-0.288228	-0.043637
O	3.128433	0.810827	0.086714
S	3.984672	-4.290633	0.928289
S	2.035161	-2.966828	3.682034
C	1.572801	-4.719264	3.349628
C	0.767107	-5.013680	2.067657
H	1.008479	-5.045859	4.244916
H	2.538543	-5.262258	3.356188
C	1.522715	-5.636806	0.880851
H	0.220262	-4.095588	1.757859
H	-0.028843	-5.734373	2.349945
C	2.424840	-4.730956	0.040921
H	0.765518	-6.060169	0.185636
H	2.109444	-6.513969	1.235597
H	1.900163	-3.790454	-0.220434
H	2.703721	-5.232363	-0.907714
H	2.388912	-2.349846	1.978833
H	2.189451	0.681523	0.459053
H	0.783735	-2.398461	3.416966



S5. Cartesians coordinates, first frequency for TS and Energies of Z-RC, IN-1, TS-1, IN-2, TS-2, Z-PC, Z-VS (*Z*-vinyl sulphide derived from propiolamide)

Z-RC structure

Energy: -5221.44098966364 Eh



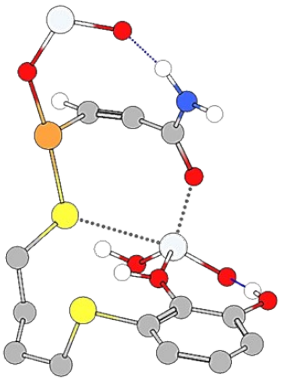
0 2

Ti	0.603920	-1.72603	3.549110
O	0.89036	-0.017980	3.72053
O	-0.29793	-2.06645	2.203300
O	2.61061	-2.067570	2.80259
C	3.129680	-1.40865	1.685110
C	3.490530	-2.20667	0.576710
C	4.123760	-1.64317	-0.543070
H	4.40938	-2.283900	-1.388460
C	4.376150	-0.26246	-0.539900
H	4.87470	0.203210	-1.403670
C	3.986580	0.533070	0.54373
H	4.16841	1.618020	0.548540
C	3.340770	-0.00099	1.689120
O	3.01332	0.803480	2.693480
S	3.166280	-3.96206	0.718180
S	1.117090	-4.28319	4.617580
C	1.203180	-5.45528	3.188840
C	0.148840	-5.23918	2.091010
H	1.17088	-6.477180	3.615870
H	2.23317	-5.301260	2.808060
C	0.683120	-5.31641	0.649590
H	-0.31551	-4.235050	2.20739
H	-0.66026	-5.987340	2.22690
C	1.390570	-4.04452	0.163560
H	-0.18754	-5.463640	-0.02343
H	1.32886	-6.211460	0.499480
H	0.86880	-3.143920	0.553110
H	1.41662	-4.002180	-0.943340
H	2.73524	-3.038740	2.539340
H	2.14307	0.476990	3.185600
Ti	-2.828000	2.50126	9.135680
Cu	-2.62540	0.06943	8.337750
O	-1.93637	1.894660	7.80128
O	-3.51517	1.085760	9.77808
C	-2.62897	-1.850100	7.908200
C	-1.91632	-1.207220	7.077930
C	-1.02650	-0.905350	5.944810
O	-0.64330	-1.88864	5.226320
N	-0.67933	0.352420	5.74277
H	-1.03914	1.085190	6.386620
H	-0.00542	0.484830	4.900420
H	-3.11300	-2.713780	8.36537
H	-0.22106	-4.367630	4.86087

IN-1 structure

Energy: -5221.4484590237 Eh

Energy: -5222.51487709561 Eh B3LYP/6311+G*/CPCM=DCM



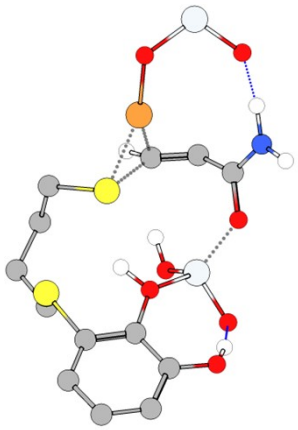
0 2

Ti	0.155034	-0.991816	1.581694
O	0.33034	0.11073	0.380952
O	-1.27852	-1.984035	1.082922
O	2.10860	-1.72960	1.396513
C	3.32774	-1.467585	0.767007
C	4.30591	-2.489032	0.828527
C	5.58817	-2.297621	0.292909
H	6.33173	-3.10328	0.367256
C	5.88243	-1.069795	-0.319838

H	6.87963	-0.89544	-0.749960
C	4.91372	-0.065583	-0.393193
H	5.12706	0.900290	-0.873438
C	3.60853	-0.222503	0.139363
O	2.77084	0.81021	0.039391
S	3.841991	-3.991878	1.676266
S	0.131269	-3.470628	3.339616
C	0.91369	-5.064978	2.860284
C	0.78821	-5.314283	1.344571
H	0.41878	-5.86870	3.440694
H	1.97473	-5.03598	3.177859
C	2.03205	-5.953655	0.706751
H	0.56892	-4.35438	0.826661
H	-0.10127	-5.949200	1.155686
C	3.09755	-4.949818	0.265809
H	1.73724	-6.50919	-0.20910
H	2.47188	-6.71578	1.387605
H	2.66064	-4.20008	-0.424820
H	3.93597	-5.45189	-0.257180
H	2.24994	-2.606000	1.90277
H	1.79218	0.5603538	0.17298
Ti	0.40056	-2.0160359	8.50743
Cu	-0.0381	-3.2417001	5.51082
O	0.59930	-0.552081	7.73525
O	0.06274	-3.256360	7.36420
C	-1.70651	-1.942116	5.33440
C	-1.14633	-0.891387	4.95388
C	-0.08173	-0.068513	4.48139
O	0.09895	0.102593	3.21022
N	0.72134	0.496175	5.37459
H	0.67628	0.166823	6.42119
H	1.49965	1.049026	5.00446
H	-2.56876	-2.523762	5.65950
H	-1.37425	-2.710046	1.74988

TS-1 structure (-157.79 cm^{-1})
Energy: -5221.43831242394 Eh
Energy: -5222.50075819525 Eh B3LYP/6311+G*/CPCM=DCM
0 2

Ti	0.667640	-0.7080499	1.669903
O	0.884663	0.450179	0.532078
O	-0.483818	-1.961630	1.00162
O	2.626805	-1.396902	1.69113
C	3.675251	-1.3398801	0.766383
C	4.378214	-2.5381792	0.515816
C	5.515073	-2.5338955	-0.30787
H	6.057668	-3.472359	-0.48533
C	5.927431	-1.3211296	-0.88228
H	6.820891	-1.296133	-1.52366
C	5.201531	-0.1453328	-0.66495
H	5.500502	0.806259	-1.12747
C	4.046471	-0.1158947	0.15263
O	3.412210	1.049078	0.33810
S	3.8061707	-4.016323	1.34100
S	1.4361845	-3.372416	3.76359
C	1.171663	-5.1495543	3.35713
C	0.597270	-5.4496833	1.96547
H	0.491055	-5.530303	4.14399
H	2.149346	-5.649305	3.51587
C	1.586515	-5.6455991	0.80756
H	-0.134299	-4.662086	1.68683
H	0.011601	-6.390015	2.05576
C	2.325026	-4.4073224	0.29632



H	1.010616	-6.045696	-0.05394
H	2.321059	-6.440245	1.06637
H	1.646101	-3.529470	0.26935
H	2.710292	-4.576816	-0.72813
H	2.709311	-2.293170	2.17556
H	2.416777	0.910237	0.45462
Ti	-0.353115	-2.0260704	8.69170
Cu	0.490382	-3.014053	5.82658
O	-0.806056	-0.659983	7.85887
O	0.603020	-3.036882	7.67454
C	-0.646710	-2.852445	4.15286
C	-1.016089	-1.620348	4.41179
C	-0.378566	-0.356276	4.43151
O	0.113425	0.133602	3.30213
N	-0.295939	0.398519	5.52413
H	-0.578971	0.022294	6.49693
H	0.186667	1.293492	5.42364
H	-1.213515	-3.767013	3.90755
H	-0.881522	-2.501801	1.71798

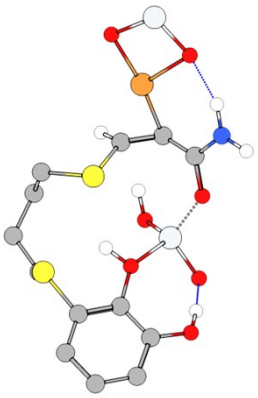
IN-2 structure

Energy: -5221.47070355175 Eh

Energy: -5222.52615406456 Eh B3LYP/6311+G*/CPCM=DCM

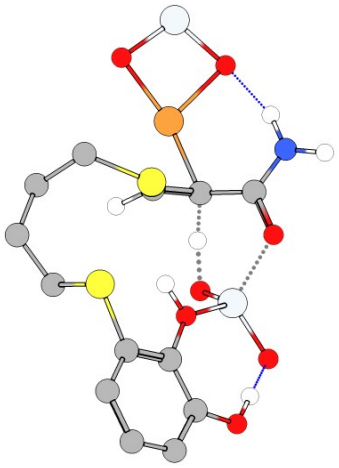
0 2

Ti	0.699420	-0.640380	1.6788300
O	0.851040	0.50221	0.5079000
O	-0.610240	-1.83464	1.229110
O	2.610620	-1.41547	1.519630
C	3.658680	-1.368940	0.5973600
C	4.390420	-2.560850	0.4017700
C	5.524560	-2.572960	-0.4246600
H	6.087530	-3.50667	-0.558630
C	5.907460	-1.379510	-1.0576200
H	6.798030	-1.36474	-1.703430
C	5.158070	-0.210730	-0.8905200
H	5.437170	0.72498	-1.3960600
C	4.004140	-0.164320	-0.0697800
O	3.356600	0.99769	0.0610200
S	3.844960	-4.007200	1.2986800
S	1.551310	-3.256410	3.8623200
C	1.364820	-5.024610	3.4050700
C	0.675590	-5.325150	2.0613900
H	0.804630	-5.47453	4.249490
H	2.389570	-5.44480	3.448510
C	1.590010	-5.633790	0.8665500
H	-0.001890	-4.48695	1.791810
H	0.020500	-6.20940	2.211500
C	2.370560	-4.464520	0.2684600
H	0.953620	-6.03436	0.048570
H	2.291190	-6.45773	1.127370
H	1.719880	-3.57239	0.161220
H	2.764630	-4.72493	-0.733280
H	2.701570	-2.29317	2.035650
H	2.369960	0.87152	0.2669200
Ti	-0.892260	-2.433110	8.8298700
Cu	-0.77496	-2.53660	6.2475200
O	-0.809180	-1.09273	7.779870
O	-0.877940	-3.77372	7.785280
C	-0.186810	-2.86366	4.249930
C	-0.647860	-1.60544	4.583850
C	-0.037260	-0.33644	4.521340
O	0.412580	0.16990	3.3763000
N	0.023910	0.47505	5.5931900



H -0.307100 0.11196 6.510210
H 0.379000 1.42215 5.4721400
H -0.856530 -3.70376 3.975160
H -1.001730 -2.25945 2.023990

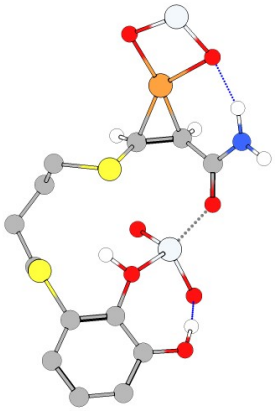
TS-2 structure (-1043.82 cm^{-1})
Energy: -5221.45600127691 Eh
0 2



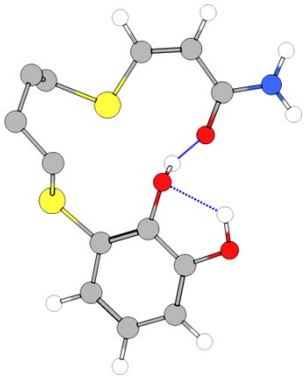
Ti -0.636109 2.636468 -0.279647
O -0.247654 3.988427 -1.162156
O -2.284732 2.150296 -0.534137
O 0.919492 1.313079 -0.846219
C 1.838433 1.188662 -1.899530
C 2.471571 -0.069740 -2.042350
C 3.419929 -0.300834 -3.050252
H 3.903479 -1.284439 -3.121640
C 3.725495 0.746402 -3.933006
H 4.462333 0.592877 -4.735792
C 3.103352 1.987466 -3.794898
H 3.336115 2.821874 -4.472607
C 2.150001 2.268297 -2.777925
O 1.665821 3.503286 -2.738496
S 2.0974932 -1.320421 -0.823687
S -0.044722 -0.723085 1.783353
C -0.204577 -2.557122 1.732876
C -0.768604 -3.196283 0.460327
H -0.854656 -2.809339 2.595704
H 0.818180 -2.926225 1.953895
C 0.134160 -3.319840 -0.774360
H -1.719018 -2.694391 0.179695
H -1.073818 -4.224686 0.750377
C 0.532782 -2.033216 -1.509799
H -0.409949 -3.951979 -1.508392
H 1.053455 -3.893900 -0.521101
H -0.271050 -1.267728 -1.464933
H 0.744930 -2.243036 -2.576049
H 1.033111 0.456639 -0.302123
H 0.901656 3.688835 -2.068015
Ti -3.802703 -1.056820 5.297742
Cu -2.94460 -0.289861 2.999057
O -3.475844 0.54952 4.800706
O -3.371208 -1.99060 3.943344
C -1.714788 -0.21984 1.427709
C -2.224117 1.05730 1.744193
C -1.468521 2.12009 2.409888
O -0.648656 2.84414 1.712630
N -1.702436 2.44558 3.683561
H -2.377884 1.88302 4.244498
H -1.265314 3.29006 4.056596
H -2.187510 -0.77092 0.594019
H -2.613313 1.61196 0.566944

Z-PC structure
Energy: -5221.49298035997 Eh
0 2
Ti 0.907307 -0.76518 1.60261
O 1.01253 0.35291 0.33293
O -0.04042 -2.08151 1.20198
O 2.92066 -1.35848 1.66848
C 3.83765 -1.36425 0.61827
C 4.51889 -2.57332 0.37191
C 5.54558 -2.63285 -0.58448
H 6.07569 -3.57864 -0.76144

C 5.85804 -1.46158 -1.29410
H 6.66491 -1.47905 -2.04275
C 5.13809 -0.27797 -1.08618
H 5.35807 0.63060 -1.66594
C 4.08351 -0.18493 -0.14057
O 3.41480 0.94846 0.02305
S 3.978713 -3.99055 1.32798
S 1.400023 -3.12740 4.02720
C 1.38689 -4.88061 3.47051
C 0.72286 -5.13445 2.10241
H 0.89801 -5.44670 4.28807
H 2.46107 -5.15416 3.48310
C 1.66065 -5.56631 0.96377
H 0.17971 -4.21936 1.76747
H -0.03728 -5.93100 2.24060
C 2.48356 -4.45038 0.32101
H 1.02628 -5.98464 0.15334
H 2.32197 -6.40291 1.28485
H 1.85588 -3.54442 0.18985
H 2.87552 -4.76200 -0.66644
H 3.02350 -2.27756 2.08903
H 2.37020 0.76512 0.19138
Ti -0.98115 -2.71606 8.63916
Cu -0.84973 -2.64732 6.07088
O -1.02295 -1.31553 7.64868
O -0.81694 -3.98441 7.51823
C -0.34362 -2.84508 4.08892
C -0.93638 -1.60682 4.40964
C -0.16949 -0.31438 4.46826
O 0.44257 0.10732 3.44657
N -0.21892 0.38259 5.60266
H -0.60352 -0.06951 6.46758
H 0.26477 1.28316 5.63872
H -0.96061 -3.62061 3.60696
H -1.99868 -1.47869 4.12950



Z-VS structure
Energy: -1581.64272400092 Eh
0 1
O 2.0269741 -1.3662373 0.942205
C 3.33936711 -1.371608 0.5264736
C 4.16993396 -2.511031 0.4747638
C 5.49226145 -2.376443 -0.0103468
H 6.1307931 -3.2704303 -0.059352
C 5.96846877 -1.129706 -0.4376675
H 6.9993280 -1.0427623 -0.812426
C 5.13979184 0.0030883 -0.421070
H 5.4906582 0.9840822 -0.7714436
C 3.82454665 -0.121793 0.0528069
O 2.9768267 0.9333904 0.088502
S 3.67715934 -4.1209948 1.057682
S 1.73209529 -3.4256719 3.523135
C 1.43901845 -5.235465 3.3529881
C 0.64732321 -5.642730 2.1041919
H 0.9308478 -5.5783247 4.277117
H 2.4534065 -5.6820397 3.351261
C 1.40995276 -5.685263 0.7699137
H -0.2388061 -4.9776932 2.009293
H 0.2419058 -6.6616520 2.288312
C 2.03276518 -4.377639 0.2661381
H 0.6948334 -6.0328998 -0.005982
H 2.1973363 -6.4719697 0.817640
H 1.3992137 -3.4958533 0.489128



H	2.1980144	-4.4240379	-0.829045
H	1.9710364	-1.2617129	1.940429
H	2.1410318	0.5345629	0.4353075
C	0.22439062	-2.952836	4.2449214
C	-0.1737133	-1.6666856	4.485074
C	0.64202516	-0.509355	4.1008567
O	1.7139407	-0.6126259	3.463404
N	0.1763949	0.7210379	4.4702728
H	-0.6636480	0.8412650	5.031794
H	0.7352154	1.5384612	4.2268202
H	-0.4531252	-3.7747985	4.533746
H	-1.1448552	-1.5023531	4.976843

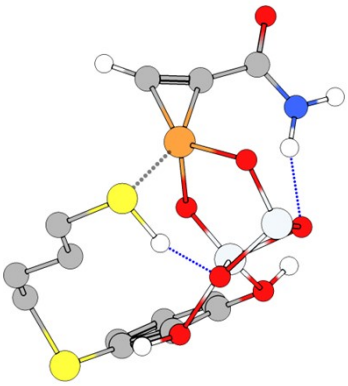
S6. Cartesians coordinates, first frequency for TS and Energies of E-RC, IN-3, TS-3, IN-4, TS-4, E-PC, E-VS (*E*-vinyl sulphide derived from propiolamide)

E-RC structure

Energy: -5221.52350020803 Eh

0 2

O	0.815858	1.31108	0.762664
Ti	0.463826	0.566730	2.420964
Ti	1.574090	-0.354470	0.261989
O	1.705821	-0.79610	2.122488
Cu	-1.405319	-1.54288	1.14528
O	0.394481	-1.28021	-0.46073
O	-1.097600	-0.11259	2.49624
O	3.397146	-1.55428	-0.30300
C	3.505932	-1.58443	-1.666383
C	3.904296	-2.74011	-2.358589
C	4.009083	-2.69266	-3.763636
H	4.340286	-3.58847	-4.307459
C	3.674551	-1.51627	-4.448494
H	3.754821	-1.47979	-5.544606
C	3.217799	-0.37800	-3.753931
H	2.920887	0.53227	-4.296894
C	3.123856	-0.42323	-2.361699
O	2.637465	0.58476	-1.546169
S	4.167032	-4.202838	-1.363807
S	-0.330903	-3.08243	2.553446
C	0.356510	-4.52655	1.636166
C	1.288803	-4.16325	0.484893
H	-0.529460	-5.08284	1.266186
H	0.864155	-5.17789	2.378975
C	1.790695	-5.38628	-0.287378
H	2.152684	-3.60452	0.906334
H	0.772228	-3.44871	-0.191443
C	2.525468	-5.06775	-1.589301
H	0.920134	-6.01937	-0.574278
H	2.423908	-6.03033	0.362460
H	1.919804	-4.40354	-2.237203
H	2.748962	-5.99389	-2.155045
H	0.789165	-2.21136	2.455473
H	3.589532	-2.48896	0.006171
H	2.143423	1.26387	-2.045958
C	-2.89063	0.534315	-0.694403
C	-2.75127	-2.122397	-0.221201
C	-2.64765	-0.863952	-0.255677
N	-1.86605	1.399721	-0.477240
O	-3.95488	0.829232	-1.238369
H	-0.97361	1.167782	-0.005299
H	-3.11811	-3.108828	-0.498489
H	-2.02306	2.365149	-0.768442



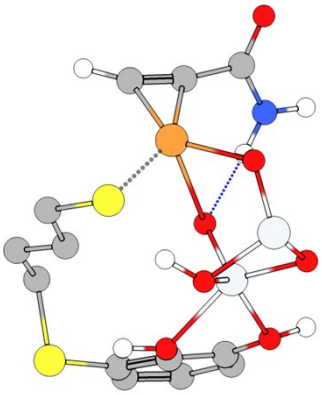
IN-3 structure

Energy: -5221.53628957496 Eh

Energy: -5222.60407945043 Eh B3LYP/6311+G*/CPCM=DCM

0 2

O	0.098693	3.484838	1.430188
Ti	-0.589881	2.7301443	2.9520232
Ti	0.601105	1.7990743	0.7945938
O	0.575363	1.185097	2.710156
Cu	-2.57217	0.3508954	2.358282
O	-0.596834	1.144009	-0.142798
O	-2.196952	2.223500	2.909631
O	2.241325	0.364376	0.316253
C	2.512916	0.4262243	-1.0235150
C	2.789427	-0.7253811	-1.778381
C	3.083221	-0.5854623	-3.148582
H	3.316933	-1.480605	-3.741557
C	3.052417	0.6851173	-3.7418337
H	3.282662	0.795173	-4.811100
C	2.703975	1.8280905	-2.9942601
H	2.638522	2.816536	-3.474641
C	2.419707	1.6871737	-1.6351017
O	1.992886	2.691970	-0.777610
S	2.656942	-2.2757854	-0.8981649
S	-1.220144	-1.0239317	3.568484
C	-0.898309	-2.398159	2.382385
C	-0.054601	-1.986184	1.178264
H	-1.874908	-2.802647	2.043084
H	-0.396348	-3.210553	2.950051
C	0.137895	-3.0910980	0.1344846
H	0.936161	-1.652368	1.562576
H	-0.523956	-1.101841	0.694938
C	0.837264	-2.6333246	-1.145816
H	-0.861362	-3.469532	-0.177112
H	0.665492	-3.967055	0.572504
H	0.384515	-1.694834	-1.524701
H	0.776822	-3.400871	-1.942692
H	0.092007	0.290801	3.014055
H	2.249005	-0.614897	0.552328
H	1.724972	3.503134	-1.251989
C	-4.217059	1.853909	0.1975190
C	-3.833010	-0.648348	1.205422
C	-3.897346	0.562300	0.8519662
N	-3.142479	2.410415	-0.419167
O	-5.353045	2.324186	0.233288
H	-2.197999	1.983594	-0.350568
H	-4.074053	-1.711130	1.200942
H	-3.269769	3.333450	-0.833832



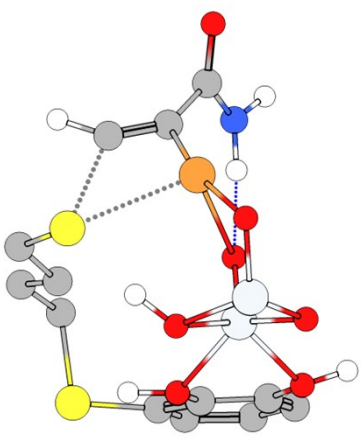
TS-3 structure (-228.13 cm^{-1})

Energy: -5221.48900988505 Eh

Energy: -5222.55760493778 Eh B3LYP/6311+G*/CPCM=DCM

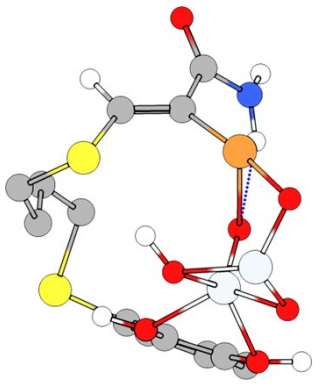
0 2

O	0.601370	3.480991	1.8115494
Ti	-0.029663	2.730401	3.3472545
Ti	0.698880	1.8371549	0.9118846
O	0.576618	0.980779	2.7452029
Cu	-2.501498	1.561981	2.622219
O	-0.530376	1.532234	-0.139939
O	-1.689992	2.824238	3.7439856
O	2.179190	0.303652	0.3223448
C	2.492848	0.433847	-1.0048090
C	2.701297	-0.684744	-1.8261440
C	3.035629	-0.479274	-3.1787876



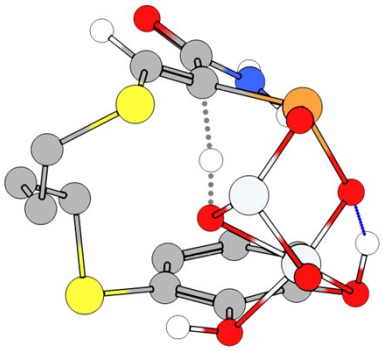
H 3.215732 -1.348452 -3.8266721
C 3.1150309 0.826782 -3.68468818
H 3.3750950 0.988267 -4.740490
C 2.8471065 1.943299 -2.86694221
H 2.8790992 2.963272 -3.279500
C 2.5232317 1.737226 -1.52475350
O 2.1840278 2.710371 -0.597974
S 2.4573672 -2.271441 -1.04021851
S -1.5545560 -1.022432 3.4151517
C -1.0989854 -2.360870 2.247022
C -0.2542614 -1.905355 1.056132
H -2.0493811 -2.813564 1.880463
H -0.5825076 -3.155240 2.826107
C -0.1047695 -2.969612 -0.036176
H 0.7462321 -1.613464 1.446715
H -0.7104404 -0.991223 0.618703
C 0.6181731 -2.493418 -1.2961830
H -1.1191833 -3.290903 -0.361214
H 0.3832339 -3.884903 0.365190
H 0.2255456 -1.512165 -1.631458
H 0.5054395 -3.216455 -2.127881
H -0.1094969 0.208802 2.952898
H 2.1309255 -0.688837 0.496418
H 1.9543712 3.564148 -1.014293
C -4.1412962 1.198070 0.031898
C -3.2911721 -0.457678 1.879509
C -3.4238370 0.639666 1.219382
N -3.2758010 1.463728 -0.991533
O -5.3551352 1.382637 -0.003898
H -2.2580463 1.506608 -0.800765
H -3.6678360 -1.479404 2.001002
H -3.6674631 1.921800 -1.815334

IN-4 structure
Energy: -5221.54266490499 Eh
Energy: -5222.60687790952 Eh B3LYP/6311+G*/CPCM=DCM
0 2
O 1.672855 1.544337 0.7665239
Ti 0.696002 0.8687767 2.133884
Ti 1.831913 -0.1301962 -0.080744
O 1.442967 -0.930010 1.778242
Cu -1.44182 -0.3606194 1.126138
O 0.736689 -0.379565 -1.280949
O -0.98436 1.1848400 2.096528
O 3.378367 -1.655382 -0.590420
C 3.704333 -1.4700905 -1.913882
C 3.846220 -2.5530338 -2.794534
C 4.200070 -2.2947696 -4.132744
H 4.326406 -3.136491 -4.827958
C 4.355846 -0.9696281 -4.566802
H 4.630129 -0.767305 -5.611942
C 4.131453 0.1146568 -3.695125
H 4.205607 1.1519825 -4.055252
C 3.787653 -0.1453776 -2.367060
O 3.467271 0.790304 -1.396595
S 3.492893 -4.1603708 -2.102197
S -0.471651 -3.4571398 2.259188
C 0.719262 -4.7658191 1.743574
C 1.603689 -4.3922250 0.542857
H 0.157006 -5.7055436 1.558769
H 1.329658 -4.9313289 2.653651
C 1.058888 -4.8266045 -0.827185
H 2.616516 -4.824478 0.6888762



H 1.726690 -3.287578 0.5537572
C 1.625934 -4.0482174 -2.011764
H -0.03777 -4.6578226 -0.862636
H 1.211813 -5.919277 -0.963638
H 1.354105 -2.973604 -1.931849
H 1.230069 -4.430713 -2.972628
H 0.839746 -1.728987 1.912617
H 3.369223 -2.651681 -0.450331
H 3.243096 1.663659 -1.7739541
C -2.500185 -2.071931 -1.035339
C -1.427649 -3.243937 0.7713392
C -1.764930 -2.025294 0.2847964
N -2.07282 -1.0880871 -1.897042
O -3.36299 -2.9016475 -1.335113
H -1.156927 -0.645203 -1.719986
H -1.775577 -4.185176 0.299589
H -2.392129 -1.171931 -2.864004

TS-4 structure (-665.60 cm^{-1})
Energy: -5221.50302734984 Eh
0 2
O 2.214358 0.3851220 2.262450
Ti 0.7399724 -0.820798 2.3551437
Ti 2.2927411 0.231063 0.4723882
O 1.524958 -1.515640 0.6312082
Cu -0.625660 0.038906 0.209065
O 1.026457 1.0575560 -0.441754
O -0.716553 0.020146 2.2044007
O 3.858974 -1.016387 -0.4904549
C 3.5703061 -1.060764 -1.840369
C 3.4635704 -2.291863 -2.513795
C 3.1541950 -2.290360 -3.886729
H 3.085449 -3.2470517 -4.424393
C 2.9070450 -1.074187 -4.542939
H 2.664907 -1.0754406 -5.615966
C 2.9328893 0.143317 -3.839127
H 2.691082 1.0958110 -4.332818
C 3.2429768 0.158138 -2.469866
O 3.156571 1.2755188 -1.676861
S 3.5399313 -3.772817 -1.506411
S -0.7482533 -3.058807 1.974875
C 0.2284161 -4.632674 1.973527
C 1.5024957 -4.680115 1.113952
H -0.479530 -5.445240 1.7050774
H 0.467931 -4.7604941 3.049455
C 1.3015179 -5.104906 -0.363102
H 2.188944 -5.3994524 1.608492
H 2.006294 -3.6926727 1.156092
C 1.7076935 -4.091277 -1.429347
H 0.227300 -5.3128385 -0.556920
H 1.819854 -6.0683721 -0.554996
H 1.235436 -3.1134828 -1.238408
H 1.397108 -4.4397995 -2.433246
H 0.546082 -1.5911178 -0.015113
H 3.778739 -1.9788731 -0.196202
H 2.145432 1.4245078 -1.450265
C -1.057289 -2.0254305 -2.018805
C -1.175996 -2.9230941 0.239135
C -0.814147 -1.8633978 -0.534390
N -0.517750 -0.990304 -2.741290
O -1.602544 -2.998444 -2.545474
H -0.023300 -0.233138 -2.2595003
H -1.717552 -3.800607 -0.1674404



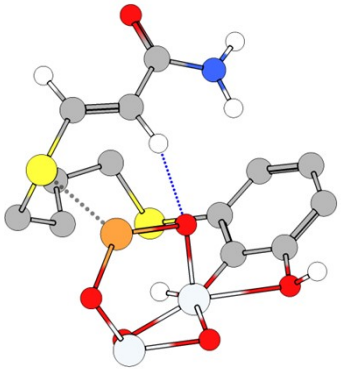
H -0.537506 -1.028742 -3.7606244

E-PC structure

Energy: -5221.5659995892 Eh

0 2

O 3.235924 0.71848 2.316822
Ti 2.851477 -0.61769 3.559089
Ti 3.027332 -0.58698 1.025688
O 3.419762 -1.88520 2.328150
Cu 0.613578 -1.16836 2.155227
O 1.407222 -0.67797 0.395200
O 1.192492 -0.81242 3.987537
O 3.999815 -1.95398 -0.475423
C 3.568756 -1.59270 -1.720241
C 3.165934 -2.53899 -2.677155
C 2.707217 -2.08964 -3.932444
H 2.405702 -2.82780 -4.688892
C 2.621341 -0.71501 -4.192623
H 2.265781 -0.36365 -5.172021
C 2.981605 0.23211 -3.210971
H 2.891038 1.31131 -3.410096
C 3.445324 -0.21250 -1.970396
O 3.768550 0.59517 -0.892767
S 3.186122 -4.24834 -2.154701
S -0.881029 -2.960449 1.972295
C 0.506789 -4.2139027 1.945128
C 1.424010 -4.1140917 0.723168
H 0.060201 -5.222937 2.064045
H 1.046018 -3.956913 2.878326
C 1.019134 -5.0276780 -0.444685
H 2.456560 -4.342947 1.059025
H 1.448467 -3.050921 0.396210
C 1.365357 -4.5067812 -1.836863
H -0.085405 -5.155466 -0.454979
H 1.432382 -6.049617 -0.299643
H 0.895439 -3.520256 -2.015757
H 1.007328 -5.202956 -2.620570
H 3.870155 -2.945104 -0.402873
H 3.374152 1.484097 -0.990470
C -1.467664 -2.228443 -2.058560
C -1.461699 -3.038333 0.285656
C -1.048563 -2.135108 -0.624539
N -0.723482 -1.405537 -2.871829
O -2.341741 -2.983451 -2.481524
H 0.047215 -0.844384 -2.506141
H -2.174114 -3.838163 0.015298
H -0.876088 -1.442178 -3.879707
H -0.299118 -1.373178 -0.326133

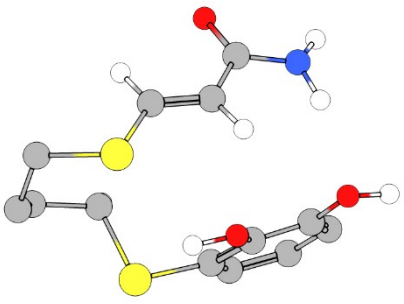


E-VS structure

Energy: -1581.64556658438 Eh

0 1

O 2.523350 -0.893895 -0.341251
C 2.7700592 -1.088620 -1.64918
C 3.2901330 -2.304406 -2.15819
C 3.5858515 -2.450269 -3.52714
H 4.010479 -3.399902 -3.883274
C 3.3331993 -1.394121 -4.40957
H 3.566385 -1.494252 -5.479340
C 2.7662652 -0.201244 -3.92509
H 2.533854 0.625095 -4.617566
C 2.4747928 -0.043604 -2.56421
O 1.867808 1.078050 -2.049368



S	3.5153570	-3.637961	-0.988867
S	0.5072954	-2.838768	1.548979
C	0.4837911	-4.669975	1.721821
C	1.7066945	-5.419776	1.178485
H	-0.462513	-5.036292	1.270778
H	0.403380	-4.834529	2.814804
C	1.7430156	-5.710448	-0.32904
H	1.739047	-6.398246	1.704709
H	2.629589	-4.882622	1.487236
C	1.9182775	-4.528948	-1.28146
H	0.802433	-6.229220	-0.622371
H	2.559218	-6.440798	-0.519277
H	1.101956	-3.786331	-1.194040
H	1.936183	-4.887163	-2.330244
H	0.181462	-0.568988	-0.270980
H	2.681821	-1.770782	0.103286
H	1.903495	1.779082	-2.727012
C	-1.296868	-1.282923	-1.800686
C	-0.463839	-2.568915	0.121172
C	-0.476388	-1.400974	-0.563515
N	-1.057000	-0.122276	-2.501788
O	-2.099114	-2.140505	-2.177371
H	-0.237397	0.452889	-2.285595
H	-1.117392	-3.391008	-0.226530
H	-1.471224	-0.055380	-3.431601

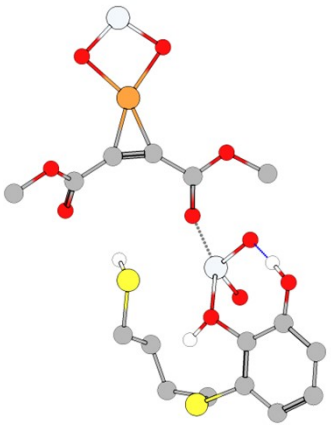
S7. Cartesians coordinates, first frequency for TS and Energies of Z-RC', IN-1', TS-1', IN-2', TS-2', Z-PC', Z-VS' (Z-vinyl sulphide derived from dimethyl acetylenedicarboxylate)

Z-RC' structure

Energy: -5508.315269684155 Eh

0 2

Ti	0.45202	-1.14172	3.64865
O	1.43694	0.17899	4.10863
O	-0.01386	-1.08313	2.05430
O	2.20078	-2.38433	3.30454
C	3.09972	-2.04587	2.28465
C	3.26937	-2.97970	1.23780
C	4.21905	-2.77752	0.22208
H	4.32552	-3.53398	-0.56680
C	4.99437	-1.60810	0.25967
H	5.75017	-1.43363	-0.52035
C	4.80704	-0.66517	1.27753
H	5.41253	0.25245	1.31340
C	3.85554	-0.83554	2.31995
O	3.76580	0.09713	3.26032
S	2.27341	-4.46522	1.31687
S	-0.29327	-3.51561	4.94773
C	-0.40656	-4.71106	3.53489
C	-1.09006	-4.14589	2.28159
H	-0.90412	-5.62425	3.91548
H	0.65290	-4.96939	3.33272
C	-0.52141	-4.69191	0.95990
H	-0.96066	-3.04022	2.24073
H	-2.18378	-4.32423	2.35353
C	0.70579	-3.90782	0.47036
H	-1.30172	-4.60100	0.17363
H	-0.30603	-5.78259	1.02497
H	0.58558	-2.82360	0.68613
H	0.87038	-4.04462	-0.61636
H	1.95181	-3.33447	3.05501
H	2.79307	0.16138	3.66684
Ti	-4.12042	1.71057	10.34403

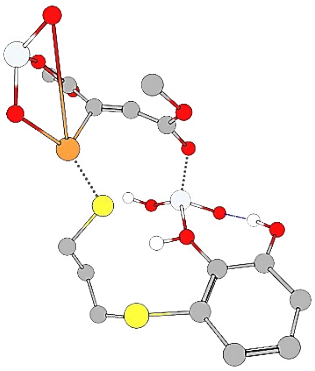


Cu	-3.07062	0.30126	8.47174
O	-3.46679	2.20193	8.84738
O	-3.88769	0.02570	10.24941
H	-1.62440	-3.22677	5.03368
C	-2.57834	-2.73534	7.71069
O	-2.01371	-3.10891	8.86618
C	-1.92881	-4.53070	9.09345
H	-1.20469	-4.65419	9.91616
H	-1.58090	-5.04853	8.17892
H	-2.92050	-4.93022	9.38762
C	-2.51688	-1.27914	7.52551
C	-2.24368	-0.24272	6.82051
C	-1.64238	0.25236	5.58638
O	-1.29425	-0.55766	4.70911
O	-1.52491	1.55702	5.51342
C	-0.90569	2.11447	4.31553
H	0.12312	1.69816	4.20138
H	-1.51063	1.83407	3.43133
H	-0.91634	3.20403	4.47403
O	-3.06346	-3.48447	6.87732

IN-1’ structure

Energy: -5508.311494150436 Eh

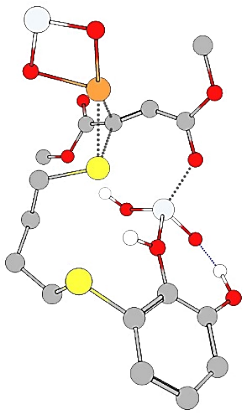
0 2



Ti	0.103280	-1.463860	1.354490
O	0.201130	-0.550520	-0.007620
O	-1.136900	-2.750090	0.953190
O	2.169830	-1.655880	1.526340
C	3.329780	-1.268370	0.863000
C	4.415490	-2.170210	0.895690
C	5.659120	-1.804100	0.350030
H	6.487720	-2.525900	0.359510
C	5.786470	-0.534020	-0.242190
H	6.750320	-0.231010	-0.686240
C	4.690520	0.336340	-0.319800
H	4.777920	1.316790	-0.814910
C	3.420730	-0.011220	0.209550
O	2.406360	0.857470	0.102490
S	4.090170	-3.776280	1.627910
S	0.807660	-3.523310	3.315820
C	1.186230	-5.293340	2.925560
C	1.024570	-5.652000	1.436760
H	0.502120	-5.896160	3.553790
H	2.219120	-5.492260	3.279610
C	2.321010	-5.757270	0.614530
H	0.337860	-4.920940	0.956270
H	0.507260	-6.633510	1.367450
C	3.010120	-4.439250	0.254100
H	2.073550	-6.254360	-0.349420
H	3.043090	-6.440170	1.117320
H	2.258260	-3.660280	0.016020
H	3.684380	-4.551890	-0.617710
H	2.389790	-2.466750	2.120040
H	1.508170	0.380900	0.084810
Ti	-0.378600	-2.784290	8.362980
Cu	0.385270	-3.261280	5.465380
O	0.085680	-1.232170	8.669600
O	0.708590	-3.612360	7.300820
C	-1.416940	-2.171310	5.493800
C	-0.984650	-1.144420	4.850900
C	-0.140000	-0.369020	4.073670
O	-0.295070	-0.215060	2.795290
O	0.874490	0.322960	4.619360

H	-1.262050	-3.306590	1.756080
C	-2.458350	-2.638860	6.348550
O	-2.245350	-2.893910	7.589020
O	-3.635960	-2.897730	5.781410
C	-4.696230	-3.488060	6.560980
H	-5.117130	-4.408340	5.894410
H	-5.555980	-2.640270	6.726740
H	-4.232150	-3.847580	7.613170
C	1.232430	0.008070	5.981090
H	1.991330	0.759740	6.274510
H	1.674310	-1.017510	6.026540
H	0.356710	0.036810	6.669220

TS-1' structure (-125.13. cm^{-1})
Energy: -5508.268539107341Eh
0 2



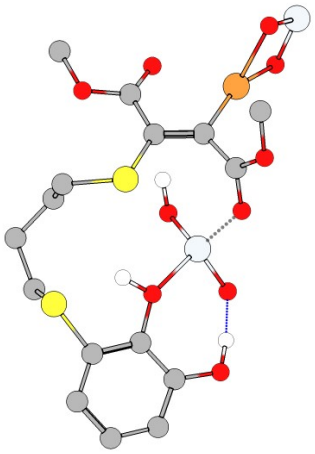
Ti	0.392740	-0.933180	1.725590
O	0.477940	0.089320	0.443310
O	-0.872540	-2.145170	1.247390
O	2.390160	-1.431740	1.536900
C	3.458860	-1.351630	0.641720
C	4.399520	-2.406350	0.718940
C	5.561900	-2.393540	-0.066000
H	6.291120	-3.211790	0.005960
C	5.760250	-1.313020	-0.944400
H	6.654950	-1.279250	-1.583690
C	4.815310	-0.286050	-1.040230
H	4.941700	0.554830	-1.737170
C	3.630330	-0.267660	-0.258600
O	2.792990	0.761540	-0.405940
S	4.002620	-3.727910	1.866270
S	1.049440	-2.900390	3.789540
C	1.004410	-4.731460	3.636680
C	0.821330	-5.299620	2.221300
H	0.187080	-5.044790	4.314140
H	1.942970	-5.087870	4.111530
C	2.081670	-5.779100	1.476640
H	0.275280	-4.566840	1.592270
H	0.140100	-6.173660	2.307070
C	2.901410	-4.719080	0.740490
H	1.754330	-6.500550	0.696800
H	2.741190	-6.358220	2.159670
H	2.247580	-4.006430	0.198650
H	3.584460	-5.187710	0.004900
H	2.640580	-2.209440	2.162560
H	1.865660	0.586760	-0.013910
Ti	0.280360	-3.988530	8.080470
Cu	0.027650	-2.574200	5.921540
O	0.875290	-2.430410	7.684850
O	-0.386440	-4.541260	6.625980
C	-1.191990	-2.226720	4.468360
C	-1.140520	-0.955490	4.800790
C	-0.225290	0.071010	4.504990
O	0.200700	0.258560	3.303300
O	0.217180	0.930040	5.415640
C	-2.273600	-3.206880	4.213050
H	-1.141300	-2.851780	1.879790
C	-0.161960	0.693490	6.787580
H	0.212950	1.564780	7.357740
H	0.303650	-0.247100	7.158880
H	-1.268140	0.611970	6.868240
O	-3.320130	-3.239370	4.824310
O	-1.961480	-4.049290	3.187650

C	-2.943900	-5.075670	2.929910
H	-2.516720	-5.698390	2.087910
H	-3.924810	-4.604900	2.635850
H	-3.097360	-5.696100	3.869690

IN-2’ structure

Energy: -5508.311829730415 Eh

0 2



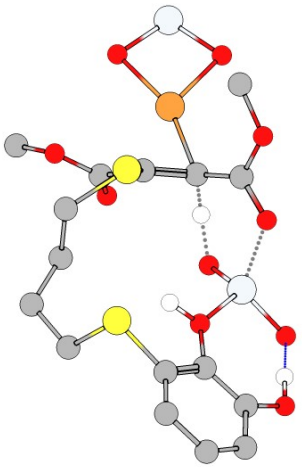
Ti	0.728069	-0.792241	1.967692
O	0.586339	0.344075	0.797387
O	-0.592072	-2.017510	1.715651
O	2.629746	-1.430897	1.423410
C	3.501846	-1.265457	0.339937
C	4.323550	-2.372600	0.024798
C	5.299145	-2.284583	-0.978527
H	5.935700	-3.153002	-1.197193
C	5.434153	-1.071896	-1.673237
H	6.191898	-0.975061	-2.465072
C	4.606122	0.014499	-1.376418
H	4.694990	0.966173	-1.920312
C	3.610237	-0.040197	-0.369294
O	2.887064	1.057626	-0.134181
S	4.094364	-3.834044	1.028228
S	1.761864	-3.180023	4.245832
C	1.943051	-4.810362	3.421723
C	1.119073	-5.032709	2.140406
H	1.744550	-5.591033	4.177988
H	3.032855	-4.814274	3.216767
C	1.910407	-5.641891	0.972143
H	0.660078	-4.078121	1.806758
H	0.265319	-5.692931	2.390631
C	2.685766	-4.638752	0.118223
H	1.202241	-6.146050	0.280183
H	2.590916	-6.444632	1.334276
H	2.020758	-3.824176	-0.233170
H	3.127437	-5.127671	-0.772529
H	2.920142	-2.325733	1.834660
H	1.976950	0.846744	0.260852
Ti	-4.211991	-0.541920	6.967298
Cu	-2.170435	-1.395266	5.576071
O	-4.029773	-0.723405	5.289947
O	-2.722996	-1.062883	7.587083
C	0.032375	-2.965167	4.708128
C	-0.412212	-1.694503	4.994238
C	0.310673	-0.470682	4.845944
O	0.577356	0.064966	3.696750
H	-0.869915	-2.469664	2.543553
O	0.704661	0.258685	5.878860
C	0.481190	-0.257323	7.208463
H	0.883996	0.510842	7.891665
H	1.025650	-1.212254	7.346484
H	-0.605063	-0.424640	7.385064
C	-0.954976	-4.043410	4.944681
O	-2.132043	-3.811728	5.220756
O	-0.473093	-5.305605	4.853753
C	-1.430277	-6.343297	5.108855
H	-0.875026	-7.294744	5.026967
H	-2.255945	-6.307979	4.369940
H	-1.865928	-6.232911	6.121338

TS-2’ structure (-831.33 cm^{-1})

Energy: -5508.27761375344 Eh

0 2

Ti	-0.636109	2.636469	-0.279648
O	-0.247654	3.988428	-1.162156
O	-2.284733	2.150296	-0.534137
O	0.919492	1.313079	-0.846220
C	1.838434	1.188662	-1.899531
C	2.471571	-0.069741	-2.042351
C	3.419930	-0.300834	-3.050252
H	3.903480	-1.284440	-3.121641
C	3.725496	0.746403	-3.933006
H	4.462334	0.592878	-4.735793
C	3.103353	1.987466	-3.794899
H	3.336115	2.821875	-4.472607
C	2.150001	2.268297	-2.777925
O	1.665822	3.503287	-2.738497
S	2.097493	-1.320421	-0.823688
S	-0.044723	-0.723086	1.783354
C	-0.204578	-2.557122	1.732877
C	-0.768604	-3.196284	0.460328
H	-0.854657	-2.809340	2.595705
H	0.818181	-2.926225	1.953895
C	0.134160	-3.319841	-0.774360
H	-1.719019	-2.694391	0.179696
H	-1.073819	-4.224686	0.750378
C	0.532783	-2.033217	-1.509800
H	-0.409949	-3.951979	-1.508392
H	1.053455	-3.893901	-0.521102
H	-0.271051	-1.267728	-1.464934
H	0.744931	-2.243037	-2.576049
H	1.033111	0.456640	-0.302124
H	0.901657	3.688836	-2.068016
Ti	-3.802703	-1.056821	5.297742
Cu	-2.944603	-0.289861	2.999057
O	-3.475844	0.549526	4.800707
O	-3.371209	-1.990609	3.943344
C	-1.714788	-0.219846	1.427710
C	-2.224118	1.057310	1.744193
C	-1.468522	2.120093	2.409888
O	-0.648656	2.844147	1.712630
N	-1.702437	2.445590	3.683562
H	-2.377885	1.883022	4.244499
H	-1.265314	3.290067	4.056597
H	-2.187511	-0.770925	0.594020
H	-2.613314	1.611964	0.566945

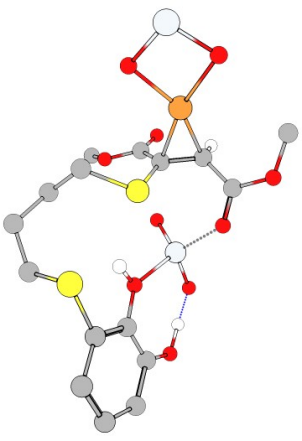


Z-PC' structure

Energy: -5508.316933808605 Eh

0 2

Ti	0.495120	-0.639730	1.597620
O	0.502270	0.509660	0.365790
O	-0.926690	-1.524150	1.601060
O	2.202040	-1.694030	0.968620
C	3.400030	-1.483620	0.296270
C	4.432670	-2.415970	0.548670
C	5.683780	-2.297870	-0.076730
H	6.476680	-3.026140	0.141430
C	5.876020	-1.230240	-0.968940
H	6.845380	-1.111310	-1.475820
C	4.853230	-0.309790	-1.218080
H	5.002530	0.531150	-1.911520
C	3.574010	-0.390200	-0.600830
O	2.666770	0.524440	-0.899190



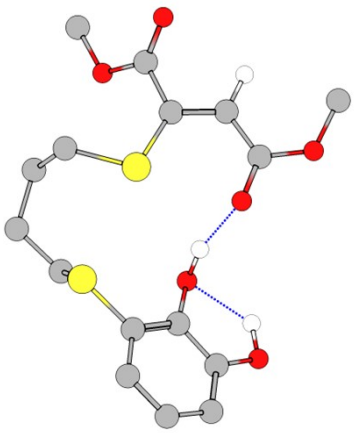
S	4.072030	-3.703060	1.743430
S	1.197680	-2.898220	3.658610
C	1.233010	-4.736190	3.577400
C	1.075240	-5.392310	2.192190
H	0.469150	-5.068230	4.308170
H	2.221110	-4.970440	4.025630
C	2.352450	-5.917760	1.511350
H	0.535360	-4.700960	1.514120
H	0.390100	-6.254040	2.332230
C	3.156890	-4.915770	0.683020
H	2.056030	-6.722840	0.805110
H	3.014470	-6.413610	2.256680
H	2.491380	-4.336970	0.009660
H	3.911350	-5.433420	0.057390
H	2.399110	-2.452290	1.614460
H	1.752600	0.498490	-0.358220
Ti	-0.118750	-4.167680	8.136930
Cu	-0.424900	-2.717150	6.038820
O	-0.144930	-2.465500	7.997170
O	-0.356310	-4.664080	6.524430
C	-0.503600	-2.474590	4.052820
C	-0.743740	-1.242680	4.731440
C	0.160330	-0.082550	4.603560
O	0.790460	0.145530	3.546660
O	0.270120	0.807880	5.572650
H	-1.819930	-0.983090	4.804350
C	-0.425980	0.626460	6.822760
H	-0.066680	1.440530	7.476230
H	-0.203590	-0.364610	7.270760
H	-1.518990	0.731700	6.669490
C	-1.751400	-3.142220	3.516120
O	-2.866920	-2.768640	3.830790
O	-1.491290	-4.191370	2.726480
C	-2.622200	-4.705060	2.010210
H	-2.261960	-5.601370	1.475070
H	-2.973750	-3.938670	1.291320
H	-3.445710	-4.963340	2.704070

Z-VS' structure

Energy: -1868.478008181368 Eh

0 2

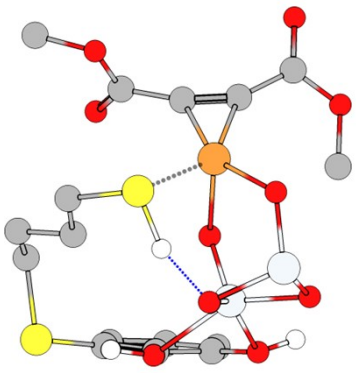
O	2.212197	-1.262242	0.772451
C	3.566543	-1.285630	0.529786
C	4.401666	-2.408143	0.707585
C	5.775347	-2.306228	0.389611
H	6.417496	-3.188183	0.526858
C	6.296466	-1.105058	-0.111325
H	7.366670	-1.038934	-0.359057
C	5.467028	0.006743	-0.325008
H	5.857000	0.951575	-0.729720
C	4.101713	-0.084750	-0.010352
O	3.260384	0.958248	-0.192078
S	3.805813	-3.956491	1.359617
S	1.321233	-3.311286	3.233417
C	1.181188	-5.143768	3.093779
C	0.720479	-5.644205	1.717105
H	0.529684	-5.516784	3.904786
H	2.213415	-5.482165	3.318277
C	1.776861	-5.687861	0.602607
H	-0.151902	-5.040375	1.394547
H	0.337810	-6.678879	1.857052
C	2.430942	-4.360791	0.198979
H	1.285409	-6.104680	-0.302474



H	2.573707	-6.418548	0.867615
H	1.709651	-3.517867	0.204960
H	2.871809	-4.437446	-0.814889
H	2.033240	-1.199496	1.752026
H	2.389175	0.607078	0.113662
C	-0.172160	-2.764758	3.966393
C	-0.363516	-1.436514	4.290331
C	0.599581	-0.385222	3.976550
O	1.619601	-0.563585	3.303652
O	0.378967	0.872224	4.436071
H	-1.302979	-1.198645	4.805131
C	-0.724027	1.171757	5.288262
H	-0.615698	2.236352	5.564890
H	-0.712477	0.556785	6.212325
H	-1.696096	1.035488	4.767621
C	-1.345266	-3.648370	4.319270
O	-2.005980	-3.526278	5.333316
O	-1.624878	-4.545742	3.347942
C	-2.765087	-5.382663	3.592167
H	-2.843831	-6.050283	2.715961
H	-3.682825	-4.770786	3.698771
H	-2.628083	-5.970886	4.521423

S8. Cartesians coordinates, first frequency for TS and Energies of E-RC', IN-3', TS-3', IN-4', TS-4', E-PC', E-VS' (*E*-vinyl sulphide derived from dimethyl acetylenedicarboxylate)

E-RC' structure
Energy: -5508.364500993257 Eh
0 2



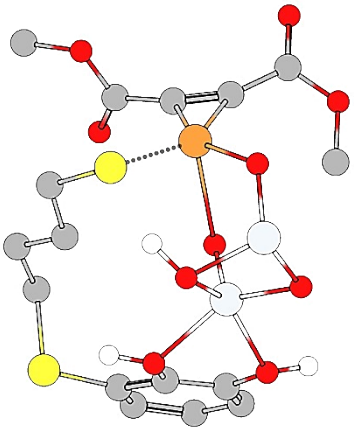
O	1.076977	1.406663	1.041284
Ti	0.648056	0.724467	2.683872
Ti	1.602911	-0.327752	0.535335
O	1.801427	-0.719473	2.405392
Cu	-1.383280	-1.442788	1.658105
O	0.271624	-1.155608	-0.043393
O	-0.967533	0.123541	2.764944
O	3.201090	-1.714327	-0.282493
C	3.074535	-1.731544	-1.647879
C	3.207454	-2.913929	-2.393938
C	3.062193	-2.857789	-3.794764
H	3.180392	-3.778588	-4.382850
C	2.748612	-1.641035	-4.415966
H	2.626230	-1.599435	-5.507947
C	2.564856	-0.467130	-3.658271
H	2.284144	0.479604	-4.144319
C	2.718119	-0.523157	-2.272011
O	2.507271	0.521494	-1.386677
S	3.481059	-4.410091	-1.455587
S	-0.203894	-2.881452	3.109536
C	0.323161	-4.397743	2.208717
C	1.036740	-4.126727	0.889297
H	-0.617456	-4.963993	2.050799
H	0.948975	-4.996933	2.902728
C	1.252830	-5.381572	0.042339
H	2.013306	-3.651734	1.125431
H	0.462777	-3.374880	0.309054
C	1.744077	-5.095610	-1.375629
H	0.275085	-5.896482	-0.082720
H	1.928806	-6.103043	0.552666
H	1.086077	-4.355743	-1.872848
H	1.756203	-6.018388	-1.987774
H	0.917057	-2.051092	2.858244

H	3.326770	-2.675870	-0.018760
H	2.006354	1.260125	-1.785463
C	-2.537702	-2.505840	0.457256
C	-2.442712	-3.923482	0.130349
O	-3.095220	-4.679418	1.047828
C	-3.112360	-6.087911	0.785201
H	-3.802928	-6.526601	1.526662
H	-2.100058	-6.526960	0.906705
H	-3.461684	-6.294682	-0.245715
O	-1.839306	-4.378997	-0.828488
C	-2.915636	-1.296208	0.348704
C	-3.838795	-0.273919	-0.189378
O	-5.004742	-0.547998	-0.403120
O	-3.351508	0.949805	-0.444825
C	-1.976123	1.259633	-0.145416
H	-1.808201	1.274777	0.949550
H	-1.282179	0.519372	-0.592794
H	-1.797090	2.262266	-0.572809

IN-3’ structure

Energy: -5508.374458821394 Eh

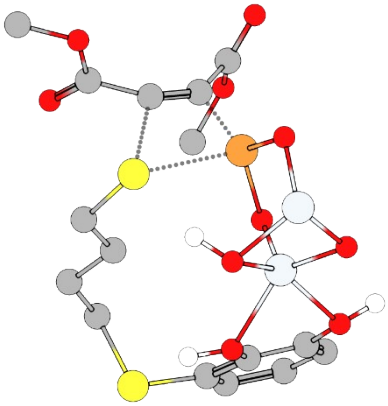
0 2



O	-0.098046	3.651071	1.244367
Ti	-0.446128	3.137572	2.952772
Ti	0.508530	1.911571	0.825854
O	0.860691	1.699113	2.795802
Cu	-2.280055	0.573050	2.601356
O	-0.757341	0.958907	0.393154
O	-1.975276	2.434982	3.193240
O	2.178752	0.577122	0.178212
C	2.083911	0.380949	-1.175908
C	2.355208	-0.865359	-1.763606
C	2.240302	-0.996881	-3.161481
H	2.465897	-1.965861	-3.628463
C	1.822633	0.095954	-3.934437
H	1.725906	-0.010597	-5.024606
C	1.500206	1.329038	-3.333289
H	1.139636	2.174750	-3.938402
C	1.621529	1.458454	-1.948932
O	1.279702	2.578483	-1.202012
S	2.763256	-2.187161	-0.633103
S	-0.768231	-0.464805	3.976315
C	-0.249730	-2.030822	3.164481
C	0.388436	-1.843795	1.788953
H	-1.145961	-2.680732	3.092526
H	0.452135	-2.537059	3.861208
C	0.681922	-3.154382	1.056932
H	1.328426	-1.262788	1.931618
H	-0.282167	-1.214580	1.166316
C	1.084979	-2.983904	-0.406020
H	-0.252280	-3.756675	1.033804
H	1.438080	-3.761016	1.602966
H	0.353804	-2.345437	-0.940552
H	1.141966	-3.959393	-0.927175
H	0.451310	0.824480	3.247004
H	2.385180	-0.332561	0.562365
H	0.740351	3.216205	-1.709596
C	-5.009333	1.182029	0.821794
O	-4.728974	2.365406	0.246949
C	-3.890435	0.395432	1.376957
C	-3.334003	-0.729488	1.604380
C	-3.127830	-2.160316	1.383667
O	-2.551834	-2.637331	0.418355

O	-3.646821	-2.890214	2.396939
C	-3.523341	-4.310884	2.260798
H	-3.917118	-4.651959	1.282907
H	-2.461086	-4.622759	2.341470
H	-4.106925	-4.747288	3.090211
O	-6.152519	0.769951	0.882638
C	-3.374684	2.848838	0.233464
H	-3.394906	3.774354	-0.370102
H	-2.678335	2.110743	-0.213446
H	-3.028651	3.070782	1.261945

TS-3' structure (-135.24 cm^{-1})
Energy: -5508.336863663772 Eh
0 2



O	1.338610	4.025180	1.676880
Ti	0.731040	3.142150	3.160880
Ti	1.510650	2.390110	0.791170
O	1.727710	1.520120	2.618220
Cu	-1.148490	1.729670	1.596790
O	0.084340	1.924140	0.020710
O	-0.935310	2.905480	3.198600
O	3.003150	1.068190	-0.241440
C	2.862550	1.254390	-1.595980
C	2.956990	0.186610	-2.502790
C	2.784760	0.444620	-3.877560
H	2.873330	-0.384180	-4.593950
C	2.488880	1.744110	-4.312040
H	2.345220	1.943080	-5.383890
C	2.358670	2.804850	-3.393820
H	2.100900	3.818310	-3.736100
C	2.539530	2.549870	-2.033580
O	2.394100	3.467660	-1.005330
S	3.253040	-1.423750	-1.789990
S	-0.411760	-0.596470	2.985770
C	0.263990	-1.914510	1.906930
C	0.656330	-1.451310	0.507380
H	-0.507500	-2.710830	1.833620
H	1.137160	-2.356110	2.434880
C	1.059240	-2.602090	-0.416560
H	1.487920	-0.719220	0.595420
H	-0.188710	-0.890180	0.059040
C	1.538120	-2.168790	-1.801060
H	0.176270	-3.262620	-0.566570
H	1.833900	-3.239410	0.066630
H	0.867530	-1.405580	-2.245100
H	1.597120	-3.027830	-2.497970
H	1.116440	0.694420	2.757120
H	3.126520	0.073780	-0.126660
H	1.899820	4.264910	-1.281430
C	-3.725160	1.319910	0.029290
O	-3.471960	1.030670	-1.282000
C	-2.772640	0.748180	0.992180
C	-2.560500	-0.289480	1.708500
C	-2.947210	-1.642950	2.099820
O	-2.741430	-2.628590	1.397460
O	-3.575310	-1.682340	3.292340
C	-3.924560	-2.990440	3.754690
H	-3.011130	-3.584720	3.964430
H	-4.500990	-2.840680	4.684710
H	-4.530570	-3.533330	3.001360
O	-4.670500	2.020840	0.326730
C	-2.338260	0.223310	-1.614850
H	-2.323170	0.166370	-2.720080

H	-2.430760	-0.801720	-1.196360
H	-1.397910	0.686220	-1.246410

IN-4’ structure
Energy: -5508.397872253430 Eh
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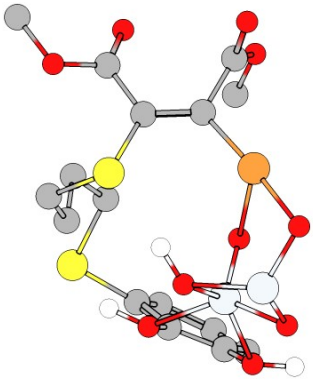
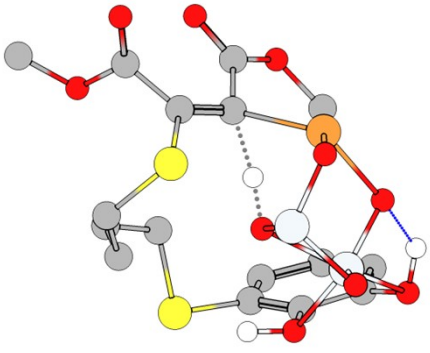


O	2.031185	1.608875	0.882991
Ti	0.975714	0.956431	2.201993
Ti	2.247645	-0.067297	0.053650
O	1.693234	-0.852750	1.861191
Cu	-1.340523	-0.268331	1.252554
O	1.141395	-0.348972	-1.115255
O	-0.702218	1.269335	2.095751
O	3.758587	-1.607302	-0.589394
C	4.026371	-1.326912	-1.910304
C	4.058174	-2.335887	-2.885383
C	4.358442	-1.983201	-4.215039
H	4.398091	-2.767949	-4.983579
C	4.565924	-0.636193	-4.547465
H	4.798646	-0.359982	-5.585767
C	4.436856	0.380907	-3.580840
H	4.538866	1.440456	-3.860471
C	4.144718	0.025538	-2.262812
O	3.890066	0.892196	-1.209664
S	3.605306	-3.969817	-2.320413
S	-0.271025	-3.296530	2.207925
C	0.974725	-4.513846	1.610126
C	1.768624	-4.090985	0.369225
H	0.460589	-5.485286	1.469883
H	1.646024	-4.618807	2.486528
C	1.147386	-4.462784	-0.982072
H	2.786813	-4.533490	0.433215
H	1.892519	-2.988607	0.412772
C	1.752159	-3.717537	-2.170655
H	0.070244	-4.195876	-0.988992
H	1.196249	-5.563006	-1.133490
H	1.580329	-2.625005	-2.064146
H	1.303093	-4.050121	-3.126907
H	1.041204	-1.627171	1.928399
H	3.681040	-2.610216	-0.546240
H	3.679742	1.799277	-1.508434
C	-3.147411	-1.720852	-0.307079
C	-1.467264	-3.147890	0.870203
C	-1.916735	-1.906107	0.517320
O	-3.006688	-1.466977	-1.633106
O	-4.249032	-1.656911	0.210800
C	-2.073358	-4.385345	0.313307
C	-1.722994	-1.669931	-2.228567
H	-1.807342	-1.310972	-3.271456
H	-1.472364	-2.751605	-2.233014
H	-0.921849	-1.102059	-1.709619
O	-2.669801	-4.439508	-0.753575
O	-1.881700	-5.485951	1.096372
C	-2.457573	-6.692970	0.585898
H	-2.204900	-7.484903	1.313828
H	-2.044545	-6.936829	-0.414209
H	-3.557089	-6.592919	0.486016

TS-4’ structure (-745.67 cm^{-1})
Energy: -5508.3353258036 Eh
0 2



O	1.548600	3.120640	2.958480
Ti	0.182230	1.869080	3.251040

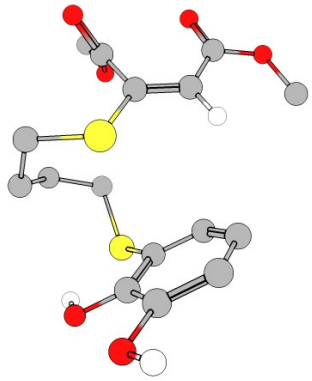
Ti	1.550390	2.725990	1.178160
O	0.556910	1.001220	1.456740
Cu	-1.449790	2.405930	1.200940
O	0.244040	3.483610	0.331080
O	-1.333740	2.649240	3.127820
O	3.048160	1.394930	0.185270
C	2.851070	1.417220	-1.173360
C	2.771030	0.224510	-1.918200
C	2.560400	0.306210	-3.307740
H	2.513800	-0.619970	-3.899640
C	2.385820	1.560660	-3.913950
H	2.215370	1.622430	-4.998210
C	2.389890	2.740080	-3.146430
H	2.205440	3.722070	-3.606150
C	2.603100	2.671790	-1.762710
O	2.512060	3.754740	-0.906120
S	2.793050	-1.297660	-0.976540
S	-1.221480	-0.680200	3.022520
C	-0.109260	-2.151650	2.818750
C	0.995350	-2.085090	1.751170
H	-0.770350	-3.030960	2.682840
H	0.330520	-2.222800	3.832860
C	0.593750	-2.513320	0.317440
H	1.809510	-2.747480	2.112830
H	1.408300	-1.056910	1.741040
C	0.954120	-1.536280	-0.797650
H	-0.505290	-2.646750	0.252890
H	1.023060	-3.510920	0.081950
H	0.519450	-0.537520	-0.598910
H	0.575230	-1.896200	-1.775140
H	-0.451230	0.789290	0.859500
H	2.980430	0.423280	0.442140
H	1.533560	3.996590	-0.818320
C	-2.733030	0.312340	-0.689060
O	-2.490350	1.105250	-1.772560
C	-1.855890	0.394030	0.545420
C	-2.095590	-0.625100	1.462810
C	-3.106950	-1.746290	1.367730
O	-4.219070	-1.730940	1.850980
O	-2.518500	-2.878390	0.858530
C	-3.283880	-4.088140	0.972410
H	-2.638830	-4.898990	0.581660
H	-3.542980	-4.287700	2.034160
H	-4.222520	-4.027180	0.385400
O	-3.690860	-0.461710	-0.749250
C	-1.386440	2.034620	-1.811110
H	-1.330720	2.432950	-2.855110
H	-0.409630	1.533450	-1.577810
H	-1.533330	2.901140	-1.096380

E-PC' structure

Energy: -5508.407935865346 Eh

0 2

O	3.673929	0.810338	2.026654
Ti	3.366385	-0.392343	3.409058
Ti	3.303605	-0.579291	0.862878
O	3.747724	-1.778978	2.238306
Cu	0.977490	-1.015657	2.283590
O	1.626272	-0.633256	0.421700
O	1.747917	-0.456008	3.989190
O	4.076262	-2.072318	-0.622996
C	3.627697	-1.713245	-1.863722
C	3.118530	-2.655125	-2.773049



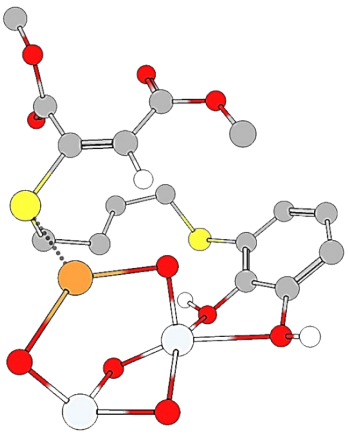
C	2.654625	-2.209933	-4.027291
H	2.262990	-2.942538	-4.746572
C	2.679305	-0.842217	-4.334468
H	2.316439	-0.495234	-5.312343
C	3.146383	0.103546	-3.398997
H	3.134023	1.179531	-3.632719
C	3.604767	-0.337748	-2.155872
O	4.012452	0.471889	-1.105243
S	3.043132	-4.342623	-2.184821
S	-0.544174	-2.748806	2.371468
C	0.750084	-4.086798	2.164941
C	1.542194	-4.015254	0.854922
H	0.223707	-5.052362	2.299040
H	1.395234	-3.895342	3.045234
C	1.011862	-4.934433	-0.258673
H	2.600968	-4.250301	1.093082
H	1.545616	-2.955104	0.515504
C	1.245974	-4.437257	-1.680168
H	-0.087716	-5.055577	-0.156581
H	1.423513	-5.960668	-0.140125
H	0.848802	-3.412880	-1.817573
H	0.746360	-5.093583	-2.418569
H	3.889081	-3.055897	-0.534447
H	3.724099	1.396758	-1.234263
C	-1.567892	-2.321408	-1.613989
C	-1.402383	-2.874867	0.798875
C	-1.029133	-2.094154	-0.247529
O	-1.167655	-1.460873	-2.591268
O	-2.274517	-3.270289	-1.920379
H	-0.212687	-1.368482	-0.073655
C	-0.419395	-0.280816	-2.277472
H	-0.225722	0.217733	-3.244621
H	0.547143	-0.507857	-1.781397
H	-1.001058	0.401735	-1.622888
C	-2.430919	-3.966817	0.736188
O	-2.144859	-5.150866	0.835729
O	-3.676299	-3.483648	0.626490
C	-4.700856	-4.468457	0.428454
H	-5.661197	-3.927161	0.485777
H	-4.646557	-5.260321	1.201973
H	-4.578926	-4.931438	-0.571342

E-VS' structure

Energy: -1868.482480502813 Eh

0 2

O	4.694327	-2.837196	-0.456298
C	3.838471	-2.127621	-1.224816
C	2.915877	-2.749460	-2.097393
C	2.038850	-1.983054	-2.890569
H	1.353356	-2.497455	-3.579753
C	2.056150	-0.588296	-2.785023
H	1.383095	0.025295	-3.402814
C	2.955936	0.040604	-1.903817
H	2.974368	1.140875	-1.822909
C	3.846657	-0.709596	-1.121202
O	4.732944	-0.164810	-0.245399
S	2.941689	-4.536183	-2.162089
S	0.708488	-1.971701	0.548641
C	1.107683	-3.329326	1.720347
C	2.084209	-4.394749	1.212783
H	0.154615	-3.751871	2.095725
H	1.565950	-2.788040	2.572254
C	1.565606	-5.424607	0.200309



H	2.415358	-4.951149	2.116719
H	2.997228	-3.897670	0.826047
C	1.389427	-4.993946	-1.259091
H	0.580327	-5.810286	0.543805
H	2.254291	-6.295917	0.217256
H	0.685044	-4.151031	-1.384622
H	0.977005	-5.841086	-1.842879
H	4.513854	-3.785114	-0.697015
H	4.618889	0.803413	-0.260903
C	-2.560525	-2.025122	-1.890609
C	-0.802028	-2.431735	-0.199715
C	-1.220336	-1.776247	-1.325290
O	-2.860807	-1.459280	-3.098460
O	-3.420033	-2.703567	-1.347454
H	-0.538901	-1.043214	-1.779684
C	-1.898979	-0.707188	-3.828272
H	-2.382442	-0.431663	-4.783714
H	-0.984976	-1.299174	-4.049383
H	-1.606735	0.225434	-3.299203
C	-1.676315	-3.464001	0.478134
O	-1.686855	-4.615922	-0.226252
C	-2.643772	-5.590539	0.212801
H	-2.422515	-6.515034	-0.348560
H	-3.662426	-5.226354	-0.029280
H	-2.566201	-5.761818	1.304753
O	-2.210757	-3.295008	1.555281

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