

## **Supporting Information**

### **On the Formation of Phosphorous Polycyclic Aromatics Hydrocarbons (PPAHs) in Astrophysical Environments**

Marco Fioroni\* Robert E. Savage, and Nathan J. DeYonker\*

213 Smith Chemistry Building, The University of Memphis, Memphis,  
TN, USA, 38152

E-mail: [mfioroni@memphis.edu](mailto:mfioroni@memphis.edu); [ndyonker@memphis.edu](mailto:ndyonker@memphis.edu)

## Index

1) ORCA Input Template

2) XYZ

3) PES

4) Energies

5) Spin Surfaces  $S=3/2$ ,  $S=1/2$ ; Figure 1

6) cis-trans-gauche, TS I (trans-cis) (Figure 1)

## ORCA Input Template

```
#
# Optimization employing DFT
#

%pal nprocs 10
  end

! UKS RIJCOSX B3LYP TightSCF SlowConv Opt
! GRID4
! GRIDX4
! D3BJ
! DIIS

%basis
basis "ma-def2-TZVPP"
AuxJK "aug-cc-pVTZ/JK"
end

%scf Maxiter=350
  end

%base "OPT"

* xyzfile 0 2 OPT.xyz

$new_job
! UKS RIJCOSX B3LYP TightSCF SlowConv MORead
! GRID4
! GRIDX4
! D3BJ
! NumFreq
! DIIS

%basis
basis "ma-def2-TZVPP"
AuxJK "aug-cc-pVTZ/JK"
end

%moinp "OPT.gbw"

%scf Maxiter=150
  end
```

```
%base "FREQ"
```

```
%freq Temp 10, 30, 100, 298.15
```

```
CentralDiff true
```

```
Increment 0.0030
```

```
end
```

```
* xyzfile 0 2 OPT.xyz
```

## XYZ Compounds

**M = multiplicity**

**Dipole = D (Debye)**

### **Compound 1**

**M=2 (D=1.045)**

C	-1.99599737579164	0.36962584642924	0.00000000000000
P	-0.44265262420836	0.37368415357076	0.00000000000000

### **Compound 1**

**M=4 (D=0.596)**

C	-2.07852756596378	0.36941022600124	0.00000000000000
P	-0.36012243403622	0.37389977399876	0.00000000000000

### **Compound 2**

**M=2 (D=1.524)**

C	-1.99208142154720	0.79118417477582	0.26958127517017
P	-0.82666727743522	-0.03291135791764	-0.32041492927715
C	-3.03342447404428	1.57043568624628	0.83191016285598
C	-4.32065286515456	1.41435328558638	0.59406788827072
H	-5.24024621563728	1.88161965701208	0.90682856110345
H	-2.72137774618145	2.36496855429709	1.51855704187685

### **Compound 2**

**M=4 (D=1.679)**

C	-2.00156336283932	0.83501621864300	0.30530038409825
P	-0.80435242077371	-0.05676652130903	-0.33827872277921
C	-2.98398497343086	1.55937172992241	0.82649833559991
C	-4.37457980036454	1.39159880711806	0.57032492165518
H	-5.26042992712496	1.89832953142938	0.91940065987468
H	-2.70953951546660	2.36210023419618	1.51728442155120

### **Compound 3**

**M=2 (D=1.580)**

C	-2.05295717091021	0.91506286590028	0.34756813094642
P	-0.90152841582178	0.10038869627478	-0.29831697857013
C	-3.08538769751492	1.65317738758877	0.93593920985678
C	-4.39493979430121	1.52692305730535	0.60873331028388
H	-5.10883731588620	2.15112717551902	1.13103701450387
H	-2.80565111994561	2.36938291247869	1.70141504770922
C	-4.92842658287665	0.61979255307661	-0.38855854285619
H	-6.01287795530559	0.64578521169620	-0.52117414968291
C	-4.22443630699128	-0.21315695952741	-1.13113043441211
H	-4.44210764044653	-0.93988290031230	-1.89698260777883

### **Compound 3**

**M=4 (D=1.896)**

C	-2.05476218943798	0.91178788626639	0.33668943771433
P	-0.77306977345761	0.14842954696189	-0.25794159988146
C	-3.04405352900274	1.60478599125581	0.90258190821680
C	-4.47042161927983	1.51518295089766	0.58138384225562
H	-5.13915963942179	2.16521257617896	1.12721148017946
H	-2.76797912157092	2.31138207781080	1.68081145097268
C	-4.97910280972023	0.65575726198060	-0.36498654034780
H	-6.05805358096051	0.67060595204546	-0.52641679272413
C	-4.22702879818415	-0.21196497188148	-1.11412226805246
H	-4.44351893896421	-0.94257927151609	-1.87668091833304

## Compound 4

M=2 (D=1.722)

C	-2.04214741916093	0.83558867827350	0.27441415997611
P	-0.91886531795346	-0.00640092925157	-0.37904004798993
C	-3.04364283371967	1.61066043941588	0.88355564246659
C	-4.36782939923872	1.52711690767404	0.61255619967009
H	-5.04433337300686	2.17926267928765	1.15084271977336
H	-2.71485978172936	2.32850520607054	1.62857485765433
C	-4.95088359477252	0.61833775977469	-0.35638901298557
C	-6.23962877441380	0.53823831113075	-0.61146790570739
H	-7.15601386651325	1.00306670038000	-0.28289479183422
H	-4.25605563949143	-0.02610575275552	-0.89075182102337

## Compound 4

M=4 (D=1.803)

C	-2.01697770539162	0.86716085943008	0.31310187970242
P	-0.88446747827383	-0.02740550162947	-0.38080954042095
C	-2.97292042357893	1.59987103885126	0.87932521941631
C	-4.41043085382632	1.50675050582518	0.58896519092466
H	-5.05965535359463	2.16612935418604	1.15001179589236
H	-2.67846703940069	2.33422170612606	1.62397898806008
C	-4.95489636623008	0.64238407578982	-0.33921717842867
C	-6.28681570159425	0.53053780968028	-0.62884542610944
H	-7.20393455984901	0.98981257326072	-0.29375202323941
H	-4.26569451826064	-0.00119242152000	-0.88335890579734

## Compound 5

M=2 (D=2.069)

C	-2.83758946615069	2.01813230782798	0.70325218529739
H	-3.65236263926425	1.95238235089545	-0.01087004509430
C	-1.74695454226148	1.17833639716008	0.53456544901491
H	-1.75357077535309	0.49063917551083	-0.30352536444067
C	-0.63785796050474	1.16296548883812	1.37876715194307
C	-0.53486105664706	2.00911819084302	2.48874800142030
C	-1.55212913334367	2.87847947329105	2.75483180774693
P	-3.03400354637432	3.19790490486723	1.98278040634926
H	0.17220522256580	0.47553372358058	1.16995837063215
H	0.34934389733352	1.95995798718564	3.11640203713098

## Compound 5

M=4 (D=1.994)

C	-2.85816382705119	1.97000857605169	0.66851958771590
H	-3.73224153729495	1.82907174479911	0.04375789898407
C	-1.77003795001903	1.18996046572440	0.49999903738428
H	-1.78466173335872	0.44156376057275	-0.28613518955411
C	-0.59735391333908	1.22843838929465	1.32700540902793
C	-0.55201047070352	1.99545454639742	2.54792869829396
C	-1.56337739217257	2.79401923066319	2.88400646954982
P	-2.92063119938187	3.41310396885689	1.84990337182490
H	0.23660656192790	0.58406576882382	1.08639240655745
H	0.31409146139307	1.87776354881607	3.19353231021583

## Compound 6

M=2

C	-2.83359416451844	2.01223234326526	0.69653259958381
H	-3.64818265554369	1.94823044924735	-0.01639630237890
C	-1.74713595270669	1.16468399189815	0.52194983344464
H	-1.74940377006790	0.47303316764548	-0.31257465856795
C	-0.65242337609538	1.16716694207619	1.37704956191381
C	-0.55405733164343	2.01488333495621	2.47454785489475
C	-1.52342740564136	2.94530134858304	2.84521683235200
P	-3.02240836991110	3.17928697705878	1.95779719155776
H	0.16214954113264	0.48159625727478	1.18287190899423
H	0.34034406216362	1.94703236015421	3.08620006478846
C	-1.27019139149396	3.77017025088358	4.03578036234621
C	-2.05282586113176	4.69119202646423	4.54594758963165
H	-0.31522863369821	3.57943100025651	4.53788111274411
H	-2.04353469084435	5.37387955023624	5.37834604869544

## Compound 7

M=2 (D=0.892)

C	-3.00662458940614	2.22306885254952	0.82527729302178
H	-3.92646323930356	2.12627599489777	0.26433769179139
C	-2.04228377741693	1.26825930027653	0.75841793641987
H	-2.22902373484228	0.39222008926733	0.14680361104418
C	-0.80213760202459	1.30284713926696	1.47104383309713
C	-0.51972892165524	2.21479687854043	2.46421299304418
C	-1.37594097766228	3.27340690980647	2.81947034881293
P	-2.64229414187769	3.76404489365399	1.65074093374047
H	-0.10238159648682	0.49724750107443	1.29576724002287
H	0.36626464522229	2.05922527964624	3.07222906251040
C	-1.29282483680720	3.96909854203584	4.03929329656658
C	-2.31474704348190	4.73720102003527	4.55316871382125
H	-0.40695721073207	3.81329196068089	4.64736873783719
H	-2.17518011435431	5.20244743302697	5.51927018537432
C	-3.61064901374803	4.83149654385502	3.95498606819142
C	-3.94029539355611	4.34668312391069	2.72932578683471
H	-4.94597947348250	4.44548348974211	2.34321938516542
H	-4.38907297838460	5.29925504773352	4.54797688270397

## Compound 8

M=2

C	-2.72404037054720	2.48297636724314	-0.25372160761010
H	-3.08130181230214	2.51893794613527	-1.27677612792656
C	-2.46571775066703	1.23885371085198	0.30527761977267
H	-2.62773511255731	0.35056500596432	-0.29464567785534
C	-2.02592567642206	1.08055526779447	1.61399880149050
C	-1.77658932972136	2.15003094740506	2.46676167728959
C	-1.93420543191541	3.49204113423204	2.11649006066438
P	-2.53533419398216	4.00405181949034	0.54641706759112
H	-1.87567925852704	0.07832884386542	1.99396686264002
H	-1.47673735736020	1.92484796899663	3.48171187105864
C	-1.62110253616793	4.56592571382139	3.06079561322233
C	-0.58389092325101	4.67798307202915	3.91305947290977
H	-2.28290493668243	5.42470573295343	3.01292340876260
H	-0.54496653260790	5.59557922717094	4.48840731476071
C	0.58086851453947	3.81753745582107	4.10481604245090
C	0.79332778986729	2.57610471477788	3.72648535716247
H	1.60689713767191	1.87266007017160	3.79953147121828
H	1.40507778063251	4.31164500127589	4.62988077239800

## Compound 8a

M=2 (D=1.912)

C	-3.03547947651500	2.40314759563636	0.10715994368786
H	-3.67256037739128	2.26411009233045	-0.75851107809261
C	-2.10049708126590	1.36366158055572	0.40725360864576
H	-1.99376483942677	0.55823294258325	-0.31081289861945
C	-1.33697261866995	1.34109721672546	1.51792256397484
C	-1.45143234235473	2.35953297255349	2.61790839421540
C	-1.95511908269476	3.72207402149314	2.18294147969307
P	-3.12974343158754	3.92433568909171	0.88385085857843
H	-0.64297926165161	0.52604260357112	1.68043662946955
C	-1.53152990886243	4.84907377901832	2.89360118232316
C	-0.52918572122084	4.78952200831999	3.84284272136312
H	-1.97588182130083	5.80790622344157	2.65131426942606
H	-0.21180360365861	5.68975805006579	4.35069547431913
C	0.15567618836479	3.56147034240883	4.09245854131317
C	-0.23501287233847	2.41708236145676	3.49534790788500
H	1.01337246068667	3.56264439327658	4.75285569448906
H	0.29161800734814	1.48765372716740	3.67314137887036
H	-2.26449421746087	1.96724440030405	3.27740332845809

## Compound 9

M=1 (D=1.660)

C	-3.56271472984583	-0.37860613738761	-0.15840462528740
C	-2.31194505727074	0.28805970543458	-0.19460155180323
C	-1.13394775103230	-0.40188897561898	-0.07496017690942
C	-3.57692560170275	-1.79725849932328	0.00513253351899
C	-2.34036377566529	-2.47683012010559	0.12421490318697
C	-1.14657452203053	-1.80112605069955	0.08532465803795
C	-4.76114611214977	0.36857893296171	-0.28158795344261
C	-6.01678961400429	-0.18126755692924	-0.25522170241457
P	-5.05985773159405	-2.76931129915546	0.06602591113963
C	-6.25438356296169	-1.55918809750336	-0.10710320306353
H	-0.19040262841074	0.12680588261176	-0.10364500701290
H	-2.30476920168779	1.36381762058698	-0.31862157816847
H	-0.21337055955041	-2.34060213831034	0.17749566764396
H	-2.35012744726536	-3.55295945265925	0.24809292747901
H	-4.66476416492906	1.44079452253433	-0.40162942613263
H	-6.86918757610421	0.48082296618910	-0.35375781171342
H	-7.28562996379517	-1.89364130262581	-0.10067356505833

## Compound 10

M=2 (D=0.820)

C	-3.23505657321742	2.28062666445356	0.30329608256475
H	-3.97633955209004	2.14619157686922	-0.47360008442520
C	-2.51874569664856	1.17486513217986	0.72832105014929
H	-2.74143780659181	0.22743953648313	0.25543124591607
C	-1.52551847655948	1.17764881022399	1.72127222399056
C	-1.11987933761764	2.32768089310672	2.43289589328091
P	-1.92001478236505	3.80127647209846	2.02313009340416
C	-3.07139350720679	3.59554815245816	0.81235178925627
H	-1.03331625846237	0.24378293441405	1.96488286188715
C	-1.36372268526587	5.11012007095488	2.92381317042407
C	-0.33789282326595	4.84539011468780	3.86901860931699
H	-1.76732103421414	6.10055135479025	2.78447387053732
H	0.02493770292164	5.68645608947098	4.44534776183626
C	0.22161988834821	3.59998906739785	4.09805259099375



C	-0.13207558488975	2.41161661790718	3.43860918926853
H	0.38069542981266	1.49623409898943	3.70857419843544
H	0.99807167256143	3.53519221551933	4.84886939415409
H	-3.65414057524908	4.42508019799513	0.44418005900963

## Compound 11

M=1

C	-3.20074362539713	2.40230988651149	0.30743607259977
H	-3.94019395317018	2.28523955358683	-0.47573905039182
C	-2.51287990765045	1.23650045206813	0.72398764761893
H	-2.77200861230402	0.30934043941031	0.23038914313077
C	-1.54684469672699	1.20231117790969	1.70184921560369
C	-1.13060021357502	2.35029856645278	2.41257160143291
P	-1.84497842174629	3.88691500786641	2.05583534576924
C	-3.00675562510920	3.66591109240113	0.81452508705263
H	-1.07952386948794	0.25297184066446	1.94400894115928
C	-1.34770546516070	5.25220524450079	2.89939658263013
C	-0.35905662615641	4.87325991368436	3.81624363029288
H	0.06142839698484	5.66444003044078	4.43678566017489
C	0.19208533039871	3.58369698557284	4.06681314078766
C	-0.14961286957056	2.40684980227452	3.42961796564377
H	0.34880462701371	1.48666070229587	3.71448774714162
H	0.95629023628799	3.52261502786104	4.83361168545955
H	-3.56753470463036	4.51349427649857	0.44752958389409

## Compound 12

M=2

C	-1.59659769785457	-0.37898213517038	-0.00016877476828
C	-0.45496071848445	0.41668116020505	0.00060594422410
C	0.81182502381111	-0.15919851379256	0.00223257905219
C	-1.48206249155973	-1.77373971453766	0.00068716477312
C	0.94999721011131	-1.55205749110839	0.00309908445714
C	-0.20951330088400	-2.28285937281983	0.00228403304943
H	1.92832491358741	-2.01449742052562	0.00434988408517
H	-2.36089947596799	-2.40493775559866	0.00010262098179
H	-2.57868173567357	0.07700083139435	-0.00143115481968
H	1.69533122291852	0.46659545323871	0.00282940471089
H	-0.55353295000399	1.49401495871502	-0.00006078574587

## Compound 13

M=1 (D=1.812)

C	-1.59250524138931	-0.31659854079022	-0.00016332622321
C	-0.42955344530604	0.44814244786246	0.00084064265913
C	0.81300959778104	-0.17901595082494	0.00224392729862
C	-1.51897782633205	-1.70010783834174	0.00022931025730
C	0.89733840800739	-1.56189859143463	0.00262979916752
C	-0.26998827544961	-2.34397170549850	0.00162668593285
H	1.85911256853623	-2.05497035822212	0.00371508496737
H	-2.41833700740741	-2.29945769738196	-0.00053951442758
H	-2.55972013362904	0.16789538910386	-0.00126122729488
H	1.71879076405045	0.41234460471939	0.00302933700421
H	-0.49160376888841	1.52807658015016	0.00051977530480
C	-0.18927192416315	-3.76028746368847	0.00201625874636
P	-0.10236371581012	-5.30308087565328	0.00229324660751

## Compound 14

M=1

C	-5.82880512758661	3.80536000422821	-0.23954795641943
C	-7.17872664612222	3.48248211002911	-0.33139474422706
C	-8.13999018437335	4.38810652222815	0.10558599882334
C	-7.75141495424568	5.61470351062411	0.63381109141808

C	-6.40149290308053	5.93758014311379	0.72565507384926
C	-5.44023263226660	5.03195765733036	0.28867628474580
H	-4.38960603281879	5.28132897065780	0.35949072222772
H	-5.07987503517727	3.10192724047940	-0.57926152848198
H	-9.19061266512817	4.13872034556741	0.03477235647668
H	-7.48035237000153	2.52806406278499	-0.74241558630925
H	-8.50034595863543	6.31815029729296	0.97349222593335
H	-6.09986549056381	6.89198913566370	1.13669606196350

## Compound 15

M=2 (D=1.263)

C	-5.62483589153958	4.33322600171580	-0.82160395706713
C	-7.10048032091127	4.06672346865424	-1.00528854259940
C	-8.04082233739509	4.66108933404343	-0.22692045789109
C	-7.69149974859896	5.55743916560908	0.80817184060200
C	-6.32974706116933	5.84422988915843	1.05392921322099
C	-5.33656812881336	5.28672930967161	0.31450402888433
C	-5.03088284459213	4.82375241006605	-2.07525722989411
H	-5.12341529064336	3.37322664828355	-0.60433729758961
H	-9.08649559934416	4.44279472593623	-0.40479496899317
H	-7.37701335574922	3.39208386281019	-1.80327299566180
H	-8.46102368489761	6.02078976568273	1.40829797355266
H	-6.07128638526720	6.52728725718415	1.85354378893212
P	-4.43056879639435	5.35882319348116	-3.38952484135112
H	-4.29814055468445	5.52200496770326	0.50151344585533

## Compound 16

M=2

C	-5.95152004875755	3.71984591182220	-0.33454110698660
C	-7.30682851736503	3.44344147021363	-0.31257470745361
C	-8.21072122341078	4.39133279314984	0.16604379997929
C	-7.74400466275746	5.61851542884167	0.62098538438228
C	-6.38439845509224	5.89701619451238	0.59797166788745
C	-5.46236020252395	4.95374081613861	0.12294628488480
C	-4.04022475218331	5.27932424413869	0.12050130992028
H	-5.25480373780694	2.98109600345277	-0.70920474424583
H	-9.26991700652720	4.17223763617084	0.18157394685257
H	-7.66585098233518	2.48714050931891	-0.66936835338274
H	-8.43907116150116	6.35954575895727	0.99289199124148
H	-6.02312209699234	6.85375970095877	0.95326883517715
P	-2.71417152835591	4.36162106962523	-0.31749339859086
H	-3.82179562439096	6.28957246269918	0.46940909033437

## Compound 17

M=2

C	-6.37047187753767	3.48157054333928	1.44116581999092
C	-7.66366090934819	3.90793387694836	1.18338340188846
C	-7.98034711101336	4.47441810725424	-0.04775997097294
C	-6.98821378435358	4.61952701992176	-1.01144731237708
C	-5.69531259713024	4.18394600306977	-0.75900964195745
C	-5.36395230854033	3.58904251700442	0.46761790014306
C	-4.02214262961378	3.11281224195754	0.78123880440288
H	-6.12785585310699	3.04466847539245	2.40141337575530
H	-8.98755098696816	4.81437998245891	-0.24758088080974
H	-8.42555926460506	3.80459450706522	1.94458708763787
H	-7.21929333480959	5.08567358462302	-1.96015229718050
H	-4.92331553657876	4.33934521206748	-1.49773854807824

P	-2.77820696921145	2.41029885752160	-0.10249758284348
H	-3.76342683261435	3.19044860851374	1.83529933759899
C	-3.46696100109847	2.15586013441681	-1.77424114540241
C	-2.70587958644666	1.94007077920424	-2.81347224943537
H	-4.55570268255741	2.12355161399876	-1.87304939446004
H	-2.79546673446598	1.72342793524234	-3.86598670390026

## Compound 18

M=2 (D=2.402)

C	-6.23376639888032	3.73868616747204	1.39182458071509
C	-7.42778527974401	4.20665481773049	0.92987393809142
C	-7.68021321692335	4.30844868139733	-0.48410190828423
C	-6.70233584667247	4.07540934169277	-1.37334829728927
C	-5.29306375179456	3.78845092633136	-0.93769591581429
C	-5.17710017502691	3.36723768753071	0.51397464763207
C	-4.06082680048779	2.70142358946513	0.97945253029197
H	-6.08869278251034	3.57868596906935	2.45325385685979
H	-8.67740614308883	4.55867497188661	-0.82204231253782
H	-8.22140400822796	4.44349915097535	1.62549969522091
H	-6.88797219581232	4.14405742090628	-2.43791770333358
H	-4.78259814636544	4.77970202424506	-0.97218812878270
P	-2.78856414970520	1.97203820607924	0.04183916406873
H	-3.98921297771957	2.56106194657955	2.05398535283887
C	-3.46356085863014	2.19094781016528	-1.60177532055673
C	-4.53379746020137	2.93700265609102	-1.91582024447545
H	-2.95734119767432	1.65318868439759	-2.39602694375999
H	-4.86767861053511	2.99639994798474	-2.94701699088481

## Compound 19

M=1 (D=1.983)

C	-6.46559618077641	4.36788303657165	0.12808347623152
C	-7.69431848460814	3.76299642086625	-0.23000142854029
C	-8.65734825993700	3.49639173858347	0.70808415832589
C	-8.43403940703819	3.82540978051351	2.06114860826521
C	-7.25599781508254	4.41080340748351	2.44240443618602
C	-6.23606358895647	4.70235415484459	1.49872083368913
C	-5.02871702587574	5.30730085429991	1.91783070999940
H	-9.58956870864954	3.03277926453428	0.41458205245752
H	-7.86062381064615	3.51121076804542	-1.26985285592790
H	-9.19716203944490	3.61269226180021	2.79797408059793
H	-7.08245511720414	4.66309138952910	3.48071940931600
P	-3.69144700485702	5.73218605360960	0.94317466723213
C	-4.27346433609085	5.20493855006280	-0.63110446355141
C	-5.48890547311436	4.62835688451263	-0.86787920006228
H	-3.60561355534740	5.35548570356964	-1.47145820022449
H	-5.74487572565340	4.34102111519733	-1.88291838539867
H	-4.94197346671770	5.52581861597608	2.97727210140426

## Compound 20

M=2

C	-6.04499141594256	3.55701705707628	-0.37779186308962
C	-7.41871128964536	3.43257978127841	-0.39091852295217
C	-8.23174239373759	4.45126561666213	0.11031957293877
C	-7.64757101117826	5.60739399939090	0.63180464378477
C	-6.27619545281298	5.75491925348292	0.65628865614980
C	-5.43083308683754	4.72608173276653	0.15336891124122
C	-4.05829220778607	4.86608040141815	0.15921994001830
H	-5.41474082560386	2.76960587338471	-0.76596843287836
H	-9.30761171209717	4.34502839358157	0.09487137265220
H	-7.86764516189564	2.53453233884106	-0.79447213248629
H	-8.27440928303277	6.39845500564962	1.02195840116528
H	-5.82330597924953	6.64974882164884	1.05901346765269

P	-2.47941890867744	4.85559074874630	0.51752894018992
H	-1.97815127150323	5.46830097607259	-0.68223295438648

## Compound 21

M=2

C	-6.15378056490219	4.02249337255461	0.29310469886636
C	-7.32424152838361	3.44687267840460	-0.18119825242583
C	-8.46288683304170	4.22390804040645	-0.36346652674847
C	-8.42282695173328	5.58020870498198	-0.05996523599803
C	-7.25704141166037	6.15454503516861	0.42733837456652
C	-6.10052888273646	5.38517435901364	0.60459999105273
C	-4.85366097144618	6.00411695299530	1.09981617249376
H	-5.27561906461321	3.41128173765618	0.44860609958536
H	-9.37444926112648	3.77567455983783	-0.73563028054819
H	-7.34870319306000	2.38801880460710	-0.40237683993965
H	-9.30140647624325	6.19488062035119	-0.20472487279466
H	-7.23028397554814	7.21192295458454	0.64753563899016
P	-3.31128641220414	5.78546014871134	0.41745146109973
H	-3.70511681794396	4.94671432074607	-0.65995879675378
C	-4.92869136383835	6.88234600089104	2.26574750902758
C	-5.99332463328197	7.11655194554957	3.00412844651288
H	-3.99147450970623	7.36954176553721	2.55088338371334
H	-6.23588714853045	7.70529799800269	3.87335902930021

## Compound 22

M=2

C	-6.59407044828903	4.27248565881753	0.82080617465787
C	-7.74592504969854	3.74935786665412	0.24915118853027
C	-8.54552707920278	4.54449142478467	-0.56472145817241
C	-8.18606270895126	5.86794249917717	-0.79767117315745
C	-7.04636136656543	6.39661349943489	-0.21084365952291
C	-6.23002788083273	5.60548966791723	0.60373090059039
C	-4.99980145660676	6.17738285117736	1.18804091349368
H	-5.97967622489804	3.65577348684937	1.46230758751395
H	-9.44250475788413	4.13695598650547	-1.01123647575693
H	-8.02052013159017	2.72071719395218	0.44177284070848
H	-8.80112385297308	6.49265920939428	-1.43163184844504
H	-6.77834768667323	7.42980367043037	-0.38115518366493
P	-3.46915551407917	5.43759672905142	1.04612781633886
H	-3.88679751858785	4.28616949598923	0.32533780727382
C	-5.01080845009902	7.47085753515237	1.85288418533885
C	-5.99783338888916	8.17536512294511	2.45354912087494
H	-4.03488656527501	7.94321801239046	1.90093540062330
H	-5.68776895040464	9.14267667586628	2.83558745003711
C	-7.40394928977305	7.89142809063247	2.74705314881640
C	-8.04443058448046	6.74597345270837	2.80282155169585
H	-7.89031058649333	5.69141198558546	2.66134954755986
H	-7.97185050775308	8.78093988458414	3.02175416466603

## Compound 23

M=2 (D2.518)

C	-6.43023576711739	4.15707831027598	0.73155267658599
C	-7.51821738649155	3.64220661347197	0.09573476960298
C	-8.50491978336253	4.50124560501547	-0.51008838122911
C	-8.43341581537770	5.83022523502897	-0.35424619556070
C	-7.36669743494604	6.48234754057429	0.47350416809218
C	-6.21923290881697	5.56002972017862	0.85013197059061

C	-5.01133822520310	6.14274223179536	1.27766310120164
H	-5.70166364581884	3.48386555066707	1.15772695606059
H	-9.30993666735322	4.05677393039678	-1.08062941467365
H	-7.64553409922845	2.56984683391217	0.03250594318172
H	-9.18614550993094	6.48159710391276	-0.78108196629269
H	-6.94620166044680	7.33817476415559	-0.06878832718333
P	-3.42626397465383	5.35191724340866	1.32581350374650
H	-3.79623585822867	4.09337198033901	0.78570395959439
C	-4.93566151034397	7.53686050157463	1.69331488811340
C	-5.90221277927777	8.28591950441194	2.27952410498817
H	-3.94477789934406	7.97619219223425	1.65653611430963
H	-5.60488281955650	9.25178370496868	2.67262507555090
C	-7.25793081363444	7.87220127936619	2.53980118451050
C	-7.94742372783323	7.02173865684944	1.76752997628458
H	-8.93670606275249	6.68862993286115	2.05585063080511
H	-7.74210565028146	8.29056156460092	3.41526526172058

## Compound 24

### M=1 (D=2.011)

C	-6.57541036755785	3.61923218350686	0.05484659467105
C	-7.74991546749459	3.28486871687695	-0.59546498578858
C	-8.61242674639325	4.29184393785108	-1.01711833450858
C	-8.29459143257527	5.60787768055962	-0.74600871899297
C	-7.12414884712972	5.97441296626439	-0.05552426218890
C	-6.21331695997136	4.95049486852381	0.31745095198601
C	-4.87767040183144	5.18443300902527	0.91445282631877
H	-5.90589026574599	2.83567927865931	0.37965074769565
H	-9.52954894666612	4.05026439286188	-1.53706629342340
H	-7.98918528404534	2.24528415707869	-0.77384312455514
H	-8.97127509214316	6.39461712862596	-1.05352916245123
C	-6.21354592119649	8.00208537206152	1.14590678575075
P	-3.57466799637867	4.21330168620415	0.37953939558494
C	-4.70147092639876	6.18160862944794	1.95323617719949
H	-3.94356266302401	5.94278183894292	2.68967285592878
C	-5.28210698425340	7.39679679884680	2.05390046189868
H	-6.33865974558606	9.07360950368870	1.24906988831293
H	-4.94711650584112	8.02512578865902	2.87105568084592
H	-2.61712202120520	4.71166111907190	1.30845717970973
C	-6.97293998884717	7.39075963969614	0.21406718769662
H	-7.64318743571497	8.02433130354706	-0.35526185169050

## Compound 25

### M=2

C	-5.83640341834971	3.75708405988757	-0.16173845643944
C	-7.19793760850379	3.60772838759874	-0.37675774148803
C	-8.08651996642729	4.59250679043644	0.04303919919548
C	-7.60088394761879	5.72737862340046	0.68351583458430
C	-6.23876219478737	5.87802348283317	0.90107322492910
C	-5.32988213379087	4.90051249207882	0.47238641889994
C	-3.87965983885087	5.09111309227159	0.67407290137660
H	-5.15321125503087	2.97519585452016	-0.46358257284785
H	-9.14910728856000	4.47186115974336	-0.12001456251492
H	-7.56842849270206	2.71404933800779	-0.86109127818155
H	-8.28446888126246	6.49844790387417	1.01327488921930
H	-5.86831590380671	6.77219589077089	1.38341034168460
P	-2.78451131044376	4.49521537009310	-0.48067881529182
H	-1.59742764039722	4.81160131142739	0.23394276017959
C	-3.49376629870794	5.82254982135377	1.89987105384601
C	-2.54184557431362	6.72027111718425	1.98964891825155
H	-4.10094028230370	5.61038275993248	2.77918502616378
H	-1.82317586502486	7.19903502165107	1.34433429356447

## Compound 27

M=2 (D=0.732)

C	-6.50988133962508	3.77522437871373	-0.12533912646820
C	-7.69404725956067	3.68407494523662	-0.84274223076265
C	-8.43694063974718	4.82571942785082	-1.12078986829396
C	-7.97655174095631	6.06226352956242	-0.67690008358649
C	-6.79268229831686	6.15597942857648	0.03728167380868
C	-6.03425689117888	5.01186052026603	0.33935468949971
C	-4.77705006523893	5.11292969850853	1.08512521166922
H	-5.95787580027744	2.87279923240135	0.10336220544788
H	-9.35901182521158	4.75506387347069	-1.68179327319838
H	-8.04058949561824	2.71609220207402	-1.18020692142973
H	-8.53727492450324	6.96051955800105	-0.90027852996975
H	-6.43340675607705	7.12944206719964	0.34037604331696
P	-3.54988524601715	3.80243331974817	0.86284411954966
H	-3.21703362203531	3.95644802191194	-0.51485393176515
C	-4.54826040697945	6.12620041909534	1.99819208179383
C	-3.36029098651220	6.34752720129120	2.70025476363806
H	-5.36430732909849	6.81318997263489	2.19218716042482
H	-3.32326132636534	7.17600745374257	3.39376423210898
C	-2.19652378926056	5.56641954183670	2.52388104383222
C	-2.12341464403858	4.48692343283596	1.69477203451528
H	-1.19654768645927	3.93387823300453	1.61003343189767
H	-1.30893592692212	5.85686354203726	3.07514527397134

## Compound 28

M=1 (D=1.431)

C	-6.24470520393384	3.90696357586533	-0.46489312402736
C	-7.44657297905148	3.78836395472256	-1.14937723243558
C	-8.46165077178643	4.71686484108894	-0.94834051352266
C	-8.26480445326664	5.76359576395572	-0.05424767502892
C	-7.06304209277529	5.88238950444831	0.63007784713864
C	-6.03000378608528	4.95844788694676	0.43284134424648
C	-4.74709948428899	5.08727437585319	1.16316714209992
H	-5.45355727531745	3.19010853362891	-0.63868857860953
H	-9.39785570088200	4.62596343761315	-1.48255824718446
H	-7.58765077389425	2.97231271528015	-1.84562982389018
H	-9.05309638954182	6.48458926394608	0.11782724693205
H	-6.93053805378893	6.68494782896122	1.34319404680660
P	-4.02619123652882	3.63184763876412	1.82640460167998
C	-4.17354645231008	6.35090206641111	1.30815508230430
C	-2.97931698314855	6.60518305525000	1.97083207364845
H	-4.68332099037857	7.19150718602504	0.85038021768186
H	-2.62278021669700	7.62637759347901	2.01045798383866
C	-2.21803258165341	5.60810102994119	2.57134138765584
C	-2.59278079341643	4.27362076198510	2.55670793753728
H	-1.94717436675937	3.55658321717107	3.05169667917517
H	-1.29618941449535	5.89044576866300	3.06689160395348

## TS I trans

M=2

C	-2.10834842420995	0.79291121861230	0.19573397727373
P	-1.07109380856679	-0.09022514475533	-0.53638203408734
C	-3.02909467336253	1.61848200937969	0.88536997206827
C	-4.34252225373536	1.61678410578132	0.71401274894327
H	-5.12862426641342	2.19317726022912	1.17584553318321
H	-2.59312997694498	2.30670388686007	1.61626061215512

C	-5.21979896631216	0.12179286718934	-0.91021674989073
C	-6.41799437100697	0.24736676371783	-1.01914386131089
H	-7.46187343564429	0.44536665223072	-1.02731494466462
H	-4.21018982380355	-0.19742961924504	-1.02967525367000

## TS I cis

M=2

C	-2.07192098195992	0.76842238169579	0.48151788051021
P	-1.01060635048822	-0.23929287273466	-0.01676030580973
C	-2.99094400058664	1.72521871264592	0.96990084898492
C	-4.30094162367873	1.74374526883479	0.77558743736358
H	-5.04356957942767	2.45467635184093	1.10938841324424
H	-2.54909254457927	2.52683108043054	1.57034884935505
C	-5.37293034130531	0.17568538152697	-0.66322417327050
H	-6.25789450237371	0.30421419398938	-0.08863574975226
C	-4.57904820652794	-0.19669008323462	-1.49569157110545
H	-3.78020186907256	-0.43421041499503	-2.15390162952007

## TS II

M=2

C	-2.07058306211660	0.96171734483193	0.39284612576807
P	-1.24809685157324	-0.02465325043960	-0.48191165511022
C	-3.07747895505888	1.71182655761050	0.99611958335177
C	-4.37508104269537	1.53865189836583	0.62359920602317
H	-5.12907261183033	2.13995510874127	1.11625809513756
H	-2.82912446795520	2.43586904098807	1.76365516659514
C	-4.840729258814091	0.61059186758271	-0.38379348431619
H	-5.92103966881445	0.60705442271206	-0.54717319531852
C	-4.10275573020776	-0.21726867203613	-1.11361969478267
H	-4.36318835160722	-0.93514431835664	-1.87745014734812

## TS III

M=2

C	-2.38900096290304	2.30476181013666	0.24197301348527
H	-2.89349149181157	2.32914383620732	-0.71869480915801
C	-1.76828537963739	1.12534375246584	0.62553059372130
H	-1.80938789401535	0.27816673397809	-0.04978693476347
C	-1.09143645757773	0.96227933772024	1.83332484770696
C	-0.98046530664049	1.98940113846839	2.77395467387728
C	-1.54038748779147	3.21142215421994	2.52196017924708
P	-2.43519820745389	3.77682325129920	1.18295809195210
H	-0.63571238475892	0.00424883318155	2.05084071431104
H	-0.44610589851996	1.80876803023794	3.70119014783256
C	-1.20309357827418	4.79273484289985	4.22173761035054
C	-1.17147443337844	4.26106121133663	5.30964770238655
H	-1.17856465326680	5.54506394151603	3.46966021914936
H	-1.17304586397074	3.66755112633227	6.19089394990145

## TS IV

M=2

C	-3.44151045109990	2.10014512484540	0.51935264282881
H	-4.38708499978354	1.86340286084641	0.04466375315430
C	-2.40462845373899	1.18855348149596	0.40484230566900
H	-2.56960181952218	0.27228907809830	-0.15047309880510
C	-1.14684567112042	1.40734368389982	0.96268140477845
C	-0.82362753624667	2.54367179709018	1.68927958976767
C	-1.71434393767667	3.58579133343543	1.95645542335445
P	-3.36229546154190	3.61269433938646	1.35960188784303
H	-0.37844206968188	0.65915410083168	0.81567153540029
H	0.18412657733110	2.63474611093423	2.07104833596921
C	-1.30008797703651	4.74133536876201	2.76554964516931

C	-0.31022093725711	4.82096804660985	3.63293674049176
H	-1.91841559359006	5.63513753379048	2.64395700607996
H	-0.00274189649867	5.64369271298171	4.26145068065501
C	0.70170715136977	3.06759685245724	4.74994209893626
C	-0.05666358799477	2.13387060278541	4.90917368583821
H	-0.84811597001938	1.42470598659355	4.92890978320872
H	1.59147263410782	3.64609098515586	4.82802657966066

## TS V

M=2

C	-2.55091923708544	2.46553171770429	-0.15897811946097
H	-2.84220976334238	2.45248697001602	-1.20298730988214
C	-2.21592516720176	1.25242005333852	0.44315082412185
H	-2.26078378445388	0.34750933875162	-0.15221587207307
C	-1.87310809636069	1.14108857943797	1.77686173228420
C	-1.75597570316261	2.24867207774654	2.63779118111689
C	-2.01231140880512	3.57811524652868	2.22751631063057
P	-2.54656267002582	4.01009563453239	0.61692805075052
H	-1.69115207847754	0.15721773193137	2.18949989508494
H	-1.76462259348714	2.05270383705071	3.70244361739769
C	-1.71967453171495	4.65795515937621	3.15617749371125
C	-0.62469840487141	4.68357525078544	3.94679474015929
H	-2.35377679282865	5.53700463594794	3.12915740953169
H	-0.45835733613100	5.55894569226807	4.56195508631312
C	0.46008609965257	3.70988581989643	3.90204716998276
C	0.39316296958795	2.50104140903593	3.37574413840426
H	1.10262816685844	1.70067088201286	3.23577118832799
H	1.41834033184943	4.06064996363898	4.29033246359915

## TS VI

M=2

C	-3.02115856688343	2.40555288439968	0.08620166022721
H	-3.67980396833060	2.26573693253790	-0.76339103525144
C	-2.19153407047581	1.32385983866379	0.45200157569345
H	-2.22257005456072	0.42563406975892	-0.15359540071938
C	-1.35334889110002	1.34830252426184	1.52718820802504
C	-1.23645999249003	2.46443835229617	2.42664447527161
C	-1.85016878380513	3.73708834799362	2.10700342868866
P	-3.04502771639875	3.94929465356097	0.81883390519988
H	-0.75926551757196	0.47270135429260	1.75546306717398
C	-1.52391285164985	4.85400921848009	2.90484962918668
C	-0.57852038903402	4.77923069461722	3.89944303723835
H	-2.02343034904868	5.79467361124110	2.70694913727831
H	-0.34158300068186	5.65501596335310	4.48819794091286
C	0.11854512530316	3.57163086224605	4.12816161017200
C	-0.17938871623981	2.45640510781589	3.40227372595023
H	0.89984677826079	3.53764001644697	4.87568217250744
H	0.34934573570380	1.52751188808927	3.57221954757952
H	-2.45390477099707	1.95498367994482	3.48542331486558

## TS VII

M=2

C	-3.02564648624900	2.13477520581769	0.82052836776850
H	-3.88445620959770	2.11487778664228	0.16484183885659
C	-1.91065916430458	1.33790893990143	0.57672712250009
H	-1.92228487088167	0.69114457201764	-0.29017107048218
C	-0.77199672363307	1.31175406466638	1.41762683438148



C	-0.59322663055859	2.04641111589390	2.56470133319019
C	-1.55800180148758	2.97379411530252	3.09396117051177
P	-3.12099399264466	2.93477149006919	2.32569782775754
H	0.03943153099866	0.66075931411213	1.11695825427829
H	0.35661436268590	1.97939032243457	3.08270938840381
C	-1.36579205447925	3.85463438213497	4.14343803985904
C	-2.31541000495569	4.83502265100824	4.53693111654223
H	-0.41798339428524	3.81496949364212	4.66850213398498
H	-2.04901184525803	5.49689073841749	5.34888583473816
C	-3.54000929688623	5.02479232027163	3.92303057332225
C	-4.06446117586234	4.26870228910182	2.85843336448704
H	-5.05385359489461	4.44604867256910	2.46852252082061
H	-4.15857864770631	5.83970252599694	4.28158534907964

## TS VIII

M=2

C	-5.73271989174820	4.69319781247853	-0.74163906830417
C	-6.99927024069311	4.09153276287314	-0.80657807652389
C	-8.01103697927357	4.50008392554244	0.04713990331709
C	-7.78274434484493	5.51392386732897	0.97280810009314
C	-6.53112785721868	6.11786168511220	1.04542306233356
C	-5.51175822118454	5.71430381917276	0.19783063538101
C	-4.66394405683354	4.27652520022514	-1.58560615569759
H	-5.81389183784530	4.18820215005460	-3.34236929228856
H	-8.98304529042544	4.02900849222795	-0.01142943949370
H	-7.17270643205838	3.31046725924453	-1.53250289136101
H	-8.57760523129334	5.83268890299318	1.63356534714490
H	-6.34974418351568	6.90622217839125	1.76355881369755
P	-3.33611508448100	3.85764168188198	-2.27975231712273
H	-4.53707034858429	6.17854026247333	0.24851037882438

## TS IX

M=2

C	-6.36746053934524	3.48512903213971	1.46859435685732
C	-7.66341651618923	3.88236076297790	1.17893243248242
C	-7.96036406613800	4.45220809138173	-0.05548170455909
C	-6.94632233706877	4.63102694615919	-0.99150162185965
C	-5.64967212917436	4.23331578398477	-0.70388495484358
C	-5.33666698726440	3.63437289584910	0.52657190541227
C	-3.99044838356871	3.18232169113798	0.85847834890403
H	-6.14068023740108	3.04184755845186	2.42987797463386
H	-8.97044153382160	4.76698863335945	-0.28056805510245
H	-8.44366363811998	3.75154477215947	1.91696194740560
H	-7.16474975373792	5.09426814108223	-1.94455859349133
H	-4.86020783028625	4.40824963782113	-1.42082604772367
P	-2.68935425014586	2.72352898979385	-0.09312016418731
H	-3.81209291616567	3.09151080742530	1.93080219662583
C	-3.77604783011527	2.03586779853106	-2.13372301517841
C	-3.07237705980676	1.82194792886732	-3.11695141894565
H	-4.75370905317035	2.01717384599709	-1.69703853130083
H	-2.23564293848055	1.74790668288083	-3.77079405512935

## TS X

M=2

C	-6.31886782262133	3.46320393036129	1.29880617424494
C	-7.57235879002051	3.83667231415675	0.84718803552041
C	-7.71927895394368	4.43027934522398	-0.41237215279107
C	-6.60845561382462	4.66057129503474	-1.19999376979993
C	-5.33535063396440	4.25181004198585	-0.76972318123760
C	-5.18051272526796	3.63665273382648	0.49583496637417
C	-3.89203939959654	3.14466809944779	0.92599485451297
H	-6.20856451923802	3.00236836848024	2.27206512511743

H	-8.69971069821890	4.73467887274737	-0.75385924784453
H	-8.44049757639551	3.67449603420688	1.47192270793380
H	-6.70982794462847	5.16533314266046	-2.15160362031620
H	-4.45878268856619	4.64389147694066	-1.26246478190450
P	-2.72467852585985	2.29284872869681	0.05412152210218
H	-3.66987208003084	3.23301494313957	1.98661044510581
C	-3.53493730468590	1.91679689710357	-1.54234473914999
C	-4.52815322262829	2.53140855245955	-2.13542396677392
H	-3.11643492943789	1.01357187772920	-1.99575568948278
H	-5.11499657107110	2.36930334579877	-3.02723268161120

## TS XI

M=2

C	-6.25099096557242	3.70404894289432	1.37592210276878
C	-7.42556542844302	4.24318149814198	0.92447879189753
C	-7.68380818144549	4.33750730293740	-0.46438781005130
C	-6.73842921734072	3.94655983750086	-1.36487728258914
C	-5.45523728159635	3.46976567327662	-0.93470880729335
C	-5.25114320696455	3.24665266857037	0.48016395924649
C	-4.07959629513728	2.63593471872930	0.96049039259455
H	-6.07301291997975	3.59757430579573	2.43834372869267
H	-8.63768842986600	4.71520485508985	-0.80697473866048
H	-8.17563624715265	4.57329911114535	1.63057098120469
H	-6.92342289273713	4.01994158243541	-2.42850598562622
H	-4.69279042651488	5.03413009011779	-0.94027852161556
P	-2.79972304995248	1.96831361570472	0.03830667223673
H	-3.97939894421442	2.56749272019855	2.03890982368427
C	-3.41796626021332	2.23133046433428	-1.59410092257744
C	-4.57314979486388	2.87737044479087	-1.90204667639842
H	-2.81751714079227	1.83978882560145	-2.40716697889049
H	-4.85824331721340	2.99347334273504	-2.94236872862336

## TS XII

M=2

C	-6.19573934828838	3.94925682025972	0.33601437121128
C	-7.43412928769608	3.41580437212548	0.01683132993977
C	-8.52964173454539	4.25075941467770	-0.18314829628052
C	-8.37810694918605	5.63015868399600	-0.05822926109119
C	-7.14737061264470	6.17385166396301	0.26824973336713
C	-6.02843084702620	5.34179097546510	0.45942751058379
C	-4.75872700856258	5.88426981949139	0.78617004998860
H	-5.34333587276080	3.30373963564027	0.49518985548782
H	-9.49455284637960	3.83087359772117	-0.43305013389233
H	-7.54590132885781	2.34368241325899	-0.07732810017432
H	-9.22618354946141	6.28339205170397	-0.21624678867963
H	-7.02718448772288	7.24344739492134	0.36455180241872
P	-3.20242746986247	6.05050585351928	0.27592129157144
H	-3.36240428677058	5.43344008920977	-1.00955423923934
C	-4.84239968154118	6.94854350026326	2.74526654166374
C	-5.96408456621380	7.22796987197659	3.13721718992047
H	-3.77930539376757	6.94587596636437	2.84203290837764
H	-7.01128472871249	7.34764787544246	3.27593423482696

## TS XIII

M=2

C	-6.59251831349473	4.37782514493220	0.67634793482801
C	-7.80193175209874	3.94719928120002	0.14531872160242
C	-8.55138460920216	4.79189355791228	-0.66485035384787
C	-8.08244780889576	6.07339059476029	-0.94113230627237
C	-6.88200471726533	6.51026728035190	-0.39790896721986
C	-6.11949167899970	5.66610202341517	0.41775213291418
C	-4.84468570269538	6.14499662301734	0.99376665249615
H	-6.01789034309370	3.72614485382636	1.31971379177959
H	-9.49323962145363	4.45622737744480	-1.07742553297264
H	-8.16193023377494	2.95231437426618	0.37118602102496
H	-8.65499110187051	6.73458575098694	-1.57818899614632
H	-6.52482795416174	7.50949121223803	-0.60409138293019
P	-3.34494398427576	5.38051162969919	0.75371719258955
H	-3.81619614461789	4.33299272834717	-0.08407749931091
C	-4.86471319961213	7.35658905632508	1.80286501652124
C	-5.92248187688035	7.97670880106288	2.30626176851039
H	-3.88396016636482	7.77929685470893	2.03680989328857
H	-5.97445235531550	8.85531119101088	2.92893308646216
C	-7.93434342011035	7.00176216239814	2.79332698984214
C	-8.09005606140240	7.06876189069143	3.99551918193075
H	-8.07921936740552	7.20423918959264	5.04948834687994
H	-8.13002958700891	6.76869842181205	1.77261830803008

## TS XIV

M=2

C	-6.47130553238584	4.21208044443000	0.86905750070356
C	-7.60696252982945	3.63378806026733	0.31914618856942
C	-8.47401504214733	4.39525652994539	-0.46680281209717
C	-8.22911823152787	5.74418192535732	-0.65146209939897
C	-7.14124065983623	6.35580602680625	-0.01217517133672
C	-6.19604300393495	5.56984632893436	0.68511376961938
C	-4.94773488867137	6.18332699487576	1.15792357226031
H	-5.79025506832331	3.61272496893922	1.45670260208603
H	-9.33426731981010	3.93035322120627	-0.92979438131039
H	-7.80730742353454	2.58368358986094	0.48411917169459
H	-8.89505811486471	6.34503373351672	-1.25592614424365
H	-6.90148802580076	7.38604208072804	-0.23197499875273
P	-3.40646097913174	5.49048493666026	0.88396055445112
H	-3.83968965634757	4.34808265865220	0.15886061205946
C	-4.93114442205370	7.45998462613865	1.85104779422551
C	-5.90580276958058	8.14880399891846	2.48980327632430
H	-3.94035763313230	7.89487363238524	1.93593591302265
H	-5.56413769076307	9.03629999887708	3.01170950920037
C	-7.32225480457624	7.87533921344288	2.68715768001298
C	-8.13964506441505	7.15192028899555	1.94876480440902
H	-9.17906443762951	6.88331323315600	2.06012064578136
H	-7.74438670170375	8.37408350790598	3.56466201271957

## TS XV

M=2

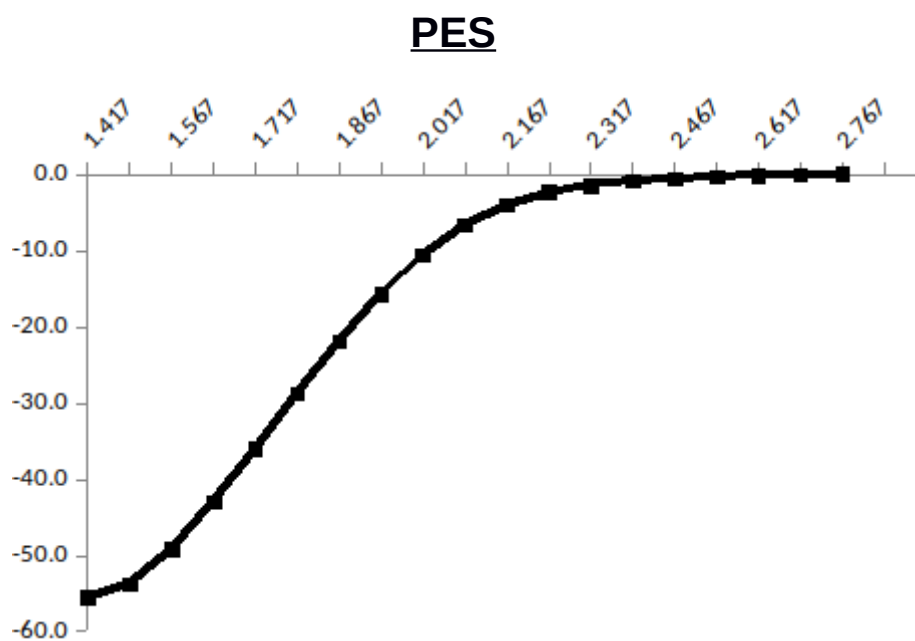
C	-6.15006191326010	4.38020284297389	0.05818989976542
C	-7.22275310075254	3.81225732751387	-0.60202134449803
C	-8.50823496296401	4.32666111620839	-0.41089520366773
C	-8.67589224988525	5.43835137439214	0.37549476599010
C	-7.57491472219207	6.12223616466153	0.96927682531634
C	-6.28404454029470	5.49206011164453	0.90310394705029
C	-5.08850656026736	5.98515194838401	1.59561536132012
H	-5.16307723788006	3.96557404031878	-0.08289705225362
H	-9.36185724556337	3.85920792242103	-0.88266843542159
H	-7.06459205310682	2.95959316739023	-1.24813084759976
H	-9.66360553788229	5.85492092253907	0.52064619208365
H	-7.22965781900830	7.20250096413948	-0.43033109053438

P	-3.83131371365391	4.99927632523947	2.21640983210142
H	-4.44723615651361	3.73785997375201	2.00055545827811
C	-4.86299798937598	7.41982425154587	1.73659116874427
C	-5.75551864480588	8.37741122199394	2.05986250858702
H	-3.82326270380931	7.72339494156230	1.67725306222646
H	-5.36460421517621	9.37574258068282	2.21852298373198
C	-7.15365235976930	8.19489126897631	2.34027520333956
C	-7.93464033428035	7.19698457978189	1.89644129983003
H	-8.98345368430702	7.22519195508115	2.16553843225490
H	-7.62386225525152	8.96601499879718	2.93911703335546

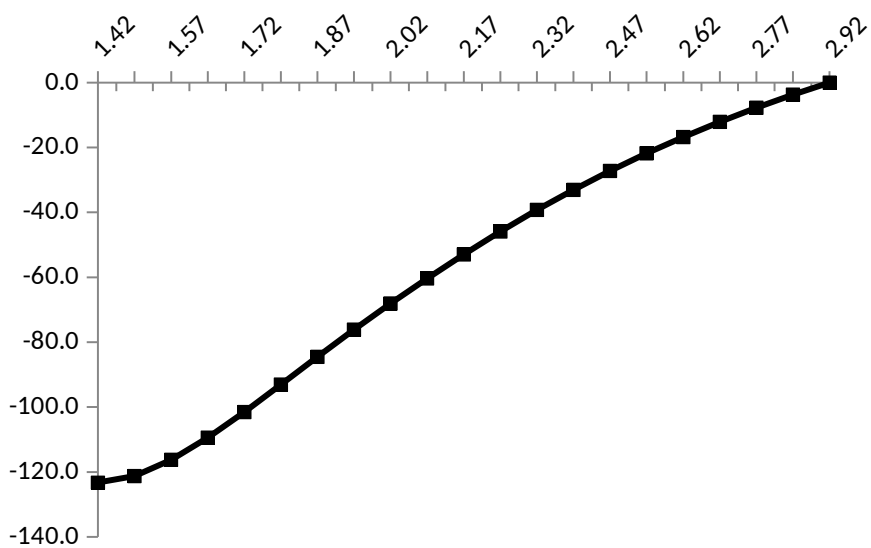
### TS 3 to 4 (*cis-trans*)

M=1

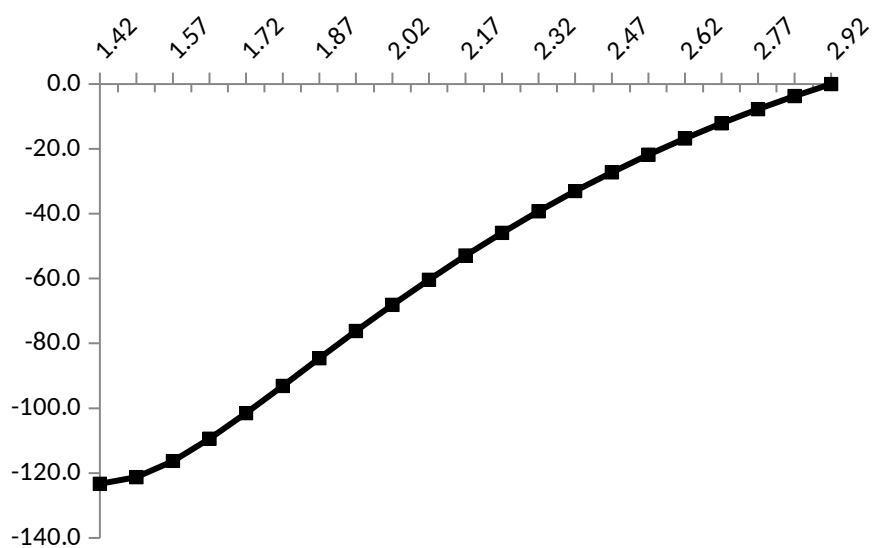
C	-1.94931365280821	1.24209993891393	0.26250060646239
P	-0.69236665233680	0.87203913414031	-0.55708082085654
C	-3.08431400723867	1.60157910754674	1.02061263843178
C	-4.35396447289363	1.34229330784585	0.67025081197744
H	-5.15077790533751	1.68301704350204	1.32251157926371
H	-2.89914446439334	2.13239960838439	1.94966885305367
C	-4.75669782738089	0.64721443131407	-0.57450011257654
H	-4.92826119738673	1.28871266756835	-1.44708547940164
C	-4.93140443701627	-0.63987459200311	-0.69449104048132
H	-5.21090538320793	-1.34088064721258	-1.46385703587296



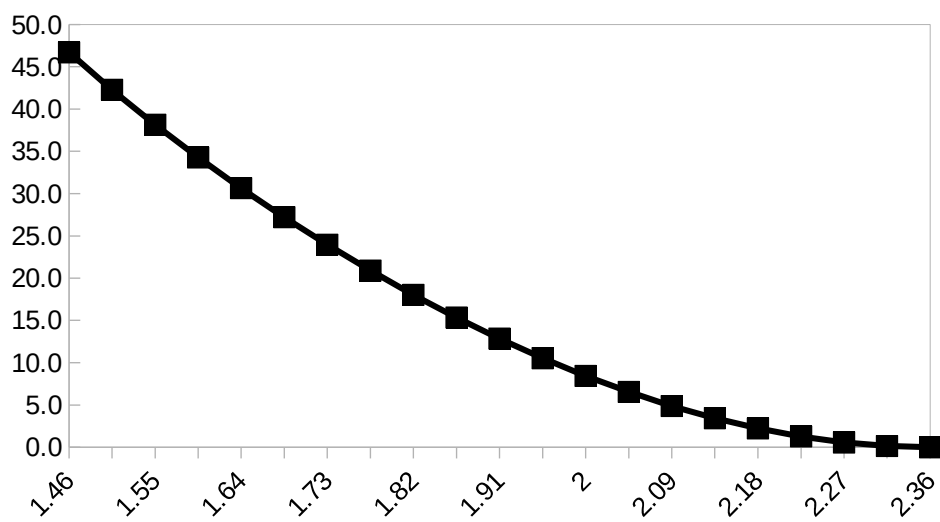
**Figure S1:** PES Compound 1  $\longrightarrow$  Compound 2



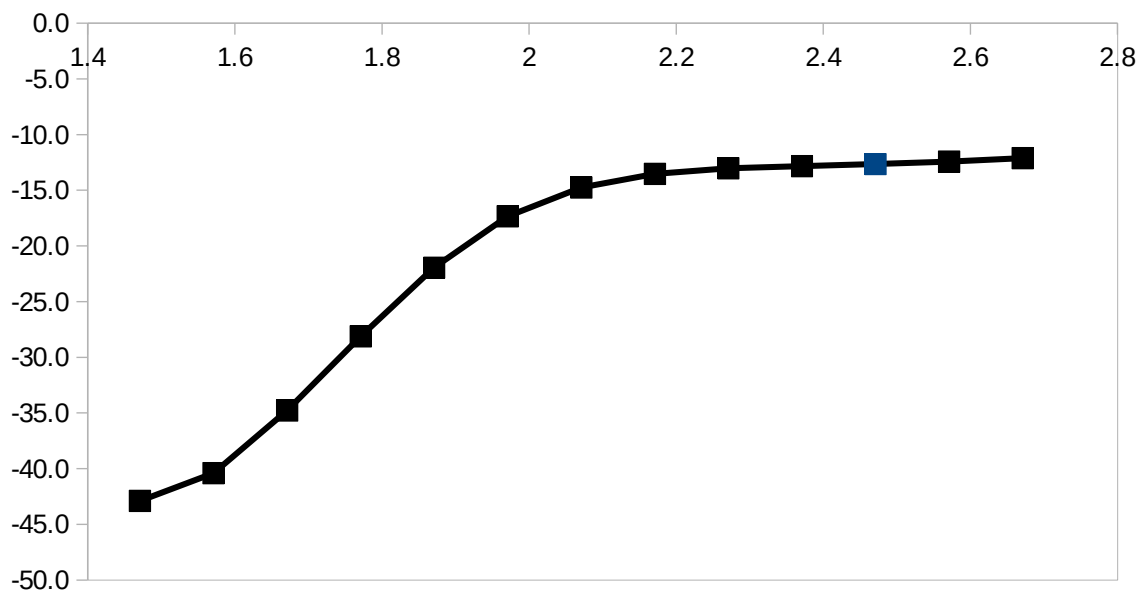
**Figure S2:** PES Compound 7  $\longrightarrow$  Compound 7a



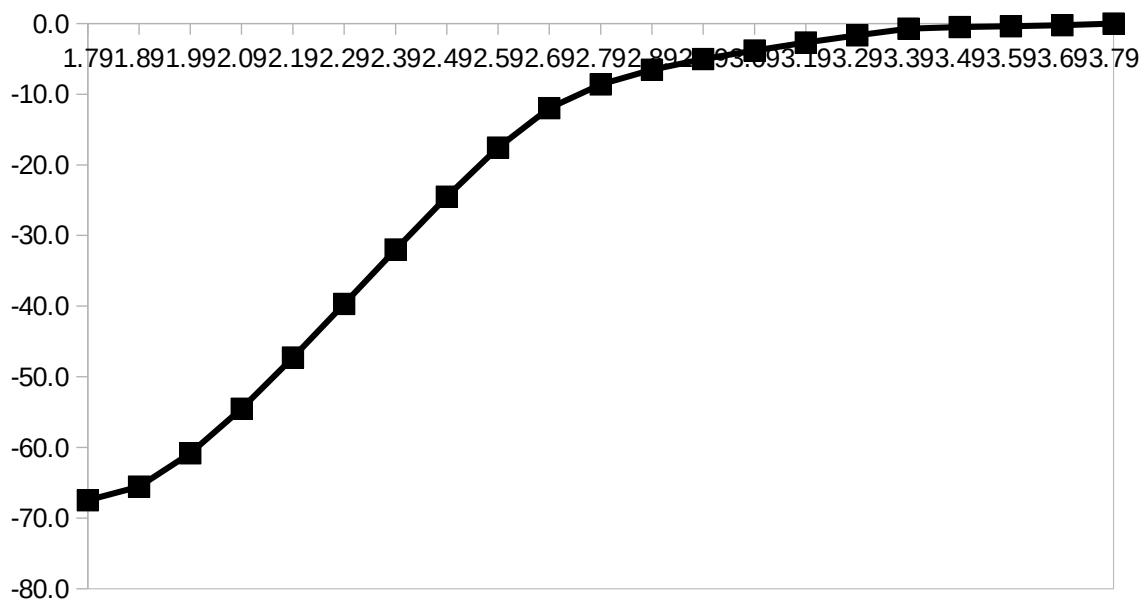
**Figure S3:** PES Compound 1+12  $\longrightarrow$  Compound 13



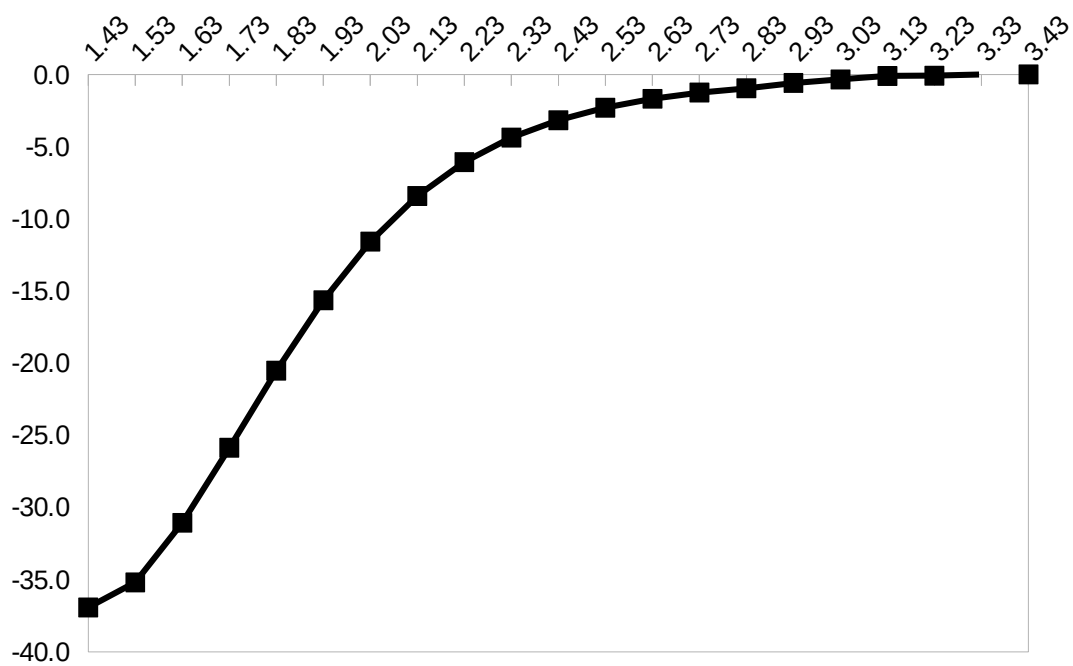
**Figure S4:** PES Compound 16  $\longrightarrow$  Compound 20



**Figure S5:** PES Compound 15  $\longrightarrow$  Compound 14



**Figure S6:** PES Compound 25  $\longrightarrow$  Compound 27



**Figure S7:** PES Compound 27  $\longrightarrow$  Compound 28



# Energies

Figure 1	B3LYP-D3	B3LYP-D3	MP2-F12	MP2-F12	CCSD-F12b	CCSD-F12b	CCSD(T)-F12b	CCSD(T)-F12b
Acetylene	-77.29175167		-77.16795132		-77.16583111		-77.180402229	
1 (CP)	-379.25834048		-378.77448937		-378.77525028		-378.792356813	
TS 1_2	-	No TS (see PES)						
2	-456.63732880	-54.7	-456.02344253	-50.8	-456.01881668	-48.8	-456.049944873	-48.4
TS 2_4 (TS I-trans)	-533.92572257	-52.6	-533.18613400	-47.5	-533.17468651	-42.5	-533.223214276	-44.0
TS 2_3 (TS I-cis)	-533.92406569	-51.6	-533.18513670	-46.9	-533.17285816	-41.4	-533.221652700	-43.0
3 (cis)	-533.99706012	-97.4	-533.25605359	-91.4	-533.24445200	-86.3	-533.292742699	-87.6
TS 3_4 (cis-trans)	-533.98704246	6.9	-533.24790723	5.8	-533.239480789	4.9	-533.290681203	2.5
4 (trans)	-533.99807379	-98.0	-533.25718975	-92.1	-533.24722077	-88.0	-533.294602263	-88.8
TS 3_5 (TS II)	-533.99559167	-96.5	-533.25529165	-90.9	-533.24128272	-84.3	-533.290885612	-86.4
5	-534.06922298	-142.7	-533.33233827	-139.3	-533.31764036	-132.2	-533.365590667	-133.3

Figure 2	B3LYP-D3	B3LYP-D3	MP2-F12	MP2-F12	CCSD-F12b	CCSD-F12b	CCSD(T)-F12b	
Acetylene	-77.29175167		-77.16795132		-77.16583111		-77.1804022285837	
5	-534.06922298		-533.33233827		-533.31764036		-533.365590666929	
H	-0.49929173		-0.50033774		-0.50033774		-0.500337739826805	
TS 5_6 (TS III)	-611.35634379	2.9	-610.49539010	3.1	-610.47250352	6.9	-610.538012137054	5.0
6	-611.41841415	-36.0	-610.55710483	-35.7	-610.53699837	-33.6	-610.600797917312	-34.4
7	-688.83407608	-113.8	-687.85863993	-119.5	-687.81967330	-106.9	-687.902315475993	-110.4
TS 6_8 (TS IV)	-688.70227227	-31.1	-687.71657663	-30.3	-687.68804109	-24.3	-687.769906894859	-27.3
8	-688.76692285	-71.7	-687.77949858	-69.8	-687.75382132	-65.6	-687.834224979216	-67.7
TS 8_8a (TS V)	-688.76294662	-69.2	-687.77663219	-68.0	-687.74640112	-60.9	-687.829851282047	-64.9
8a	-688.81866117	-104.1	-687.839489748	-107.5	-687.808319045	-99.8	-687.889788426166	-102.5
TS 8a_9 (TS VI)	-688.79675023	-90.4	-687.822124876	-96.6	-687.779075555	-81.4	-687.863921777965	-86.3
9	-688.30817929	-97.1	-687.34096741	-108.6	-687.29641428	-92.5	-687.379438567082	-96.2
TS 7_10 (TS VII)	-688.81793914	-103.7	-687.841939206	-109.0	-687.799218236	-94.1	-687.88373138196	-98.7
10	-688.82156056	-105.9	-687.85141018	-114.9	-687.80168521	-95.6	-687.886413055653	-100.4
11	-688.20529107	-32.5	-687.23984283	-45.1	-687.19089471	-26.3	-687.276499984845	-31.7

Figure 3	B3LYP-D3	B3LYP-D3	MP2-F12	MP2-F12	CCSD-F12b	CCSD-F12b	CCSD(T)-F12b	CCSD(T)-F12b
1 (CP)	-379.25834048		-378.77448937		-378.77525028		-378.792356813194	
12	-231.43238570		-231.05532067		-231.04072072		-231.086664305907	
	-	No TS (see PES)						
13	-610.89668236	-129.2	-610.05379217	-140.6	-610.01732761	-126.4	-610.083163030082	-128.1

Figure 4	B3LYP-D3	B3LYP-D3	MP2-F12	MP2-F12	CCSD-F12b	CCSD-F12b
1 (CP)	-379.25834048		-378.77448937		-378.77525028	
H	-0.49929173		-0.50033774		-0.50033774	
Acetylene	-77.29175167		-77.16795132		-77.16583111	
14	-232.10621745		-231.73356822		-231.71675281	
<b>TS_14_15</b>	-	<b>No TS (see PES)</b>				
15	-611.41958730	-34.5	-610.56165270	-33.6	-610.53967203	-29.9
<b>TS_16_20</b>	-	<b>No TS (see PES)</b>				
20	-611.44836699	-52.6	-610.58267392	-46.8	-610.56340380	-44.8
<b>TS_15_16 (TS VIII)</b>	<b>-611.39328904</b>	<b>-18.0</b>	<b>-610.54577691</b>	<b>-23.7</b>	<b>-610.50973817</b>	<b>-11.1</b>
16	-611.47492580	-69.3	-610.61545582	-67.4	-610.59384531	-63.9
<b>TS_16_17 (TS IX)</b>	<b>-688.75434898</b>	<b>-61.5</b>	<b>-687.77111800</b>	<b>-59.7</b>	<b>-687.73747783</b>	<b>-50.0</b>
17	-688.77720044	-75.9	-687.78948108	-71.2	-687.76562324	-67.6
<b>TS_17_18 (TS X)</b>	<b>-688.76967641</b>	<b>-71.1</b>	<b>-687.78170210</b>	<b>-66.3</b>	<b>-687.75301804</b>	<b>-59.7</b>
18	-688.82543002	-106.1	-687.83988005	-102.8	-687.81681323	-99.8
<b>TS_20_21 (TS XII)</b>	<b>-688.72244186</b>	<b>-41.5</b>	<b>-687.73611932</b>	<b>-37.7</b>	<b>-687.70578990</b>	<b>-30.1</b>
25	-688.77296864	-73.2	-687.78683562	-69.5	-687.76244423	-65.6
<b>TS_25_27</b>	-	<b>No TS (see PES)</b>				
21	-688.77620380	-75.2	-687.78920385	-71.0	-687.76498229	-67.2
<b>TS_21_22 (TS XIII)</b>	<b>-766.06258612</b>	<b>-71.9</b>	<b>-764.95136874</b>	<b>-67.4</b>	<b>-764.91768619</b>	<b>-59.0</b>
22	-766.12406192	-110.4	-765.01158582	-105.2	-764.98011446	-98.2
27	-766.22601057	-174.4	-765.12409963	-175.8	-765.08252442	-162.4
<b>TS_18_19(TS XI)</b>	<b>-688.79860803</b>	<b>-89.3</b>	<b>-687.82344599</b>	<b>-92.5</b>	<b>-687.78106003</b>	<b>-77.3</b>
19	-688.30836686	-95.0	-687.34048680	-103.4	-687.29662664	-87.3
<b>TS_27_28</b>	-	<b>No TS (see PES)</b>				
28	-765.67393136	-141.3	-764.58443497	-151.1	-764.53287865	-131.5
<b>TS_22_23 (TS XIV)</b>	<b>-766.12237841</b>	<b>-109.4</b>	<b>-765.00887250</b>	<b>-103.5</b>	<b>-764.97429341</b>	<b>-94.5</b>
23	-766.17181038	-140.4	-765.06434159	-138.3	-765.03151635	-130.4
<b>TS_23_24 (TS XV)</b>	<b>-766.12361061</b>	<b>-110.2</b>	<b>-765.01980604</b>	<b>-110.3</b>	<b>-764.97489922</b>	<b>-94.9</b>
24	-765.63266276	-115.4	-764.53516497	-120.2	-764.48902358	-104.0

## Spin Surfaces S=3/2, S=1/2; Figure 1

With the involvement of radical species, a possible spin crossover between the S=1/2 and the S=3/2 surfaces was analyzed (DFT level of theory) to check the existence of low energy intersections.

As a result a  $\Delta\Delta G_{S=3/2-1/2}$  of 64.4 (Compound **1**), 46.0 (**2**), 33.3 (**3**), 35.1 (**4**) and 61.5 (**5**) kcal/mol was obtained.

No thermal spin crossover is expected.

**1**

G=H-TS (TZVP) -379.15564727

**2**

G=H-TS (TZVP) -456.56396196

**3**

G=H-TS (TZVP) -533.94403292

**4**

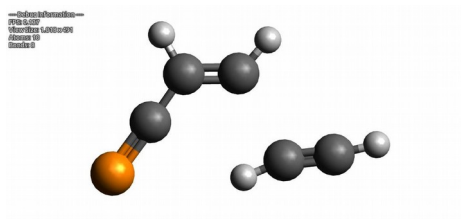
G=H-TS (TZVP) -533.94215571

**5**

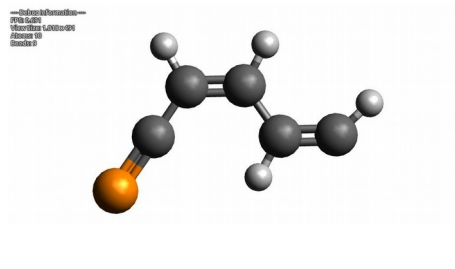
G=H-TS (TZVP) -533.97121636

*cis-trans-gauche, TS I (trans-cis)* (Figure 1)

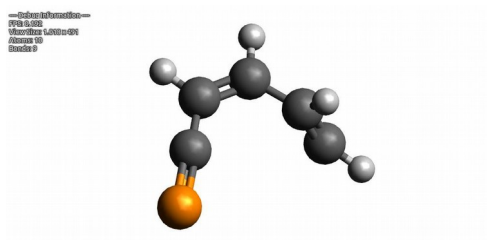
**TS I *trans***



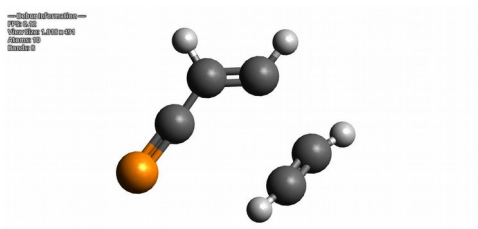
***trans***



***gauche TS***



**TS I *cis***



***cis***

