

Aromaticity can enhance the reactivity of P-donor/borole

Frustrated Lewis Pairs

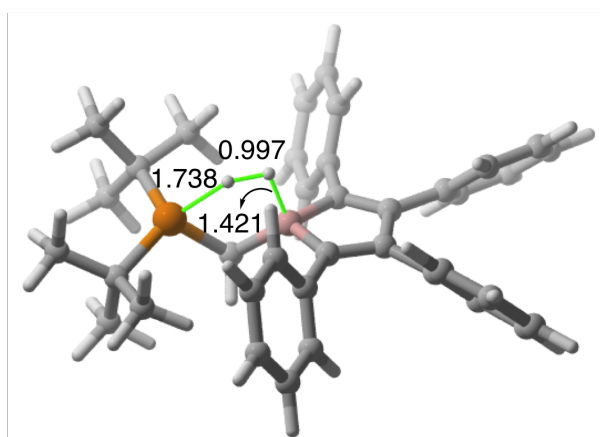
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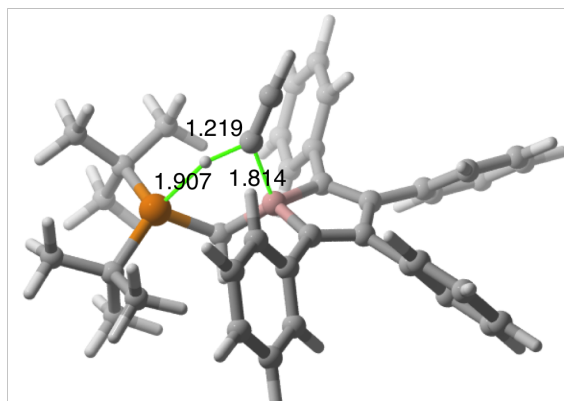
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Contents:

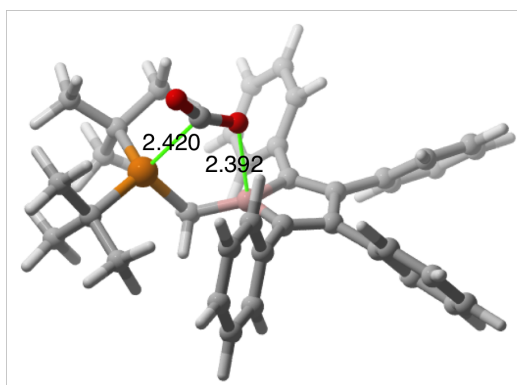
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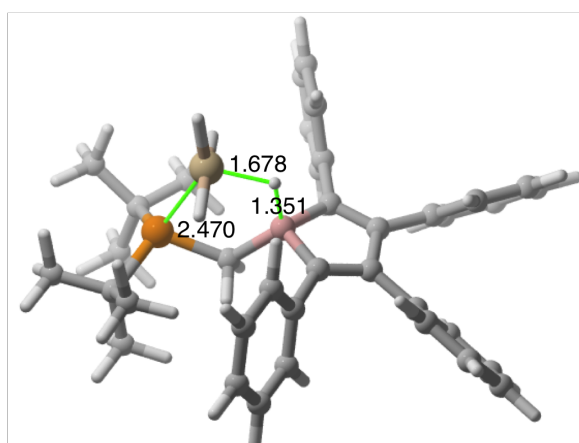
TS-2a (H₂)



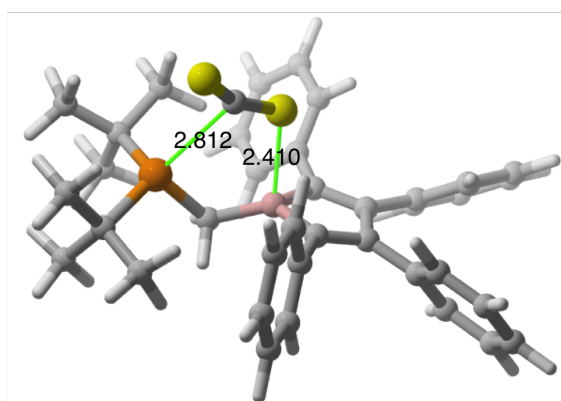
TS-2a (HCCH)



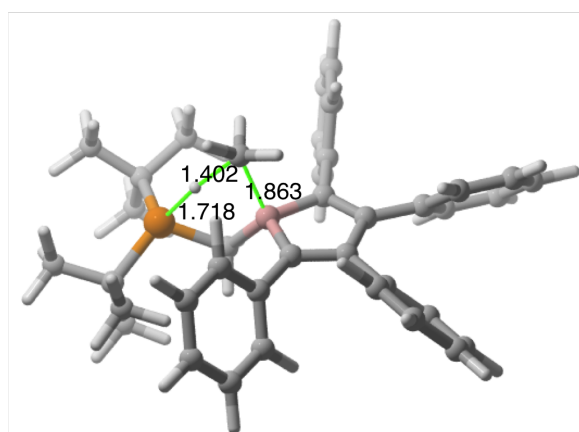
TS-2a (CO₂)



TS-2a (SiH₄)



TS-2a (CS₂)



TS-2a (CH₄)

Figure S1. Transition states for the FLP **2a**-mediated small molecule activation reactions considered in this study. Bond lengths are given in angstroms. All data have been computed at the M06-2X/def2-SVP level.

Computational details

Geometry optimizations of the molecules were performed without symmetry constraints using the Gaussian09 suite of programs¹ employing the meta-hybrid M06-2X exchange-correlation functional² combined with the double- ζ quality def2-SVP basis set.³ Reactants and products were characterized by frequency calculations, and have positive definite Hessian matrices. Transition structures (TS's) show only one negative eigenvalue in their diagonalized force constant matrices, and their associated eigenvectors were confirmed to correspond to the motion along the reaction coordinate under consideration using the Intrinsic Reaction Coordinate (IRC) method.⁴ In addition, the vibrational calculation provides the thermal Gibbs energy corrections by using the gas ideal-rigid-rotor-harmonic-oscillator approximation. Solvent effects were taken into account by means of the Polarizable Continuum Model (PCM)⁵ using the gas-phase optimized geometries at the same DFT level in conjunction with the triple- ζ quality def2-TZVPP basis set.³ This level is denoted PCM(solvent)/M06-2X/def2-TZVPP//M06-2X/def2-SVP. Moreover, more accurate energies were computed at the Domain Based Local Pair-Natural Coupled-Cluster (DLPNO-CCSD(T))⁶ as implemented in Orca 4.0.1⁷ using the def2-TZVP basis sets³ and the SMD⁸ solvation model on the M06-2X/def2-SVP geometries. This level is denoted SMD(solvent)DLPNO-CCSD(T)/def2-TZVP//M06-2X-def2-SVP.

¹ Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

² Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* **2008**, *120*, 215.

³ F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297.

⁴ C. Gonzalez, H. B. Schlegel, *J. Phys. Chem.* **1990**, *94*, 5523.

⁵ a) S. Miertuš, E. Scrocco, J. Tomasi, *Chem. Phys.* **1981**, *55*, 117; b) J. L. Pascual-Ahuir, E. Silla, I. Tuñón, *J. Comp. Chem.* **1994**, *15*, 1127; c) Barone, V.; Cossi, M. *J. Phys. Chem. A*, **1998**, *102*, 1995.

⁶ C. Riplinger, B. Sandhoefer, A. Hansen, F. Neese, *J. Chem. Phys.* **2013**, *139*, 134101.

⁷ F. Neese, *WIREs Comput. Mol. Sci.* **2018**, *8*, e1327.

⁸ A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* **2009**, *113*, 6378.

The aromaticity of the considered species has been assessed by the computation of the NICS⁹ values computed at the [3,+1] ring critical point of the electron density¹⁰ using the gauge invariant atomic orbital (GIAO) method,¹¹ at the B3LYP¹² level using the def2-SVP basis set, with the optimized M06-2X/def2-SVP geometries. This scheme is denoted as GIAO-B3LYP/def2-SVP//M06-2X/def2-SVP.

⁹ Z. Chen, C. S. Wannere, C. Corminboeuf, R. Puchta, P. v. R. Schleyer, *Chem. Rev.* **2005**, *105*, 3842.

¹⁰ R. F. W. Bader, *Atoms in Molecules -A Quantum Theory*; Clarendon Press: Oxford, 1990.

¹¹ K. Wolinski, J. F. Hilton, P. Pulay, *J. Am. Chem. Soc.* **1990**, *112*, 8251.

¹² a) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648; b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B: Condens. Matter Mater. Phys.* **1988**, *37*, 785; c) S. H. Vosko, L. Wilk, M. Nusair, *Can. J. Phys.* **1980**, *58*, 1200.

Cartesian coordinates (in Å) and total energies (in a.u., ZVPE included) of all the stationary points discussed in the text. All calculations have been performed at the level M06-2x/def2-SVP level.

```

1: E= -1182.931488
C      0.492412000      0.150388000     -1.044210000
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H      0.562690000      0.949563000     -1.801015000
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B     -1.006775000      0.148114000     -0.539354000
C     -1.801575000     -1.212897000     -0.462781000
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C	3.895366000	2.593415000	-1.540342000
C	4.790589000	2.584493000	-0.474506000
C	-0.408919000	2.534438000	-0.071325000
C	0.164354000	3.370075000	0.889272000
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C	-0.082282000	4.739445000	0.895759000
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C	1.351824000	-2.314539000	2.226620000
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H	3.237539000	-5.126446000	1.474675000
C	5.162035000	-2.289904000	-1.679544000
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H	5.888865000	-2.847832000	-2.291895000
C	5.624498000	-3.738950000	0.287159000
H	6.428971000	-4.197782000	-0.310132000
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F	-0.681242000	-3.102191000	-2.315389000
F	-2.132271000	-5.371997000	-2.309898000
F	-3.845184000	-5.881365000	-0.270652000
F	-4.082217000	-4.121930000	1.777318000
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C	1.770138000	0.718784000	-0.391273000
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C	4.194931000	3.459241000	0.464516000
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C	5.421288000	1.657605000	-0.575633000
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C	3.195735000	-3.705561000	0.357604000
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C	0.927457000	-4.278392000	-0.255806000
H	-0.369411000	-2.600677000	-0.717243000
C	2.208515000	-4.667817000	0.136890000
H	4.193732000	-4.010575000	0.676043000
H	0.153527000	-5.030346000	-0.417107000
H	2.437434000	-5.725442000	0.278626000
C	-1.105728000	0.257558000	2.172359000
H	-0.627981000	-0.693546000	1.886801000
H	-0.472201000	1.083682000	1.814999000
H	-1.125665000	0.311379000	3.272910000
C	-3.383542000	-0.700782000	2.355559000
H	-2.972719000	-1.707117000	2.185382000
H	-3.373352000	-0.505354000	3.440624000
H	-4.431148000	-0.701155000	2.026837000
C	-3.080180000	1.756548000	1.943821000
H	-2.969422000	1.962337000	3.022049000
H	-2.527795000	2.538686000	1.400895000
H	-4.147337000	1.852679000	1.699450000
C	-3.923762000	-0.115458000	-2.494690000
H	-3.014815000	0.177558000	-3.043116000
H	-3.934694000	-1.212346000	-2.420194000
H	-4.790775000	0.201313000	-3.097717000
C	-5.258530000	0.030928000	-0.407879000
H	-6.132687000	0.219969000	-1.052669000
H	-5.209829000	-1.052547000	-0.216826000
H	-5.437632000	0.543490000	0.547897000
C	-4.069401000	2.055003000	-1.286713000
H	-4.100847000	2.595586000	-0.332318000
H	-3.218721000	2.437126000	-1.868821000
H	-4.986973000	2.309687000	-1.843617000

H2: E= -1.153268

H	0.000000000	0.000000000	0.376836000
H	0.000000000	0.000000000	-0.376836000

CO2: E= -188.358325

C	0.000000000	0.000000000	0.000000000
O	0.000000000	0.000000000	1.156136000
O	0.000000000	0.000000000	-1.156136000

CS2: E= -834.155508

C	0.000000000	0.000000000	0.000000000
S	0.000000000	0.000000000	1.553532000
S	0.000000000	0.000000000	-1.553532000

C2H2: E= -77.205496

C	0.000000000	0.000000000	0.602879000
C	0.000000000	0.000000000	-0.602879000
H	0.000000000	0.000000000	-1.677248000
H	0.000000000	0.000000000	1.677248000

CH4: E= -40.405313

C	0.000000000	0.000000000	0.000000000
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H	0.633190000	0.633190000	0.633190000
H	-0.633190000	-0.633190000	0.633190000
H	0.633190000	-0.633190000	-0.633190000
H	-0.633190000	0.633190000	-0.633190000

SiH4: E= -291.722060

Si	0.000000000	0.000000000	0.000000000
H	0.857365000	0.857365000	0.857365000
H	-0.857365000	-0.857365000	0.857365000
H	0.857365000	-0.857365000	-0.857365000
H	-0.857365000	0.857365000	-0.857365000

Activation of H₂

TS-1 (H2): E= -1184.046348

C	0.211444000	0.460487000	0.881206000
H	0.169463000	1.445374000	1.366971000
H	0.316132000	-0.290702000	1.677155000
H	-0.628251000	0.387490000	-1.362596000
P	1.647932000	0.355004000	-0.252153000
H	0.364966000	0.188698000	-1.365446000
B	-1.079829000	0.068620000	-0.068133000
C	2.894441000	-0.865598000	0.451856000
C	2.319981000	2.096720000	-0.468161000
C	1.102491000	2.974342000	-0.808921000
H	0.569060000	2.606142000	-1.697771000
H	0.379997000	3.037148000	0.015058000
H	1.454391000	3.995214000	-1.026186000
C	3.271007000	2.134321000	-1.672727000
H	4.204466000	1.587720000	-1.493081000
H	2.792172000	1.717787000	-2.571454000
H	3.534486000	3.182367000	-1.886846000
C	3.016818000	2.642038000	0.779307000
H	3.249688000	3.709081000	0.630201000
H	2.378202000	2.559484000	1.672043000
H	3.965101000	2.121702000	0.978060000
C	2.258983000	-2.251748000	0.256058000
H	1.283059000	-2.342046000	0.758149000
H	2.103795000	-2.476467000	-0.809039000
H	2.932238000	-3.014527000	0.678885000
C	4.213216000	-0.804155000	-0.324137000
H	4.053934000	-0.856291000	-1.411737000
H	4.782281000	0.108102000	-0.094025000
H	4.837203000	-1.664331000	-0.034102000
C	3.158049000	-0.635689000	1.944047000
H	3.585388000	0.354960000	2.146249000
H	2.242299000	-0.745038000	2.540405000
H	3.877695000	-1.391773000	2.298202000
C	-1.236940000	-1.529994000	-0.183668000
C	-1.597473000	-2.262923000	0.961712000
C	-0.980531000	-2.261738000	-1.351080000
H	-1.820324000	-1.726322000	1.889667000
H	-0.708944000	-1.728433000	-2.267144000
C	-1.681028000	-3.653555000	0.947536000
C	-1.059076000	-3.656756000	-1.378484000
H	-1.963933000	-4.193508000	1.853553000
H	-0.848792000	-4.196443000	-2.304155000
C	-1.403774000	-4.358543000	-0.226043000
H	-1.463834000	-5.448177000	-0.240709000
C	-4.801230000	1.180087000	-0.500799000
C	-4.849044000	2.391189000	0.191122000

C	-3.612284000	0.456153000	-0.559319000
H	-5.779796000	2.959128000	0.243437000
H	-3.591551000	-0.496213000	-1.096311000
C	-3.699577000	2.865947000	0.819436000
C	-2.434622000	0.913912000	0.058593000
H	-3.726947000	3.808115000	1.370529000
C	-2.513380000	2.133847000	0.748664000
H	-1.630197000	2.526845000	1.259262000
H	-5.698100000	0.796687000	-0.991447000

TS-2a (H2) : E= -1798.854537

C	1.808719000	0.245659000	0.898149000
H	1.902043000	1.171784000	1.486876000
H	1.835145000	-0.603962000	1.597799000
H	0.900355000	0.266160000	-1.340113000
P	3.213669000	0.072700000	-0.274385000
H	1.853531000	-0.027603000	-1.352203000
B	0.447358000	0.170980000	0.003121000
C	-0.730995000	1.261123000	0.077086000
C	-0.386864000	-1.201878000	-0.077738000
C	4.479000000	-1.104470000	0.483913000
C	3.924515000	1.790241000	-0.566287000
C	-1.706097000	-0.894502000	-0.027816000
C	-1.914135000	0.596760000	0.025382000
C	-0.573524000	2.730808000	0.132843000
C	-0.088686000	3.345771000	1.298382000
C	-0.853702000	3.540535000	-0.976888000
C	0.118996000	4.723256000	1.350125000
H	0.116344000	2.727940000	2.176313000
C	-0.640537000	4.917082000	-0.928128000
H	-1.243080000	3.074674000	-1.884640000
C	-0.149368000	5.514285000	0.233030000
H	0.491732000	5.181687000	2.268134000
H	-0.864547000	5.529506000	-1.803587000
H	0.015441000	6.592215000	0.269472000
C	-3.256899000	1.222318000	-0.059908000
C	-3.624956000	2.284478000	0.778248000
C	-4.183053000	0.771979000	-1.013861000
C	-4.880116000	2.879254000	0.664649000
H	-2.916472000	2.642765000	1.526664000
C	-5.434452000	1.370661000	-1.131041000
H	-3.914002000	-0.057768000	-1.670331000
C	-5.788918000	2.425891000	-0.290750000
H	-5.149339000	3.703437000	1.327346000
H	-6.138478000	1.007749000	-1.881770000
H	-6.771513000	2.892231000	-0.380134000
C	0.187707000	-2.562588000	-0.131405000
C	0.866608000	-2.997017000	-1.280969000
C	0.096621000	-3.441814000	0.958673000
C	1.425407000	-4.271728000	-1.344338000
H	0.935217000	-2.325167000	-2.140153000
C	0.672352000	-4.710312000	0.902132000
H	-0.442375000	-3.119291000	1.852137000
C	1.338542000	-5.131130000	-0.249221000
H	1.937323000	-4.595032000	-2.253036000
H	0.593296000	-5.379437000	1.760897000
H	1.781155000	-6.127347000	-0.295662000
C	-2.821974000	-1.868835000	0.047332000
C	-2.876469000	-2.983276000	-0.801910000
C	-3.837730000	-1.704194000	1.001892000
C	-3.915013000	-3.906792000	-0.697838000

H	-2.095412000	-3.119475000	-1.551800000
C	-4.871252000	-2.630667000	1.110015000
H	-3.812093000	-0.836503000	1.664253000
C	-4.914896000	-3.734951000	0.258707000
H	-3.942903000	-4.766410000	-1.369561000
H	-5.649293000	-2.487687000	1.861763000
H	-5.727469000	-4.458728000	0.339950000
C	2.731962000	2.703748000	-0.890469000
H	2.145893000	2.334663000	-1.745053000
H	2.050691000	2.823602000	-0.038585000
H	3.113900000	3.703170000	-1.153012000
C	4.838616000	1.756717000	-1.800257000
H	5.758517000	1.182992000	-1.637002000
H	4.315075000	1.334002000	-2.670812000
H	5.129694000	2.788857000	-2.052150000
C	4.674982000	2.356767000	0.640718000
H	4.935486000	3.408782000	0.440182000
H	4.055848000	2.336570000	1.550777000
H	5.611343000	1.816160000	0.840286000
C	3.889716000	-2.512451000	0.319967000
H	2.893727000	-2.613523000	0.779495000
H	3.793937000	-2.782347000	-0.740771000
H	4.560014000	-3.241258000	0.803502000
C	5.815533000	-1.043323000	-0.260175000
H	5.686967000	-1.163469000	-1.346447000
H	6.353185000	-0.103988000	-0.070287000
H	6.454566000	-1.867848000	0.093903000
C	4.698760000	-0.819604000	1.974524000
H	5.095342000	0.187053000	2.157620000
H	3.770998000	-0.935105000	2.550669000
H	5.427969000	-1.546258000	2.368621000

TS-2b (H2) : E= -3781.541945

C	2.223297000	1.620084000	0.946933000
H	1.840581000	2.401963000	1.618019000
H	2.750584000	0.884937000	1.575127000
H	1.320951000	1.137355000	-1.277795000
P	3.439871000	2.288891000	-0.277889000
H	2.207765000	1.456321000	-1.300307000
B	1.061961000	0.868372000	0.097835000
C	-0.519612000	1.218103000	0.105542000
C	1.008162000	-0.748383000	0.064980000
C	5.172064000	1.874369000	0.344475000
C	3.173545000	4.147871000	-0.409221000
C	-0.288971000	-1.127999000	0.080364000
C	-1.199528000	0.047782000	0.074327000
C	-1.225415000	2.510355000	0.012902000
C	-1.121692000	3.475588000	1.014652000
C	-2.058023000	2.813002000	-1.069850000
C	-1.786118000	4.693898000	0.947368000
C	-2.740825000	4.023776000	-1.159786000
C	-2.605494000	4.967121000	-0.145113000
C	-2.667537000	-0.098115000	-0.013276000
C	-3.522740000	0.479027000	0.926464000
C	-3.246128000	-0.820443000	-1.058205000
C	-4.905014000	0.343704000	0.831909000
C	-4.623349000	-0.977605000	-1.167491000
C	-5.454603000	-0.390132000	-0.216526000
C	2.123602000	-1.709082000	0.077815000
C	3.097511000	-1.677894000	-0.921087000
C	2.254744000	-2.706088000	1.051679000

C	4.163632000	-2.567101000	-0.954416000
C	3.312041000	-3.613361000	1.038687000
C	4.270014000	-3.545093000	0.029854000
C	-0.798785000	-2.514195000	0.093404000
C	-0.427220000	-3.444911000	-0.877970000
C	-1.689748000	-2.932818000	1.083199000
C	-0.922015000	-4.745874000	-0.866876000
C	-2.203086000	-4.224902000	1.110200000
C	-1.814244000	-5.134330000	0.129298000
C	1.654299000	4.360888000	-0.457018000
H	1.163890000	3.731637000	-1.216854000
H	1.196568000	4.155267000	0.518170000
H	1.447961000	5.413238000	-0.709874000
C	3.770245000	4.622351000	-1.742393000
H	4.858113000	4.487419000	-1.791977000
H	3.318970000	4.087031000	-2.590569000
H	3.560329000	5.696403000	-1.867388000
C	3.741344000	4.961119000	0.754872000
H	3.414298000	6.008571000	0.652410000
H	3.375978000	4.592148000	1.725196000
H	4.839696000	4.959109000	0.766984000
C	5.328221000	0.358081000	0.162182000
H	4.601304000	-0.202509000	0.770251000
H	5.209193000	0.061228000	-0.889984000
H	6.335040000	0.055919000	0.491661000
C	6.228591000	2.581901000	-0.509329000
H	6.083363000	2.386455000	-1.582611000
H	6.232399000	3.668298000	-0.345825000
H	7.224318000	2.202656000	-0.230705000
C	5.367742000	2.216847000	1.825304000
H	5.336609000	3.295922000	2.014838000
H	4.613211000	1.731899000	2.460803000
H	6.356346000	1.850110000	2.146252000
F	3.042603000	-0.745710000	-1.865544000
F	5.087996000	-2.465653000	-1.895765000
F	5.281368000	-4.392735000	0.017897000
F	3.415028000	-4.535327000	1.980381000
F	1.373303000	-2.798423000	2.037407000
F	0.398447000	-3.100243000	-1.854587000
F	-0.563453000	-5.607641000	-1.801988000
F	-2.294316000	-6.362738000	0.142987000
F	-3.041272000	-4.597434000	2.061184000
F	-2.054073000	-2.089643000	2.039550000
F	-2.473616000	-1.354860000	-1.994010000
F	-5.146566000	-1.659950000	-2.170415000
F	-6.762788000	-0.524840000	-0.313272000
F	-5.696649000	0.896666000	1.734075000
F	-3.030028000	1.167327000	1.944325000
F	-0.340663000	3.253117000	2.066521000
F	-1.641013000	5.592501000	1.906767000
F	-3.241078000	6.121094000	-0.223198000
F	-3.510483000	4.284382000	-2.202405000
F	-2.203722000	1.946572000	-2.063661000

TS-3 (H2) : E= -1260.111724

C	-1.090116000	0.832297000	0.643933000
H	-1.007547000	0.296920000	1.600484000
H	-1.170671000	1.907729000	0.865913000
H	-0.390253000	0.699909000	-1.629201000
P	-2.547821000	0.341986000	-0.318957000
H	-1.425496000	0.494535000	-1.574481000

B	0.188058000	0.554202000	-0.353672000
C	1.357279000	-0.452289000	-0.261975000
C	1.691551000	0.842541000	-0.228560000
C	-3.904082000	1.613265000	-0.051367000
C	-3.029871000	-1.406810000	0.155397000
C	1.963268000	-1.777318000	-0.133678000
C	2.909271000	-2.032665000	0.874011000
C	1.608619000	-2.826436000	-0.995953000
C	3.477985000	-3.295775000	1.014588000
H	3.188243000	-1.221974000	1.550679000
C	2.192065000	-4.085009000	-0.865690000
H	0.880456000	-2.636887000	-1.787345000
C	3.124655000	-4.326644000	0.143172000
H	4.206726000	-3.475756000	1.807088000
H	1.914813000	-4.884984000	-1.554545000
H	3.574940000	-5.314832000	0.250076000
C	2.868292000	1.701611000	-0.131791000
C	2.722044000	3.081252000	0.074154000
C	4.165291000	1.174771000	-0.257018000
C	3.837388000	3.910437000	0.169359000
H	1.713745000	3.491695000	0.158058000
C	5.279180000	2.003977000	-0.170735000
H	4.285734000	0.103560000	-0.431872000
C	5.119207000	3.373992000	0.047331000
H	3.707584000	4.981568000	0.334015000
H	6.280149000	1.581400000	-0.275181000
H	5.993723000	4.023253000	0.115678000
C	-1.721990000	-2.211588000	0.202288000
H	-1.172900000	-2.149430000	-0.747980000
H	-1.041125000	-1.868131000	0.993245000
H	-1.964336000	-3.269183000	0.392270000
C	-3.921277000	-2.001131000	-0.943456000
H	-4.890009000	-1.491724000	-1.024677000
H	-3.424035000	-1.956836000	-1.923445000
H	-4.119171000	-3.059688000	-0.711198000
C	-3.731653000	-1.487617000	1.513000000
H	-3.884510000	-2.546833000	1.776603000
H	-3.129754000	-1.026283000	2.310101000
H	-4.719579000	-1.005336000	1.495350000
C	-3.427411000	2.865286000	-0.804846000
H	-2.458336000	3.227956000	-0.430769000
H	-3.326429000	2.670454000	-1.882259000
H	-4.163543000	3.673062000	-0.666974000
C	-5.227652000	1.144140000	-0.660981000
H	-5.106313000	0.832431000	-1.709469000
H	-5.667738000	0.310712000	-0.095445000
H	-5.948575000	1.976736000	-0.637719000
C	-4.095437000	1.954756000	1.430029000
H	-4.440432000	1.091150000	2.013199000
H	-3.164249000	2.324315000	1.881901000
H	-4.853715000	2.749443000	1.523346000

add-1 (H2) : E= -1184.077889

C	-0.278566000	0.566926000	0.515789000
H	-0.311544000	0.018581000	1.470598000
H	-0.195701000	1.638317000	0.743331000
H	0.643784000	0.120455000	-1.643295000
P	-1.846778000	0.361415000	-0.294983000
H	-1.748367000	0.903422000	-1.592574000
B	1.041374000	0.139329000	-0.470769000
C	1.646614000	-1.312108000	-0.069628000

C	2.111871000	-2.200047000	-1.054552000
C	1.804130000	-1.730204000	1.263443000
C	2.679690000	-3.434934000	-0.738087000
C	2.370406000	-2.961573000	1.599065000
C	2.807351000	-3.824780000	0.594778000
C	2.133996000	1.339836000	-0.329399000
C	3.408148000	1.178758000	0.234320000
C	1.810881000	2.632658000	-0.781391000
C	4.304964000	2.244629000	0.350627000
C	2.692402000	3.705737000	-0.672434000
C	3.951397000	3.514530000	-0.099375000
H	3.250303000	-4.789545000	0.848931000
H	2.477182000	-3.246609000	2.648101000
H	3.026967000	-4.096587000	-1.534762000
H	2.023626000	-1.906736000	-2.105159000
H	1.488829000	-1.065463000	2.075479000
H	0.833768000	2.800309000	-1.251127000
H	2.404155000	4.692943000	-1.041219000
H	4.651251000	4.347738000	-0.011511000
H	5.289052000	2.080044000	0.795580000
H	3.711655000	0.189869000	0.588473000
C	-3.192081000	1.405289000	0.478404000
C	-2.288638000	-1.433323000	-0.538312000
C	-3.773189000	-1.618907000	-0.869250000
H	-3.940773000	-2.687269000	-1.072957000
H	-4.434862000	-1.333928000	-0.040562000
H	-4.067873000	-1.061760000	-1.770887000
C	-1.458712000	-1.964083000	-1.717068000
H	-1.694992000	-1.432473000	-2.650801000
H	-0.381858000	-1.886048000	-1.530076000
H	-1.709062000	-3.027392000	-1.855308000
C	-1.920643000	-2.204182000	0.736869000
H	-0.836786000	-2.176016000	0.920078000
H	-2.447559000	-1.825514000	1.625743000
H	-2.208740000	-3.257602000	0.599594000
C	-4.372998000	1.589176000	-0.483748000
H	-4.930677000	0.663526000	-0.661712000
H	-5.072749000	2.318021000	-0.046463000
H	-4.042455000	1.991010000	-1.453780000
C	-2.569023000	2.787718000	0.739848000
H	-2.106727000	3.213538000	-0.164560000
H	-3.366245000	3.473751000	1.063308000
H	-1.810486000	2.755073000	1.532256000
C	-3.648230000	0.800008000	1.810409000
H	-2.799690000	0.639399000	2.492519000
H	-4.343556000	1.498062000	2.301931000
H	-4.173693000	-0.155730000	1.677580000

add-2a (H2) : E= -1798.897769

C	1.611538000	0.305243000	0.674477000
H	1.672589000	1.299434000	1.147361000
H	1.420890000	-0.438918000	1.461917000
H	0.852491000	0.460863000	-1.608982000
P	3.217696000	0.008300000	-0.035122000
H	3.101673000	-0.770061000	-1.202196000
B	0.396336000	0.250235000	-0.479723000
C	-0.795879000	1.287474000	-0.148349000
C	-0.421403000	-1.140598000	-0.419970000
C	4.282903000	-1.039874000	1.075312000
C	3.977148000	1.609441000	-0.608975000
C	-1.731522000	-0.872652000	-0.171437000

C	-1.962895000	0.602423000	-0.037152000
C	-0.605281000	2.752459000	-0.133537000
C	-0.100983000	3.406863000	1.003286000
C	-0.806070000	3.515531000	-1.294525000
C	0.198524000	4.769545000	0.978896000
H	0.040358000	2.833983000	1.923856000
C	-0.508404000	4.876420000	-1.319994000
H	-1.197891000	3.019351000	-2.184625000
C	0.001712000	5.509875000	-0.185854000
H	0.582066000	5.256715000	1.877774000
H	-0.678164000	5.448659000	-2.234180000
H	0.233928000	6.575856000	-0.207319000
C	-3.310214000	1.211739000	0.094262000
C	-3.551049000	2.237689000	1.019531000
C	-4.370413000	0.796929000	-0.727381000
C	-4.806705000	2.834296000	1.117619000
H	-2.739211000	2.563906000	1.671098000
C	-5.624844000	1.394002000	-0.631240000
H	-4.202524000	-0.003063000	-1.451188000
C	-5.849190000	2.415097000	0.292670000
H	-4.971010000	3.629566000	1.846966000
H	-6.433841000	1.058967000	-1.282805000
H	-6.833541000	2.879879000	0.370949000
C	0.208458000	-2.469309000	-0.505080000
C	1.097501000	-2.759579000	-1.556964000
C	0.017231000	-3.456375000	0.479751000
C	1.753682000	-3.987259000	-1.632727000
H	1.240397000	-2.006061000	-2.335595000
C	0.687842000	-4.676186000	0.414537000
H	-0.671690000	-3.250548000	1.302050000
C	1.559409000	-4.949937000	-0.641424000
H	2.421294000	-4.196019000	-2.471774000
H	0.524873000	-5.424241000	1.192990000
H	2.076121000	-5.909597000	-0.695171000
C	-2.810184000	-1.879363000	-0.011164000
C	-2.949948000	-2.933188000	-0.926262000
C	-3.705821000	-1.811098000	1.067109000
C	-3.945573000	-3.894103000	-0.763900000
H	-2.265114000	-2.988471000	-1.774667000
C	-4.700887000	-2.772317000	1.230804000
H	-3.616848000	-0.991036000	1.782603000
C	-4.824994000	-3.818002000	0.315947000
H	-4.038819000	-4.704759000	-1.488806000
H	-5.386370000	-2.702525000	2.077245000
H	-5.607122000	-4.568564000	0.442055000
C	2.880178000	2.450227000	-1.284061000
H	2.458203000	1.948101000	-2.164122000
H	2.048369000	2.687906000	-0.606526000
H	3.337207000	3.398159000	-1.608102000
C	5.083807000	1.332217000	-1.635087000
H	5.941636000	0.796961000	-1.210259000
H	4.699831000	0.760342000	-2.492859000
H	5.449972000	2.297127000	-2.018079000
C	4.532487000	2.382838000	0.592498000
H	4.878272000	3.367322000	0.242680000
H	3.760872000	2.559331000	1.357435000
H	5.388093000	1.875515000	1.060403000
C	3.662369000	-2.446148000	1.011018000
H	2.587439000	-2.451693000	1.249122000
H	3.779060000	-2.897801000	0.015444000
H	4.174333000	-3.090348000	1.742398000

C	5.735039000	-1.112302000	0.596174000
H	5.806527000	-1.421593000	-0.457451000
H	6.264404000	-0.157630000	0.722176000
H	6.263860000	-1.866715000	1.198889000
C	4.218654000	-0.514995000	2.515093000
H	4.628793000	0.499007000	2.615031000
H	3.189597000	-0.512782000	2.899829000
H	4.814534000	-1.182361000	3.156459000

add-2b (H2) : E= -3781.589413

C	-2.015073000	1.554849000	-0.784253000
H	-1.592649000	2.378940000	-1.375402000
H	-2.292724000	0.757307000	-1.489779000
H	-1.231531000	1.361585000	1.489528000
P	-3.505019000	2.174945000	-0.018684000
H	-3.737297000	1.481898000	1.186149000
B	-0.946628000	0.963663000	0.362872000
C	0.640897000	1.226501000	0.122163000
C	-0.947704000	-0.656480000	0.312992000
C	-5.017621000	1.804239000	-1.041821000
C	-3.291884000	3.956914000	0.474050000
C	0.319036000	-1.102152000	0.132066000
C	1.272806000	0.027670000	0.055980000
C	1.405217000	2.487227000	0.208603000
C	1.199045000	3.547799000	-0.676129000
C	2.373173000	2.693355000	1.201150000
C	1.903823000	4.743097000	-0.601627000
C	3.097325000	3.879543000	1.297821000
C	2.862885000	4.910187000	0.392877000
C	2.733903000	-0.178402000	-0.040405000
C	3.486327000	0.401042000	-1.063364000
C	3.412590000	-0.968204000	0.889142000
C	4.860177000	0.203358000	-1.162437000
C	4.783597000	-1.188380000	0.805273000
C	5.508496000	-0.598411000	-0.226931000
C	-2.132025000	-1.525847000	0.302508000
C	-3.135533000	-1.399493000	1.270472000
C	-2.370317000	-2.464212000	-0.713132000
C	-4.299035000	-2.159767000	1.245861000
C	-3.523925000	-3.244914000	-0.752293000
C	-4.495870000	-3.092160000	0.232630000
C	0.746979000	-2.511694000	0.014750000
C	0.396708000	-3.468135000	0.969210000
C	1.509788000	-2.941174000	-1.073281000
C	0.789171000	-4.798480000	0.849818000
C	1.921597000	-4.262418000	-1.209093000
C	1.556280000	-5.195198000	-0.242110000
C	-1.875542000	4.126690000	1.045538000
H	-1.709657000	3.511576000	1.939119000
H	-1.108576000	3.866735000	0.305743000
H	-1.746530000	5.185464000	1.317531000
C	-4.311832000	4.334005000	1.555822000
H	-5.347613000	4.307249000	1.196921000
H	-4.226255000	3.679258000	2.435395000
H	-4.101352000	5.362473000	1.886451000
C	-3.439214000	4.856745000	-0.759283000
H	-3.205814000	5.890863000	-0.464339000
H	-2.735330000	4.576529000	-1.558060000
H	-4.460363000	4.849947000	-1.164291000
C	-5.239010000	0.288155000	-0.907315000
H	-4.352447000	-0.294995000	-1.202761000

H	-5.511682000	0.009997000	0.122031000
H	-6.068378000	-0.007125000	-1.567831000
C	-6.261904000	2.529397000	-0.521541000
H	-6.439055000	2.330518000	0.546118000
H	-6.208107000	3.615481000	-0.676160000
H	-7.137845000	2.159993000	-1.076500000
C	-4.759030000	2.159088000	-2.511259000
H	-4.598038000	3.234715000	-2.660734000
H	-3.890941000	1.619729000	-2.914675000
H	-5.639964000	1.866965000	-3.102859000
F	0.284235000	3.442895000	-1.642014000
F	2.619361000	1.755965000	2.105206000
F	3.998034000	4.038825000	2.253469000
F	3.539569000	6.041366000	0.481201000
F	1.664813000	5.719341000	-1.463782000
F	2.897648000	1.154163000	-1.981553000
F	5.551698000	0.756391000	-2.145285000
F	6.810907000	-0.795911000	-0.317510000
F	5.404140000	-1.937945000	1.700779000
F	2.749885000	-1.513507000	1.899839000
F	1.836697000	-2.083202000	-2.030904000
F	2.637353000	-4.642511000	-2.254538000
F	1.930215000	-6.455636000	-0.364672000
F	0.446319000	-5.684880000	1.769212000
F	-0.323515000	-3.127403000	2.028468000
F	-3.017896000	-0.505951000	2.247926000
F	-1.505196000	-2.613470000	-1.707317000
F	-3.711585000	-4.114339000	-1.730726000
F	-5.605057000	-3.808928000	0.192258000
F	-5.244872000	-1.962333000	2.153230000

add-3 (H2) : E= -1260.141512

C	0.870462000	-1.434474000	0.277278000
H	0.568313000	-1.236891000	1.315147000
H	1.118704000	-2.500182000	0.172532000
H	0.037174000	-1.331223000	-1.957659000
P	2.311933000	-0.466222000	-0.114112000
H	2.056450000	0.282402000	-1.281947000
B	-0.318234000	-0.990529000	-0.825482000
C	-1.191444000	0.305244000	-0.543349000
C	-1.813826000	-0.855582000	-0.360563000
C	3.732083000	-1.554551000	-0.630133000
C	2.681489000	0.836635000	1.160357000
C	-1.416196000	1.746557000	-0.511233000
C	-2.207386000	2.348943000	0.483593000
C	-0.785123000	2.584530000	-1.448043000
C	-2.362333000	3.732296000	0.536145000
H	-2.690688000	1.710150000	1.226318000
C	-0.955326000	3.966248000	-1.406392000
H	-0.161739000	2.123489000	-2.218333000
C	-1.741187000	4.548448000	-0.410253000
H	-2.976108000	4.178855000	1.321045000
H	-0.468465000	4.596452000	-2.153445000
H	-1.867983000	5.631471000	-0.371592000
C	-3.138747000	-1.401069000	-0.081134000
C	-3.295499000	-2.776330000	0.151980000
C	-4.286834000	-0.588242000	-0.056859000
C	-4.549683000	-3.321347000	0.417649000
H	-2.406978000	-3.409932000	0.116581000
C	-5.541191000	-1.132617000	0.200060000
H	-4.180005000	0.479525000	-0.258749000

C	-5.677671000	-2.501244000	0.443337000
H	-4.650828000	-4.393058000	0.599468000
H	-6.421922000	-0.487503000	0.207953000
H	-6.662038000	-2.927334000	0.645313000
C	1.340543000	1.496521000	1.519066000
H	0.875515000	1.976595000	0.646394000
H	0.611684000	0.788156000	1.935808000
H	1.532898000	2.274440000	2.274166000
C	3.601172000	1.915010000	0.573712000
H	4.603271000	1.539726000	0.334814000
H	3.164580000	2.364607000	-0.330616000
H	3.714301000	2.717598000	1.318693000
C	3.312340000	0.198143000	2.400912000
H	3.385487000	0.957964000	3.193882000
H	2.703477000	-0.633105000	2.787644000
H	4.328306000	-0.171553000	2.199744000
C	3.243470000	-2.230174000	-1.923676000
H	2.289873000	-2.759917000	-1.783599000
H	3.101367000	-1.498405000	-2.732150000
H	4.000605000	-2.960045000	-2.249068000
C	5.002868000	-0.753030000	-0.922925000
H	4.815864000	0.085421000	-1.610934000
H	5.462244000	-0.361272000	-0.004437000
H	5.737166000	-1.419353000	-1.401651000
C	4.011847000	-2.622222000	0.433411000
H	4.373264000	-2.189523000	1.375722000
H	3.122011000	-3.228889000	0.650034000
H	4.793406000	-3.298854000	0.054357000

Activation of CO₂

TS-1 (CO₂) : E= -1371.282585

C	0.648073000	-0.205274000	2.189500000
O	-0.474985000	-0.485039000	1.911051000
C	0.190639000	-0.365348000	-1.158194000
H	0.197983000	-1.367215000	-1.604468000
H	0.378351000	0.351435000	-1.975208000
O	1.497232000	0.039735000	2.970959000
B	-1.218883000	-0.003336000	-0.497220000
P	1.613912000	-0.255417000	0.026124000
C	2.470009000	-1.929015000	-0.132848000
C	3.807256000	-1.888830000	0.615962000
H	3.693196000	-1.455301000	1.621433000
H	4.185393000	-2.917436000	0.729119000
H	4.567930000	-1.315904000	0.066841000
C	1.541974000	-2.919115000	0.591297000
H	0.511493000	-2.894066000	0.205879000
H	1.930405000	-3.941627000	0.458890000
H	1.501594000	-2.710729000	1.670275000
C	2.693914000	-2.408368000	-1.570597000
H	3.317136000	-1.718432000	-2.153048000
H	3.208650000	-3.382729000	-1.543399000
H	1.748944000	-2.558490000	-2.111729000
C	2.724186000	1.169240000	-0.504302000
C	3.504923000	0.924713000	-1.795379000
H	4.030094000	1.850421000	-2.082964000
H	4.265114000	0.140064000	-1.673280000
H	2.842067000	0.644697000	-2.628786000
C	1.812610000	2.391220000	-0.681642000
H	1.165436000	2.558957000	0.193887000
H	2.443561000	3.284320000	-0.814953000

H	1.165024000	2.307933000	-1.564802000
C	3.681752000	1.465707000	0.661267000
H	4.422569000	0.670921000	0.810375000
H	4.230313000	2.395906000	0.443053000
H	3.131865000	1.597814000	1.604320000
C	-2.377727000	-1.058766000	-0.392920000
C	-3.641851000	-0.677228000	0.091725000
C	-2.214301000	-2.401347000	-0.777460000
C	-4.686075000	-1.592374000	0.204242000
H	-3.807671000	0.361731000	0.383973000
C	-3.251700000	-3.324455000	-0.671359000
H	-1.255725000	-2.741732000	-1.175527000
C	-4.491436000	-2.919844000	-0.176023000
H	-5.656177000	-1.269443000	0.585713000
H	-3.096063000	-4.360759000	-0.975673000
H	-5.307359000	-3.639865000	-0.090490000
C	-1.523977000	1.527427000	-0.244339000
C	-1.810229000	2.091756000	1.009365000
C	-1.542423000	2.382109000	-1.359993000
C	-2.068514000	3.456406000	1.143734000
H	-1.818593000	1.451778000	1.893071000
C	-1.821223000	3.742157000	-1.235126000
H	-1.336160000	1.978379000	-2.356567000
C	-2.073964000	4.286452000	0.023312000
H	-2.270571000	3.873571000	2.132032000
H	-1.833529000	4.379840000	-2.120975000
H	-2.278996000	5.352990000	0.129841000

TS-2a (CO2) : E= -1986.084220

C	-1.937914000	-0.281103000	2.184044000
O	-0.887307000	0.177460000	1.865313000
C	-1.652925000	0.224850000	-1.105856000
H	-1.757383000	1.140028000	-1.702894000
H	-1.740498000	-0.636826000	-1.785973000
O	-2.680990000	-0.776329000	2.947347000
P	-3.070356000	0.108381000	0.081333000
C	-3.730378000	1.878483000	0.181984000
C	-5.079176000	1.872298000	0.910699000
H	-5.029476000	1.294557000	1.846774000
H	-5.347927000	2.909210000	1.168105000
H	-5.887982000	1.465346000	0.287716000
C	-2.721466000	2.654819000	1.043916000
H	-1.695896000	2.582141000	0.654568000
H	-3.000524000	3.721040000	1.047089000
H	-2.721089000	2.302389000	2.085734000
C	-3.864423000	2.595969000	-1.166021000
H	-4.473335000	2.041361000	-1.891021000
H	-4.346534000	3.572705000	-0.997604000
H	-2.881783000	2.803786000	-1.613060000
C	-4.341919000	-1.073356000	-0.660519000
C	-5.113419000	-0.524237000	-1.860365000
H	-5.757551000	-1.319095000	-2.271772000
H	-5.763769000	0.318439000	-1.586680000
H	-4.434962000	-0.196323000	-2.663118000
C	-3.587991000	-2.342959000	-1.083753000
H	-2.914101000	-2.711853000	-0.294890000
H	-4.324114000	-3.134979000	-1.294228000
H	-2.998079000	-2.195931000	-1.999374000
C	-5.301472000	-1.461326000	0.476366000
H	-5.920473000	-0.619879000	0.811191000
H	-5.979512000	-2.253554000	0.120516000

H	-4.745941000	-1.844126000	1.345437000
B	-0.223145000	0.124807000	-0.431602000
C	0.891030000	1.251125000	-0.350485000
C	0.564841000	-1.228476000	-0.175519000
C	1.878294000	-0.906052000	-0.143215000
C	2.072243000	0.608213000	-0.190195000
C	0.668555000	2.710890000	-0.341144000
C	0.026467000	3.343380000	-1.416945000
C	1.026661000	3.486721000	0.772201000
C	-0.255853000	4.708368000	-1.379826000
H	-0.237847000	2.756634000	-2.300151000
C	0.740831000	4.849174000	0.810913000
H	1.521818000	2.999938000	1.614842000
C	0.094451000	5.464843000	-0.262196000
H	-0.751155000	5.183561000	-2.228698000
H	1.020190000	5.435242000	1.688195000
H	-0.130625000	6.531912000	-0.228747000
C	3.391301000	1.250759000	0.001489000
C	3.791891000	2.324244000	-0.807366000
C	4.251658000	0.816120000	1.021080000
C	5.018581000	2.949505000	-0.598784000
H	3.129963000	2.665167000	-1.605375000
C	5.472852000	1.450269000	1.235611000
H	3.954673000	-0.021936000	1.654485000
C	5.861297000	2.516611000	0.424953000
H	5.317635000	3.781131000	-1.238719000
H	6.126781000	1.106283000	2.038356000
H	6.821494000	3.008295000	0.589232000
C	-0.032063000	-2.583487000	-0.147884000
H	0.281633000	-2.975943000	-2.243581000
C	3.015824000	-1.852304000	-0.161695000
C	3.035809000	-2.990018000	0.658273000
C	4.088940000	-1.637042000	-1.040796000
C	4.100081000	-3.887344000	0.597972000
H	2.213048000	-3.163540000	1.352628000
C	5.144934000	-2.541122000	-1.108446000
H	4.089423000	-0.752015000	-1.679949000
C	5.155545000	-3.668041000	-0.286260000
H	4.103693000	-4.764413000	1.247073000
H	5.966127000	-2.362302000	-1.804196000
H	5.987136000	-4.372870000	-0.333387000
C	-0.562321000	-3.094103000	1.047873000
C	-0.135615000	-3.359934000	-1.309871000
C	-1.172725000	-4.346722000	1.080051000
H	-0.473771000	-2.504994000	1.963139000
C	-0.752571000	-4.610318000	-1.278710000
C	-1.275173000	-5.107192000	-0.085165000
H	-1.573317000	-4.727790000	2.021075000
H	-0.819824000	-5.202755000	-2.193010000
H	-1.756809000	-6.085868000	-0.061447000

TS-2b (CO2) : E= -3968.768210

C	-2.430888000	-0.209172000	2.420692000
O	-1.570475000	0.167565000	1.698612000
C	-2.525371000	-0.234266000	-0.872331000
H	-2.634548000	0.566392000	-1.616050000
H	-2.471924000	-1.173092000	-1.443765000
O	-3.053586000	-0.492130000	3.344070000
P	-4.051716000	-0.340731000	0.191748000
C	-4.841411000	1.379079000	-0.003779000
C	-6.306222000	1.334573000	0.444494000

H	-6.433517000	0.788423000	1.391515000
H	-6.663603000	2.365284000	0.598914000
H	-6.951343000	0.876427000	-0.317812000
C	-4.071005000	2.274898000	0.980265000
H	-2.991125000	2.286818000	0.766165000
H	-4.436977000	3.311949000	0.898779000
H	-4.218437000	1.945838000	2.020750000
C	-4.762112000	2.002377000	-1.400750000
H	-5.184159000	1.352914000	-2.178884000
H	-5.334359000	2.944682000	-1.403277000
H	-3.734006000	2.256009000	-1.689361000
C	-5.102152000	-1.677019000	-0.645678000
C	-5.486257000	-1.360202000	-2.091022000
H	-5.969969000	-2.239170000	-2.547975000
H	-6.200230000	-0.526476000	-2.147860000
H	-4.606157000	-1.105999000	-2.701654000
C	-4.269853000	-2.968970000	-0.600691000
H	-3.970018000	-3.211633000	0.429978000
H	-4.886954000	-3.801285000	-0.974488000
H	-3.369472000	-2.926469000	-1.230840000
C	-6.358336000	-1.940072000	0.198966000
H	-7.081435000	-1.118539000	0.154943000
H	-6.861291000	-2.843141000	-0.181934000
H	-6.098572000	-2.118622000	1.253384000
B	-1.136878000	-0.075373000	-0.092882000
C	-0.164074000	1.208303000	-0.186257000
C	-0.055204000	-1.273610000	-0.020133000
C	1.178036000	-0.719819000	-0.057064000
C	1.108736000	0.777894000	-0.115679000
C	-0.568285000	2.620989000	-0.124365000
C	-1.281577000	3.217373000	-1.164782000
C	-0.324132000	3.395119000	1.012068000
C	-1.794272000	4.505192000	-1.064737000
C	-0.819727000	4.691556000	1.133883000
C	-1.559107000	5.245771000	0.092089000
C	2.299143000	1.648544000	-0.063533000
C	2.521754000	2.627061000	-1.035083000
C	3.231840000	1.534253000	0.968581000
C	3.632462000	3.463266000	-0.983624000
C	4.353226000	2.354781000	1.035721000
C	4.550678000	3.323635000	0.054376000
C	-0.317094000	-2.717562000	-0.114785000
C	2.465036000	-1.440582000	-0.038586000
C	2.749536000	-2.387426000	0.947584000
C	3.445207000	-1.193600000	-1.001583000
C	3.967263000	-3.060128000	0.981105000
C	4.670896000	-1.849610000	-0.984546000
C	4.930096000	-2.787447000	0.012796000
C	-1.243076000	-3.335802000	0.726961000
C	0.293040000	-3.536578000	-1.074714000
C	-1.562556000	-4.684359000	0.637017000
C	0.000077000	-4.893827000	-1.180826000
C	-0.930769000	-5.471718000	-0.321153000
F	3.044595000	0.638923000	1.928837000
F	5.218834000	2.233486000	2.026055000
F	5.605505000	4.112612000	0.110914000
F	3.826909000	4.380001000	-1.914844000
F	1.677513000	2.770312000	-2.044767000
F	3.202850000	-0.333437000	-1.981007000
F	5.579946000	-1.604574000	-1.910761000
F	6.087592000	-3.417086000	0.037264000

F	4.218919000	-3.946172000	1.927891000
F	1.862067000	-2.657933000	1.891940000
F	1.151892000	-3.028062000	-1.947160000
F	0.590288000	-5.634480000	-2.101551000
F	-1.222694000	-6.753085000	-0.426212000
F	-2.474537000	-5.210389000	1.435977000
F	-1.886483000	-2.612540000	1.642574000
F	-1.511106000	2.535913000	-2.281114000
F	-2.501404000	5.024450000	-2.052646000
F	-2.037616000	6.470666000	0.200002000
F	-0.594169000	5.395889000	2.228743000
F	0.362142000	2.888470000	2.025511000

TS1-3 (CO2) : E= -1447.365320

C	1.090886000	-0.176680000	-1.444633000
H	1.297019000	-1.090129000	-2.024171000
H	1.302333000	0.707667000	-2.064685000
P	2.284811000	-0.019720000	-0.061422000
C	1.931853000	-1.395154000	1.165352000
C	3.156945000	-1.623816000	2.057099000
H	3.506148000	-0.677166000	2.495782000
H	2.870407000	-2.296032000	2.881196000
H	3.986782000	-2.099312000	1.516274000
C	0.790900000	-0.888215000	2.064241000
H	-0.130480000	-0.688728000	1.499987000
H	0.557828000	-1.665762000	2.809028000
H	1.086330000	0.027248000	2.595378000
C	1.505306000	-2.693212000	0.473970000
H	2.272275000	-3.072006000	-0.216345000
H	1.329185000	-3.466880000	1.238887000
H	0.564508000	-2.559497000	-0.081689000
C	3.977918000	-0.170620000	-0.873126000
C	4.286889000	-1.573017000	-1.401344000
H	5.237666000	-1.547553000	-1.958522000
H	4.399307000	-2.306682000	-0.590976000
H	3.509432000	-1.932791000	-2.092262000
C	3.972242000	0.826076000	-2.044898000
H	3.623790000	1.822004000	-1.730077000
H	4.999297000	0.926143000	-2.428591000
H	3.340477000	0.481053000	-2.874936000
C	5.059433000	0.278563000	0.122002000
H	5.186191000	-0.425015000	0.952747000
H	6.022032000	0.342832000	-0.409622000
H	4.834323000	1.267068000	0.547502000
B	-0.406729000	-0.081765000	-0.997368000
C	-1.726671000	-0.657308000	-0.660807000
C	-1.598417000	0.703339000	-0.610980000
C	-2.678549000	-1.731014000	-0.383739000
C	-2.531744000	-2.977334000	-1.010299000
C	-3.719015000	-1.552964000	0.541364000
C	-3.421615000	-4.013520000	-0.740220000
H	-1.713796000	-3.118461000	-1.719583000
C	-4.594586000	-2.596871000	0.826936000
H	-3.821858000	-0.591693000	1.048743000
C	-4.453318000	-3.825368000	0.180024000
H	-3.306655000	-4.975213000	-1.242617000
H	-5.392854000	-2.451864000	1.556361000
H	-5.145955000	-4.639866000	0.397675000
C	-2.350429000	1.924664000	-0.342571000
H	-4.295639000	1.009571000	-0.561170000
C	-1.653098000	3.118713000	-0.103571000

C	-3.754720000	1.933811000	-0.348402000
C	-2.354521000	4.294708000	0.152793000
H	-0.560563000	3.108247000	-0.117470000
C	-4.449828000	3.115245000	-0.110489000
C	-3.749512000	4.295151000	0.148762000
H	-1.807927000	5.218012000	0.349728000
H	-5.540722000	3.118444000	-0.125596000
H	-4.295200000	5.220062000	0.343345000
O	1.682836000	2.705430000	-0.033148000
C	2.162541000	2.009518000	0.816150000
O	2.623972000	1.958662000	1.917167000

add-1 (CO2) : E= -1371.320067

C	-0.954408000	0.041478000	1.564931000
O	0.326519000	0.036526000	1.472838000
C	-0.153788000	0.058621000	-1.097609000
H	-0.105374000	0.983354000	-1.688108000
H	-0.087973000	-0.797719000	-1.782233000
O	-1.639631000	0.070610000	2.554803000
B	1.052890000	0.024542000	0.106980000
P	-1.676418000	-0.000299000	-0.178100000
C	-2.658789000	1.566563000	-0.354957000
C	-3.915906000	1.531344000	0.521603000
H	-3.684961000	1.195714000	1.543151000
H	-4.327762000	2.550693000	0.577766000
H	-4.693096000	0.883581000	0.094115000
C	-1.718447000	2.679330000	0.143036000
H	-0.751262000	2.691589000	-0.382204000
H	-2.209425000	3.649302000	-0.028697000
H	-1.522060000	2.585273000	1.221186000
C	-3.019267000	1.803955000	-1.825089000
H	-3.691409000	1.028825000	-2.218207000
H	-3.540187000	2.770468000	-1.906094000
H	-2.125979000	1.850627000	-2.464367000
C	-2.529595000	-1.645220000	-0.325048000
C	-3.076764000	-1.832791000	-1.742985000
H	-3.463610000	-2.858922000	-1.839569000
H	-3.906734000	-1.143706000	-1.954068000
H	-2.297575000	-1.694156000	-2.507284000
C	-1.436851000	-2.690015000	-0.032787000
H	-1.021706000	-2.580258000	0.980767000
H	-1.892683000	-3.689193000	-0.104239000
H	-0.598124000	-2.647349000	-0.742188000
C	-3.646874000	-1.783369000	0.717174000
H	-4.518441000	-1.164263000	0.472756000
H	-3.977312000	-2.833440000	0.726293000
H	-3.297546000	-1.520999000	1.725490000
C	1.927778000	1.381720000	0.018020000
C	2.652203000	1.696012000	-1.143935000
C	1.969013000	2.312262000	1.066068000
C	3.374920000	2.881775000	-1.261430000
H	2.657947000	0.992211000	-1.982397000
C	2.688957000	3.504894000	0.959310000
H	1.428714000	2.095269000	1.990623000
C	3.393117000	3.796027000	-0.206763000
H	3.929663000	3.094889000	-2.177582000
H	2.701805000	4.208235000	1.794614000
H	3.957488000	4.726328000	-0.293278000
C	1.901131000	-1.348751000	0.028772000
C	2.240768000	-2.053132000	1.194694000
C	2.337097000	-1.890382000	-1.190897000

C	2.969745000	-3.241913000	1.146598000
H	1.918456000	-1.659293000	2.161592000
C	3.072549000	-3.074845000	-1.251645000
H	2.097186000	-1.378046000	-2.128639000
C	3.389119000	-3.758989000	-0.078597000
H	3.214099000	-3.767944000	2.071872000
H	3.399097000	-3.466176000	-2.217465000
H	3.961230000	-4.687655000	-0.118906000

add-2a (CO2) : E= -1986.125880

C	-2.392961000	-0.139366000	1.468761000
O	-1.134457000	0.147081000	1.499226000
C	-1.380343000	0.229687000	-1.078051000
H	-1.322802000	1.220646000	-1.551318000
H	-1.184178000	-0.538510000	-1.836242000
O	-3.128930000	-0.371116000	2.389471000
P	-2.989363000	0.026587000	-0.322963000
C	-3.944957000	1.633465000	-0.259861000
C	-5.280812000	1.423446000	0.462665000
H	-5.126949000	0.966782000	1.451421000
H	-5.750313000	2.408316000	0.609509000
H	-5.982010000	0.805129000	-0.113968000
C	-3.096529000	2.627809000	0.549898000
H	-2.103622000	2.795804000	0.110151000
H	-3.622872000	3.594558000	0.556906000
H	-2.968438000	2.308514000	1.593786000
C	-4.148934000	2.194724000	-1.671839000
H	-4.774804000	1.552116000	-2.303234000
H	-4.650640000	3.170828000	-1.585038000
H	-3.187943000	2.364053000	-2.179401000
C	-3.973936000	-1.464794000	-0.869548000
C	-4.864096000	-1.107085000	-2.065791000
H	-5.331431000	-2.034383000	-2.430885000
H	-5.670362000	-0.410280000	-1.802279000
H	-4.281012000	-0.680008000	-2.895752000
C	-2.990222000	-2.559821000	-1.300922000
H	-2.282568000	-2.823661000	-0.504758000
H	-3.573813000	-3.461826000	-1.541074000
H	-2.422655000	-2.280560000	-2.199212000
C	-4.811153000	-1.989477000	0.305553000
H	-5.502236000	-1.239756000	0.710355000
H	-5.404679000	-2.843013000	-0.057190000
H	-4.170443000	-2.335988000	1.127082000
B	-0.296282000	0.126716000	0.223058000
C	0.812725000	1.303821000	0.139472000
C	0.661639000	-1.179237000	0.184750000
C	1.940894000	-0.768970000	0.017114000
C	2.031516000	0.738656000	-0.014400000
C	0.472211000	2.738595000	0.224149000
C	0.218959000	3.507916000	-0.923077000
C	0.253936000	3.330767000	1.478430000
C	-0.238962000	4.822167000	-0.821832000
H	0.379790000	3.061161000	-1.907923000
C	-0.197323000	4.644936000	1.580672000
H	0.432744000	2.735931000	2.376033000
C	-0.451910000	5.394845000	0.431259000
H	-0.428606000	5.401873000	-1.727302000
H	-0.354853000	5.087311000	2.566237000
H	-0.809218000	6.422591000	0.513027000
C	3.326749000	1.459196000	-0.101320000
C	3.529838000	2.478117000	-1.041423000

C	4.376508000	1.139347000	0.773289000
C	4.742020000	3.163975000	-1.102410000
H	2.727759000	2.725242000	-1.737297000
C	5.586072000	1.826354000	0.715561000
H	4.235907000	0.343593000	1.507448000
C	5.773843000	2.841404000	-0.223465000
H	4.880421000	3.952832000	-1.843797000
H	6.388781000	1.567164000	1.407848000
H	6.723195000	3.377475000	-0.270474000
C	0.179213000	-2.569391000	0.270946000
H	0.995471000	-3.199803000	-1.621919000
C	3.123849000	-1.656756000	-0.103588000
C	3.305178000	-2.711105000	0.803504000
C	4.074970000	-1.477751000	-1.119457000
C	4.397820000	-3.567431000	0.694455000
H	2.575813000	-2.850501000	1.603408000
C	5.165586000	-2.337798000	-1.231534000
H	3.955739000	-0.653872000	-1.826078000
C	5.331439000	-3.385198000	-0.325419000
H	4.522618000	-4.379167000	1.413072000
H	5.894328000	-2.185994000	-2.029637000
H	6.189031000	-4.054580000	-0.410548000
C	-0.582805000	-2.974678000	1.383114000
C	0.396883000	-3.499765000	-0.758806000
C	-1.111898000	-4.263338000	1.456688000
H	-0.744124000	-2.269191000	2.201009000
C	-0.140881000	-4.783268000	-0.687733000
C	-0.901784000	-5.169886000	0.417439000
H	-1.692792000	-4.558919000	2.332594000
H	0.036651000	-5.490413000	-1.500272000
H	-1.319983000	-6.176264000	0.471839000

add-2b (CO2) : E= -3968.809123

C	-2.709397000	2.103863000	1.381969000
O	-1.553486000	1.526645000	1.479046000
C	-1.683157000	1.494052000	-1.110535000
H	-1.028880000	2.119266000	-1.728896000
H	-2.053986000	0.669251000	-1.733118000
O	-3.439568000	2.462959000	2.261625000
P	-3.031908000	2.467126000	-0.451183000
C	-2.677522000	4.294557000	-0.588336000
C	-3.862012000	5.121071000	-0.078737000
H	-4.182813000	4.792251000	0.920835000
H	-3.538177000	6.170403000	-0.004136000
H	-4.719349000	5.087666000	-0.765129000
C	-1.459220000	4.561519000	0.309669000
H	-0.636479000	3.870068000	0.093766000
H	-1.099531000	5.583201000	0.113741000
H	-1.714891000	4.484556000	1.375541000
C	-2.330262000	4.654976000	-2.038352000
H	-3.128351000	4.391151000	-2.744685000
H	-2.179317000	5.743833000	-2.094210000
H	-1.394885000	4.176997000	-2.359622000
C	-4.743405000	1.925562000	-0.953989000
C	-5.055139000	2.447171000	-2.361015000
H	-6.017989000	2.023026000	-2.684867000
H	-5.151198000	3.541351000	-2.383120000
H	-4.291799000	2.141114000	-3.092694000
C	-4.749751000	0.391247000	-0.962717000
H	-4.483057000	-0.024699000	0.021034000
H	-5.769742000	0.054247000	-1.202308000

H	-4.074812000	-0.028819000	-1.721020000
C	-5.787523000	2.415201000	0.060898000
H	-5.916910000	3.502937000	0.039471000
H	-6.753566000	1.959578000	-0.204909000
H	-5.531252000	2.118035000	1.086477000
B	-0.888441000	0.916039000	0.270579000
C	0.734798000	1.103969000	0.209425000
C	-0.960909000	-0.712461000	0.278815000
C	0.270115000	-1.203643000	0.046571000
C	1.288312000	-0.115966000	0.039901000
C	1.599340000	2.289743000	0.382463000
C	1.637516000	3.347272000	-0.525663000
C	2.475398000	2.371525000	1.471376000
C	2.464317000	4.451591000	-0.359597000
C	3.319577000	3.462726000	1.661184000
C	3.315103000	4.507264000	0.741208000
C	2.736012000	-0.393992000	-0.070697000
C	3.525648000	0.210160000	-1.050199000
C	3.362808000	-1.269242000	0.818058000
C	4.891417000	-0.039039000	-1.141569000
C	4.725330000	-1.540375000	0.740957000
C	5.490087000	-0.919510000	-0.243717000
C	-2.176238000	-1.539886000	0.344377000
C	0.622345000	-2.617393000	-0.195099000
C	0.295657000	-3.626004000	0.712680000
C	1.319431000	-2.985133000	-1.347433000
C	0.644616000	-4.953592000	0.481667000
C	1.683922000	-4.304075000	-1.596626000
C	1.342850000	-5.291165000	-0.675413000
C	-2.876622000	-1.681470000	1.546705000
C	-2.691268000	-2.188443000	-0.777981000
C	-4.050667000	-2.426425000	1.625349000
C	-3.868306000	-2.929151000	-0.727494000
C	-4.547371000	-3.049783000	0.481964000
F	-0.340848000	-3.333832000	1.836174000
F	0.331603000	-5.892536000	1.356799000
F	1.681626000	-6.546783000	-0.897240000
F	2.334562000	-4.626649000	-2.701312000
F	1.637764000	-2.061369000	-2.244937000
F	2.655334000	-1.850236000	1.776186000
F	5.300588000	-2.365537000	1.597519000
F	6.783667000	-1.164496000	-0.326859000
F	5.622054000	0.542959000	-2.076941000
F	2.980621000	1.036936000	-1.931304000
F	0.852519000	3.321916000	-1.605558000
F	2.450586000	5.440297000	-1.238886000
F	4.108929000	5.547644000	0.912426000
F	4.127979000	3.511106000	2.705567000
F	2.523431000	1.393234000	2.361533000
F	-2.090785000	-2.049406000	-1.956598000
F	-4.356008000	-3.498110000	-1.818375000
F	-5.665530000	-3.749418000	0.543923000
F	-4.691953000	-2.556655000	2.772928000
F	-2.419775000	-1.107917000	2.643499000

INT-3 (CO2) : E= -1447.364813

C	1.076577000	-0.207785000	-1.443027000
H	1.279252000	-1.125006000	-2.016989000
H	1.295528000	0.676610000	-2.060481000
P	2.273509000	-0.054664000	-0.076844000
C	1.913079000	-1.352637000	1.217759000

C	3.134658000	-1.540026000	2.123989000
H	3.471200000	-0.572059000	2.522966000
H	2.844140000	-2.181258000	2.970772000
H	3.968602000	-2.033332000	1.605880000
C	0.763606000	-0.811315000	2.085276000
H	-0.155348000	-0.643006000	1.507631000
H	0.532757000	-1.561023000	2.858297000
H	1.054455000	0.125992000	2.578452000
C	1.493664000	-2.675988000	0.569275000
H	2.269984000	-3.083304000	-0.094046000
H	1.306304000	-3.417197000	1.362432000
H	0.560450000	-2.563291000	-0.003924000
C	3.971786000	-0.195663000	-0.863642000
C	4.285945000	-1.615906000	-1.340822000
H	5.239285000	-1.603828000	-1.893178000
H	4.397769000	-2.319931000	-0.504364000
H	3.514197000	-2.002477000	-2.023739000
C	3.961307000	0.762388000	-2.067836000
H	3.605336000	1.764744000	-1.784734000
H	4.989637000	0.854095000	-2.449359000
H	3.334957000	0.385125000	-2.887862000
C	5.045875000	0.291916000	0.121531000
H	5.161390000	-0.374335000	0.983878000
H	6.010514000	0.323834000	-0.408806000
H	4.823542000	1.299111000	0.500056000
B	-0.421500000	-0.097076000	-0.994499000
C	-1.751195000	-0.650942000	-0.666485000
C	-1.596773000	0.707486000	-0.605343000
C	-2.720763000	-1.710772000	-0.398725000
C	-2.574098000	-2.964772000	-1.009895000
C	-3.778115000	-1.512702000	0.502716000
C	-3.479329000	-3.989484000	-0.747530000
H	-1.743435000	-3.120956000	-1.701098000
C	-4.669837000	-2.544922000	0.780658000
H	-3.881420000	-0.545298000	0.998149000
C	-4.527577000	-3.781484000	0.149431000
H	-3.363905000	-4.957398000	-1.237769000
H	-5.481453000	-2.384665000	1.491900000
H	-5.232833000	-4.586745000	0.360868000
C	-2.311028000	1.947780000	-0.325600000
H	-4.286226000	1.101221000	-0.556514000
C	-1.572021000	3.114196000	-0.073773000
C	-3.714336000	2.003786000	-0.331764000
C	-2.234226000	4.309847000	0.196191000
H	-0.479687000	3.067196000	-0.090111000
C	-4.368850000	3.205532000	-0.081378000
C	-3.628302000	4.357775000	0.191392000
H	-1.656577000	5.211559000	0.404185000
H	-5.458994000	3.246394000	-0.097523000
H	-4.142854000	5.298479000	0.395138000
O	1.706421000	2.570492000	-0.136263000
C	2.179617000	1.811878000	0.688359000
O	2.647369000	1.839130000	1.807577000

add-3 (CO2) : E= -1447.378239

C	-0.846909000	-0.638994000	-0.996008000
H	-0.650819000	0.002587000	-1.864528000
H	-0.891559000	-1.685797000	-1.332482000
P	-2.372766000	-0.242341000	-0.164842000
B	0.294601000	-0.449855000	0.210313000
C	1.522345000	0.497247000	0.131744000

C	1.786020000	-0.812705000	0.097976000
C	-3.734438000	-1.474613000	-0.456900000
C	-2.808405000	1.561954000	-0.305421000
C	2.188527000	1.795549000	0.035201000
C	3.126812000	2.045607000	-0.981439000
C	1.888031000	2.834254000	0.931674000
C	3.740104000	3.290576000	-1.097157000
H	3.365336000	1.244357000	-1.684470000
C	2.514144000	4.074119000	0.824150000
H	1.169968000	2.648026000	1.733227000
C	3.438821000	4.310047000	-0.193653000
H	4.463532000	3.465071000	-1.895865000
H	2.279428000	4.863603000	1.540547000
H	3.924064000	5.283429000	-0.281284000
C	2.926818000	-1.724527000	0.025133000
C	2.722649000	-3.104361000	-0.120161000
C	4.246028000	-1.247661000	0.108970000
C	3.801448000	-3.982728000	-0.195459000
H	1.697534000	-3.477340000	-0.169257000
C	5.324073000	-2.124696000	0.040787000
H	4.412315000	-0.176158000	0.238362000
C	5.105708000	-3.495047000	-0.115917000
H	3.625490000	-5.053766000	-0.310801000
H	6.342850000	-1.739459000	0.112178000
H	5.952015000	-4.181909000	-0.170013000
C	-1.484292000	2.331730000	-0.168980000
H	-0.985569000	2.120451000	0.788127000
H	-0.768091000	2.101669000	-0.969080000
H	-1.708959000	3.408541000	-0.206461000
C	-3.743484000	1.987906000	0.835266000
H	-4.743020000	1.546634000	0.747944000
H	-3.333921000	1.722744000	1.819622000
H	-3.855395000	3.082127000	0.790200000
C	-3.447352000	1.845818000	-1.668113000
H	-3.571450000	2.934036000	-1.779304000
H	-2.817731000	1.493808000	-2.499277000
H	-4.442680000	1.386833000	-1.756607000
C	-3.236862000	-2.803797000	0.135313000
H	-2.275751000	-3.121017000	-0.295598000
H	-3.131700000	-2.738344000	1.226948000
H	-3.978678000	-3.584059000	-0.093219000
C	-5.018212000	-1.053815000	0.265141000
H	-4.820176000	-0.826589000	1.322849000
H	-5.490725000	-0.184328000	-0.213456000
H	-5.735111000	-1.888118000	0.217845000
C	-3.970993000	-1.637209000	-1.962960000
H	-4.333425000	-0.712609000	-2.432191000
H	-3.056896000	-1.956816000	-2.484469000
H	-4.735914000	-2.414049000	-2.117270000
O	-0.462689000	-0.618843000	1.560096000
C	-1.738742000	-0.510341000	1.599453000
O	-2.487000000	-0.564288000	2.543280000

Activation of CS₂

TS-1 (CS₂) : E= -2017.071682

C	0.965010000	-0.472985000	2.257847000
S	-0.518255000	-1.026839000	2.058711000
C	-0.012953000	-0.453615000	-1.165019000
H	-0.073569000	-1.500891000	-1.487703000
H	0.017581000	0.153060000	-2.089753000

S	2.230873000	-0.070853000	3.112971000
B	-1.351241000	-0.011557000	-0.411842000
P	1.603477000	-0.229345000	-0.282756000
C	2.526516000	-1.834810000	-0.701462000
C	3.982528000	-1.722417000	-0.233856000
H	4.043625000	-1.367590000	0.806681000
H	4.453166000	-2.717844000	-0.281432000
H	4.573344000	-1.049599000	-0.871139000
C	1.847601000	-2.933206000	0.133946000
H	0.767192000	-3.005978000	-0.063868000
H	2.302718000	-3.905779000	-0.112998000
H	1.980741000	-2.759368000	1.211325000
C	2.485003000	-2.249244000	-2.176614000
H	2.996998000	-1.535706000	-2.832269000
H	2.991047000	-3.222820000	-2.285664000
H	1.457129000	-2.376872000	-2.544652000
C	2.489613000	1.256644000	-1.053210000
C	3.066946000	1.029480000	-2.450971000
H	3.452747000	1.986500000	-2.840127000
H	3.903108000	0.317325000	-2.443804000
H	2.304047000	0.665911000	-3.156122000
C	1.483424000	2.412393000	-1.119253000
H	0.992600000	2.596924000	-0.151854000
H	2.022617000	3.328818000	-1.408756000
H	0.697037000	2.240869000	-1.867086000
C	3.602187000	1.666324000	-0.074688000
H	4.381987000	0.900643000	0.028983000
H	4.082622000	2.588117000	-0.440709000
H	3.189693000	1.866807000	0.925261000
C	-2.616313000	-0.956222000	-0.408056000
C	-2.518617000	-2.342595000	-0.626045000
C	-3.898197000	-0.428953000	-0.173814000
C	-3.641359000	-3.164946000	-0.613109000
H	-1.538538000	-2.797271000	-0.792399000
C	-5.031096000	-1.242237000	-0.170610000
H	-4.008204000	0.642794000	0.007077000
C	-4.904056000	-2.612511000	-0.390157000
H	-3.535438000	-4.238537000	-0.777285000
H	-6.015402000	-0.805719000	0.007533000
H	-5.787964000	-3.252979000	-0.384388000
C	-1.566728000	1.527638000	-0.099386000
C	-1.417777000	2.177300000	1.133904000
C	-1.950820000	2.313151000	-1.202083000
C	-1.613274000	3.554964000	1.253619000
H	-1.138628000	1.605719000	2.019967000
C	-2.149964000	3.687173000	-1.088483000
H	-2.094721000	1.840414000	-2.179505000
C	-1.972349000	4.316532000	0.143864000
H	-1.482526000	4.034284000	2.225583000
H	-2.443058000	4.269367000	-1.964185000
H	-2.121747000	5.393266000	0.238750000

TS-2a (CS2) : E= -2631.878285

C	-1.487023000	0.268869000	-1.142364000
H	-1.496262000	1.198811000	-1.726070000
H	-1.487764000	-0.567682000	-1.858984000
P	-3.073688000	0.150361000	-0.187881000
C	-3.770984000	1.914754000	-0.290655000
C	-5.223318000	1.907511000	0.200370000
H	-5.326979000	1.358393000	1.149274000
H	-5.549132000	2.945793000	0.374143000

H	-5.908511000	1.466587000	-0.537661000
C	-2.936352000	2.748400000	0.695622000
H	-1.865935000	2.753030000	0.435346000
H	-3.285293000	3.793919000	0.668023000
H	-3.041120000	2.378505000	1.726394000
C	-3.695838000	2.591478000	-1.663739000
H	-4.181041000	2.011336000	-2.458095000
H	-4.204169000	3.568290000	-1.601919000
H	-2.657275000	2.797310000	-1.958993000
C	-4.177877000	-1.056562000	-1.147059000
C	-4.704841000	-0.558423000	-2.492558000
H	-5.232511000	-1.380070000	-3.005618000
H	-5.418211000	0.269490000	-2.376772000
H	-3.886998000	-0.225212000	-3.149779000
C	-3.350473000	-2.331303000	-1.372344000
H	-2.829618000	-2.658951000	-0.458125000
H	-4.026475000	-3.143951000	-1.683560000
H	-2.600304000	-2.212981000	-2.166257000
C	-5.344761000	-1.432321000	-0.218885000
H	-6.012653000	-0.587355000	-0.010563000
H	-5.945494000	-2.224084000	-0.695097000
H	-4.971884000	-1.819550000	0.741941000
B	-0.113680000	0.154784000	-0.344873000
C	1.030746000	1.271270000	-0.325707000
C	0.702272000	-1.203845000	-0.158879000
C	2.018990000	-0.879938000	-0.184340000
C	2.217142000	0.624369000	-0.218850000
C	0.787877000	2.728144000	-0.272862000
C	0.197776000	3.396216000	-1.357245000
C	1.055246000	3.459632000	0.894181000
C	-0.123606000	4.750344000	-1.274674000
H	0.002444000	2.844512000	-2.280005000
C	0.728073000	4.811436000	0.979195000
H	1.522051000	2.951556000	1.741368000
C	0.133006000	5.460895000	-0.102548000
H	-0.579654000	5.252165000	-2.130196000
H	0.939371000	5.361446000	1.897782000
H	-0.124282000	6.518921000	-0.034008000
C	3.541312000	1.267419000	-0.056951000
C	3.899815000	2.381400000	-0.830285000
C	4.448916000	0.795695000	0.904195000
C	5.130162000	3.007636000	-0.645519000
H	3.202614000	2.753337000	-1.582972000
C	5.674512000	1.428685000	1.094153000
H	4.185974000	-0.073418000	1.510163000
C	6.020482000	2.535018000	0.318423000
H	5.395065000	3.870894000	-1.258191000
H	6.365401000	1.052377000	1.850224000
H	6.983906000	3.026430000	0.463572000
C	0.114307000	-2.563068000	-0.164547000
H	0.550997000	-2.940993000	-2.240563000
C	3.145601000	-1.838122000	-0.259040000
C	3.182981000	-2.978887000	0.555867000
C	4.187055000	-1.632718000	-1.177243000
C	4.232753000	-3.889123000	0.453842000
H	2.383122000	-3.144480000	1.278853000
C	5.229660000	-2.548859000	-1.285658000
H	4.173817000	-0.744759000	-1.812494000
C	5.257452000	-3.678960000	-0.468202000
H	4.249221000	-4.768828000	1.099236000
H	6.026978000	-2.377782000	-2.010612000

H	6.077807000	-4.393858000	-0.548878000
C	-0.477078000	-3.087620000	0.995429000
C	0.083843000	-3.334627000	-1.334999000
C	-1.086522000	-4.340770000	0.983862000
H	-0.442380000	-2.507411000	1.919640000
C	-0.530341000	-4.586229000	-1.347975000
C	-1.122005000	-5.092297000	-0.190967000
H	-1.537078000	-4.730354000	1.898628000
H	-0.544713000	-5.172219000	-2.268795000
H	-1.603327000	-6.071338000	-0.203313000
S	-0.623857000	0.461047000	1.990295000
C	-1.976821000	-0.289382000	2.363838000
S	-3.044818000	-1.061914000	3.204470000

TS-2b (CS2) : E= -4614.560308

C	-2.188824000	0.727368000	-0.996865000
H	-1.933682000	1.586049000	-1.631032000
H	-2.328723000	-0.121645000	-1.681911000
P	-3.819917000	1.021879000	-0.166836000
C	-4.034899000	2.904394000	-0.306393000
C	-5.487516000	3.278896000	0.009177000
H	-5.848225000	2.784635000	0.924271000
H	-5.553009000	4.367568000	0.164923000
H	-6.165597000	3.024359000	-0.818092000
C	-3.133811000	3.492862000	0.790958000
H	-2.077624000	3.220245000	0.636562000
H	-3.201056000	4.593290000	0.766722000
H	-3.432054000	3.149803000	1.792906000
C	-3.629277000	3.526693000	-1.647176000
H	-4.135854000	3.062777000	-2.502613000
H	-3.898118000	4.596018000	-1.636911000
H	-2.545646000	3.477196000	-1.821483000
C	-5.086099000	0.111655000	-1.243288000
C	-5.300510000	0.682681000	-2.644304000
H	-5.954982000	0.008978000	-3.222153000
H	-5.786382000	1.668175000	-2.614077000
H	-4.350932000	0.778381000	-3.192913000
C	-4.584708000	-1.337806000	-1.357153000
H	-4.236998000	-1.725705000	-0.383615000
H	-5.410285000	-1.982413000	-1.698980000
H	-3.770231000	-1.445727000	-2.087708000
C	-6.411348000	0.073965000	-0.466596000
H	-6.855242000	1.068383000	-0.337640000
H	-7.137229000	-0.546739000	-1.015980000
H	-6.271527000	-0.370267000	0.531076000
B	-0.922948000	0.364629000	-0.084302000
C	0.432070000	1.231488000	-0.085740000
C	-0.332600000	-1.132678000	-0.029827000
C	1.012048000	-1.052482000	-0.114749000
C	1.472669000	0.375335000	-0.088197000
C	0.519567000	2.696681000	0.036979000
C	0.140832000	3.539834000	-1.008807000
C	0.882801000	3.295639000	1.244452000
C	0.070962000	4.919161000	-0.852448000
C	0.829379000	4.675970000	1.424528000
C	0.418928000	5.488639000	0.370812000
C	2.897923000	0.752720000	-0.013990000
C	3.464648000	1.650403000	-0.921117000
C	3.725345000	0.217806000	0.975219000
C	4.807529000	2.007869000	-0.845975000
C	5.070126000	0.560084000	1.068407000

C	5.610171000	1.459931000	0.151823000
C	-1.154924000	-2.359530000	-0.050277000
C	1.974772000	-2.159671000	-0.294101000
C	2.044227000	-3.248105000	0.576710000
C	2.889190000	-2.119686000	-1.350561000
C	2.985127000	-4.259894000	0.405655000
C	3.840890000	-3.116089000	-1.538382000
C	3.886856000	-4.190553000	-0.653196000
C	-1.587941000	-2.977770000	1.126723000
C	-1.643964000	-2.873098000	-1.251711000
C	-2.477503000	-4.048221000	1.109225000
C	-2.530981000	-3.944103000	-1.295307000
C	-2.947788000	-4.536791000	-0.107998000
S	-1.385693000	0.657543000	2.052984000
C	-2.792920000	-0.066978000	2.298221000
S	-3.917481000	-0.911706000	2.948195000
F	2.730622000	2.167538000	-1.893293000
F	5.328650000	2.852872000	-1.717506000
F	6.882038000	1.796194000	0.234388000
F	5.831307000	0.053898000	2.021627000
F	3.223060000	-0.625666000	1.867356000
F	2.851904000	-1.115151000	-2.216152000
F	4.687862000	-3.056905000	-2.550211000
F	4.781368000	-5.144649000	-0.820631000
F	3.035952000	-5.276715000	1.247008000
F	1.222231000	-3.328394000	1.609613000
F	1.258815000	2.536827000	2.265759000
F	1.159803000	5.217199000	2.583200000
F	0.354672000	6.796648000	0.531309000
F	-0.328726000	5.688130000	-1.850043000
F	-0.194125000	3.025665000	-2.184995000
F	-1.176102000	-2.537125000	2.304480000
F	-2.877459000	-4.603082000	2.239988000
F	-3.796718000	-5.546958000	-0.132331000
F	-3.013655000	-4.363473000	-2.452670000
F	-1.322058000	-2.287720000	-2.399625000

TS1-3 (CS2) : E= -2093.156146

C	0.594753000	-1.560985000	0.604745000
H	0.730070000	-1.580916000	1.700504000
H	0.551577000	-2.609726000	0.271005000
P	2.069609000	-0.687311000	-0.057405000
C	3.539474000	-1.591131000	0.725031000
C	4.832002000	-1.223011000	-0.012739000
H	4.936013000	-0.131295000	-0.111420000
H	5.692237000	-1.594232000	0.567277000
H	4.888601000	-1.674676000	-1.012584000
C	3.657638000	-1.067561000	2.166069000
H	2.729454000	-1.204529000	2.740552000
H	4.458487000	-1.623919000	2.679065000
H	3.914350000	0.000853000	2.187612000
C	3.363177000	-3.112398000	0.781752000
H	3.249480000	-3.567081000	-0.209882000
H	4.254741000	-3.556956000	1.253978000
H	2.494460000	-3.394164000	1.394340000
C	2.022839000	-0.972275000	-1.930407000
C	2.358910000	-2.400893000	-2.365610000
H	2.213851000	-2.483286000	-3.455617000
H	3.402509000	-2.667993000	-2.152781000
H	1.701278000	-3.142958000	-1.888163000
C	0.599786000	-0.648329000	-2.405187000

H	0.271796000	0.351407000	-2.085056000
H	0.582865000	-0.671689000	-3.506232000
H	-0.134425000	-1.385623000	-2.047970000
C	2.982773000	0.024791000	-2.596432000
H	4.030541000	-0.147425000	-2.318012000
H	2.904375000	-0.080222000	-3.690771000
H	2.730335000	1.060404000	-2.327421000
S	1.101280000	1.390214000	2.230409000
C	2.103054000	1.544100000	0.997772000
S	3.136463000	2.460413000	0.184154000
C	-2.241209000	-0.798065000	0.257713000
C	-1.588413000	0.392259000	0.112110000
C	-3.578517000	-1.387277000	0.213678000
C	-4.627509000	-0.762881000	-0.479196000
C	-3.818530000	-2.617680000	0.842309000
C	-5.886964000	-1.352914000	-0.533568000
H	-4.439373000	0.182384000	-0.991728000
C	-5.083391000	-3.197929000	0.803428000
H	-2.997037000	-3.109774000	1.366373000
C	-6.119534000	-2.567115000	0.114110000
H	-6.693054000	-0.863183000	-1.082203000
H	-5.261336000	-4.150303000	1.305202000
H	-7.109252000	-3.024986000	0.076194000
C	-1.820876000	1.818189000	-0.103841000
C	-0.767229000	2.631243000	-0.546755000
C	-3.067405000	2.406416000	0.162293000
C	-0.958425000	3.995798000	-0.741952000
H	0.213521000	2.185917000	-0.724037000
C	-3.253941000	3.773949000	-0.018471000
H	-3.882790000	1.783751000	0.535045000
C	-2.202234000	4.569084000	-0.476990000
H	-4.223390000	4.224462000	0.200088000
H	-2.351581000	5.640618000	-0.619758000
B	-0.764054000	-0.810376000	0.367866000
H	-0.127444000	4.614327000	-1.084040000

add-1 (CS2) : E= -2017.123446

C	-1.318377000	0.331967000	1.506502000
S	0.337349000	0.372701000	1.881862000
C	0.008365000	0.274120000	-1.022602000
H	0.034175000	1.295297000	-1.429014000
H	0.140406000	-0.421046000	-1.865217000
S	-2.575259000	0.517290000	2.555263000
B	1.240039000	0.113906000	0.097858000
P	-1.621130000	0.052877000	-0.296489000
C	-2.770079000	1.379415000	-0.957317000
C	-4.238952000	1.127275000	-0.601059000
H	-4.375701000	0.992391000	0.479938000
H	-4.822611000	2.005019000	-0.919539000
H	-4.642731000	0.253306000	-1.131408000
C	-2.309591000	2.712126000	-0.345741000
H	-1.248955000	2.917304000	-0.554287000
H	-2.899510000	3.521382000	-0.802316000
H	-2.468977000	2.736253000	0.739951000
C	-2.618120000	1.460172000	-2.485047000
H	-2.917984000	0.534318000	-2.991370000
H	-3.277816000	2.264303000	-2.845693000
H	-1.593293000	1.710378000	-2.790212000
C	-2.233035000	-1.701813000	-0.513820000
C	-2.621178000	-1.922819000	-1.981681000
H	-2.804608000	-2.997988000	-2.129242000

H	-3.543911000	-1.388740000	-2.249001000
H	-1.821373000	-1.625029000	-2.676055000
C	-1.068134000	-2.630600000	-0.143826000
H	-0.698038000	-2.443476000	0.875029000
H	-1.435499000	-3.667443000	-0.186483000
H	-0.217473000	-2.542466000	-0.832571000
C	-3.423143000	-2.028252000	0.397553000
H	-4.285384000	-1.370130000	0.238603000
H	-3.735750000	-3.059795000	0.171973000
H	-3.144808000	-1.976843000	1.457012000
C	2.284607000	1.351566000	-0.034320000
C	3.644192000	1.168552000	-0.324149000
C	1.843637000	2.678875000	0.115433000
C	4.514306000	2.251302000	-0.477078000
H	4.038013000	0.155384000	-0.431600000
C	2.699552000	3.766668000	-0.033799000
H	0.798559000	2.867288000	0.384544000
C	4.045748000	3.554968000	-0.336942000
H	5.567417000	2.071410000	-0.702600000
H	2.320332000	4.782488000	0.094881000
H	4.725049000	4.401292000	-0.453147000
C	1.950481000	-1.338295000	0.049653000
C	2.180233000	-2.153438000	1.166740000
C	2.402876000	-1.827983000	-1.189579000
C	2.799795000	-3.400286000	1.056628000
H	1.855031000	-1.817713000	2.154923000
C	3.023677000	-3.070406000	-1.314152000
H	2.274500000	-1.216252000	-2.088981000
C	3.218367000	-3.868635000	-0.186759000
H	2.954689000	-4.008869000	1.949790000
H	3.359209000	-3.417093000	-2.293796000
H	3.698961000	-4.844329000	-0.277902000

add-2a (CS2) : E= -2631.937043

C	1.321507000	-0.019956000	1.051716000
H	1.240105000	0.844333000	1.723471000
H	1.210016000	-0.929509000	1.659848000
P	2.967506000	-0.021783000	0.320011000
C	3.799231000	1.642701000	0.577744000
C	5.303304000	1.560778000	0.296981000
H	5.515619000	1.054021000	-0.655255000
H	5.691038000	2.589073000	0.233030000
H	5.841218000	1.053724000	1.109555000
C	3.151983000	2.641083000	-0.394864000
H	2.055706000	2.658597000	-0.314550000
H	3.518476000	3.647611000	-0.140188000
H	3.427537000	2.424100000	-1.436014000
C	3.561687000	2.124539000	2.016383000
H	3.849044000	1.382104000	2.774234000
H	4.179410000	3.021689000	2.175986000
H	2.515968000	2.418428000	2.179168000
C	3.914426000	-1.522508000	0.926651000
C	4.002529000	-1.446740000	2.457362000
H	4.421481000	-2.396031000	2.824996000
H	4.673752000	-0.640501000	2.786999000
H	3.020601000	-1.308990000	2.932453000
C	3.080890000	-2.741182000	0.498247000
H	3.008711000	-2.807300000	-0.596962000
H	3.589234000	-3.648198000	0.859559000
H	2.061898000	-2.747553000	0.910558000
C	5.325824000	-1.681685000	0.345127000

H	6.027900000	-0.933004000	0.726483000
H	5.694831000	-2.669940000	0.660446000
H	5.326938000	-1.646215000	-0.750827000
B	0.123909000	0.029617000	-0.089329000
C	-0.914312000	1.264587000	0.009809000
C	-0.903882000	-1.216760000	-0.097523000
C	-2.168982000	-0.734052000	-0.022826000
C	-2.176058000	0.770492000	0.019485000
C	-0.502488000	2.684453000	0.014130000
C	-0.102218000	3.308852000	1.207190000
C	-0.390895000	3.409657000	-1.181882000
C	0.401952000	4.608956000	1.205715000
H	-0.200880000	2.762750000	2.149862000
C	0.115068000	4.708828000	-1.184719000
H	-0.696652000	2.935178000	-2.116524000
C	0.519523000	5.311558000	0.006574000
H	0.701621000	5.077038000	2.145614000
H	0.194506000	5.254731000	-2.126521000
H	0.915394000	6.328273000	0.001114000
C	-3.422647000	1.575569000	0.010164000
C	-3.600608000	2.633439000	0.912174000
C	-4.444488000	1.303673000	-0.912223000
C	-4.763009000	3.401878000	0.891328000
H	-2.818385000	2.845443000	1.641992000
C	-5.603629000	2.075279000	-0.936926000
H	-4.323340000	0.478678000	-1.617015000
C	-5.768021000	3.126212000	-0.034081000
H	-4.884334000	4.218236000	1.605276000
H	-6.385510000	1.853510000	-1.665132000
H	-6.678837000	3.727057000	-0.050632000
C	-0.505484000	-2.637601000	-0.028360000
H	-1.218401000	-2.886362000	1.989067000
C	-3.395628000	-1.563798000	0.062879000
C	-3.566996000	-2.657878000	-0.797503000
C	-4.394443000	-1.295252000	1.011173000
C	-4.698028000	-3.465420000	-0.709314000
H	-2.800262000	-2.867206000	-1.545149000
C	-5.523125000	-2.106896000	1.102990000
H	-4.281195000	-0.440538000	1.681204000
C	-5.679833000	-3.193637000	0.242745000
H	-4.813920000	-4.309475000	-1.391186000
H	-6.287881000	-1.887399000	1.849960000
H	-6.567238000	-3.825050000	0.311304000
C	0.141277000	-3.272446000	-1.101105000
C	-0.702490000	-3.367962000	1.155081000
C	0.577407000	-4.592107000	-0.990873000
H	0.301224000	-2.718272000	-2.028488000
C	-0.255032000	-4.683139000	1.268847000
C	0.390669000	-5.299805000	0.196587000
H	1.071628000	-5.070313000	-1.838838000
H	-0.417438000	-5.231380000	2.198698000
H	0.738420000	-6.330487000	0.283216000
S	0.997540000	0.088335000	-1.866251000
C	2.641134000	-0.150030000	-1.496681000
S	3.868282000	-0.346101000	-2.576471000

add-2b (CS2) : E= -4614.619222

C	-2.213772000	-0.435474000	-1.023174000
H	-2.247406000	0.381777000	-1.753036000
H	-2.002451000	-1.354850000	-1.586791000
P	-3.828536000	-0.596794000	-0.232738000

C	-4.887784000	0.908263000	-0.618093000
C	-6.371931000	0.626520000	-0.361311000
H	-6.539280000	0.229648000	0.649915000
H	-6.915828000	1.579205000	-0.450559000
H	-6.793345000	-0.066772000	-1.102513000
C	-4.432686000	2.054684000	0.299939000
H	-3.343525000	2.202250000	0.280192000
H	-4.907979000	2.982257000	-0.055936000
H	-4.739395000	1.881520000	1.339766000
C	-4.676739000	1.324020000	-2.082867000
H	-4.810942000	0.494886000	-2.792028000
H	-5.425748000	2.093357000	-2.324301000
H	-3.687692000	1.772874000	-2.248251000
C	-4.562141000	-2.260446000	-0.680390000
C	-4.832796000	-2.263963000	-2.191668000
H	-5.108295000	-3.286451000	-2.491843000
H	-5.671006000	-1.604074000	-2.456991000
H	-3.950790000	-1.969748000	-2.779648000
C	-3.492554000	-3.308825000	-0.331185000
H	-3.201189000	-3.259352000	0.729763000
H	-3.919473000	-4.307079000	-0.512723000
H	-2.590503000	-3.219351000	-0.952131000
C	-5.845139000	-2.623696000	0.078644000
H	-6.664841000	-1.919322000	-0.096669000
H	-6.168197000	-3.611065000	-0.286149000
H	-5.671617000	-2.693184000	1.158293000
B	-1.016768000	-0.164040000	0.077882000
C	-0.169188000	1.212576000	-0.050403000
C	0.209120000	-1.228495000	0.091054000
C	1.374931000	-0.543429000	0.057559000
C	1.146924000	0.928280000	0.021258000
C	-0.743197000	2.569668000	-0.067149000
C	-1.348638000	3.078427000	-1.217529000
C	-0.779424000	3.366734000	1.078974000
C	-2.009742000	4.299972000	-1.228853000
C	-1.432623000	4.598314000	1.092975000
C	-2.048458000	5.065322000	-0.065180000
C	2.247942000	1.909632000	0.096387000
C	2.402885000	2.920661000	-0.854157000
C	3.187187000	1.841994000	1.127404000
C	3.447240000	3.837263000	-0.778771000
C	4.243904000	2.742083000	1.217975000
C	4.370902000	3.744503000	0.259522000
C	0.147669000	-2.693841000	-0.058729000
C	2.725782000	-1.136786000	0.000695000
C	3.151132000	-2.086141000	0.931991000
C	3.624396000	-0.768030000	-1.002292000
C	4.424331000	-2.645335000	0.871709000
C	4.904593000	-1.306041000	-1.076543000
C	5.303791000	-2.249796000	-0.133247000
C	-0.496047000	-3.520898000	0.864614000
C	0.709142000	-3.322224000	-1.178006000
C	-0.605532000	-4.895008000	0.681917000
C	0.620872000	-4.697648000	-1.379138000
C	-0.039746000	-5.488552000	-0.443175000
S	-1.832755000	-0.075927000	1.877405000
C	-3.448135000	-0.516372000	1.570005000
S	-4.634411000	-0.720847000	2.688846000
F	3.072109000	0.909255000	2.062719000
F	5.114939000	2.662125000	2.208010000
F	5.364819000	4.608240000	0.336542000

F	3.577435000	4.784182000	-1.691829000
F	1.561170000	3.014118000	-1.873393000
F	3.251424000	0.099011000	-1.934006000
F	5.732799000	-0.944426000	-2.040886000
F	6.512498000	-2.774685000	-0.193479000
F	4.806778000	-3.539821000	1.765821000
F	2.346403000	-2.472370000	1.909782000
F	-0.202288000	2.947619000	2.192515000
F	-1.465432000	5.329129000	2.193185000
F	-2.672285000	6.228476000	-0.060024000
F	-2.610774000	4.729634000	-2.326749000
F	-1.341399000	2.365304000	-2.342125000
F	1.327144000	-2.604193000	-2.106639000
F	1.153347000	-5.254354000	-2.453957000
F	-0.142140000	-6.791232000	-0.629360000
F	-1.261249000	-5.634098000	1.561140000
F	-1.068942000	-2.998976000	1.939256000

INT-3 (CS2) : E= -2093.174852

H	0.888360000	-1.727954000	-1.410934000
H	1.044482000	-0.199195000	-2.333249000
P	2.206163000	-0.165839000	-0.233569000
B	-0.616781000	-0.255320000	-0.878591000
C	-2.003981000	-0.675734000	-0.609621000
C	-1.735048000	0.662012000	-0.553460000
C	2.242521000	1.709731000	-0.134712000
C	3.744398000	-0.933479000	-1.000037000
C	-3.075935000	-1.649853000	-0.438898000
C	-4.424292000	-1.300906000	-0.610321000
C	-2.742308000	-2.972881000	-0.114204000
C	-5.420600000	-2.261420000	-0.460103000
H	-4.682201000	-0.273712000	-0.877224000
C	-3.743212000	-3.925281000	0.058275000
H	-1.688352000	-3.228276000	0.015328000
C	-5.081248000	-3.571734000	-0.118263000
H	-6.466898000	-1.988577000	-0.605561000
H	-3.479182000	-4.949661000	0.325157000
H	-5.864106000	-4.321309000	0.008933000
C	-2.400554000	1.918571000	-0.205161000
C	-1.930616000	3.140114000	-0.708018000
C	-3.501905000	1.921121000	0.664973000
C	-2.559651000	4.334988000	-0.368209000
H	-1.066046000	3.143496000	-1.373804000
C	-4.118364000	3.117746000	1.019028000
H	-3.858151000	0.973258000	1.073751000
C	-3.652905000	4.325922000	0.497983000
H	-2.191533000	5.278569000	-0.774100000
H	-4.967912000	3.109181000	1.703390000
H	-4.141530000	5.262472000	0.771115000
C	3.432973000	-2.421923000	-1.236896000
H	3.032759000	-2.905951000	-0.333583000
H	2.722234000	-2.571428000	-2.060960000
H	4.370722000	-2.927828000	-1.512088000
C	4.968858000	-0.845247000	-0.079412000
H	5.222201000	0.183099000	0.202926000
H	4.817521000	-1.419094000	0.842467000
H	5.824514000	-1.272700000	-0.625934000
C	4.053841000	-0.261469000	-2.344082000
H	4.867408000	-0.821870000	-2.830668000
H	3.193119000	-0.273989000	-3.029072000
H	4.395024000	0.775744000	-2.223167000

C	1.218736000	2.144209000	0.927096000
H	0.217869000	1.734947000	0.735139000
H	1.539369000	1.839675000	1.930825000
H	1.142127000	3.242680000	0.896935000
C	3.620968000	2.255681000	0.256368000
H	3.962668000	1.820953000	1.204882000
H	4.377033000	2.081033000	-0.521565000
H	3.524692000	3.345247000	0.384507000
C	1.825401000	2.285307000	-1.496706000
H	2.497571000	1.983459000	-2.312165000
H	0.797904000	1.997594000	-1.758871000
H	1.859011000	3.383813000	-1.426672000
S	0.730756000	-2.104698000	1.489288000
C	1.928702000	-0.946380000	1.426442000
S	2.968406000	-0.395175000	2.612734000
C	0.839919000	-0.634348000	-1.342330000

add-3 (CS2) : E= -2093.189841

H	-0.402763000	-0.021368000	-1.889661000
H	-0.656789000	-1.669965000	-1.264490000
P	-2.232925000	-0.182994000	-0.322803000
B	0.534294000	-0.385633000	0.164880000
C	1.778685000	0.544917000	0.093035000
C	2.027000000	-0.764190000	0.044876000
C	-3.522088000	-1.355874000	-1.005906000
C	-2.570121000	1.636051000	-0.588470000
C	2.425391000	1.853646000	0.027241000
C	3.437076000	2.114368000	-0.912300000
C	2.026242000	2.891962000	0.884519000
C	4.030332000	3.372046000	-0.989567000
H	3.744169000	1.316572000	-1.591938000
C	2.632526000	4.143964000	0.817344000
H	1.243598000	2.695552000	1.620493000
C	3.633909000	4.390685000	-0.122679000
H	4.810012000	3.557460000	-1.730652000
H	2.319914000	4.934724000	1.501637000
H	4.102792000	5.374174000	-0.180842000
C	3.110685000	-1.738181000	-0.038446000
C	2.807734000	-3.106617000	-0.098334000
C	4.460479000	-1.347565000	-0.048032000
C	3.820122000	-4.059408000	-0.180193000
H	1.758453000	-3.408580000	-0.074038000
C	5.472497000	-2.299543000	-0.126030000
H	4.704141000	-0.285261000	0.017320000
C	5.155588000	-3.657885000	-0.196886000
H	3.568853000	-5.120417000	-0.227600000
H	6.516942000	-1.982620000	-0.130195000
H	5.950808000	-4.402446000	-0.261358000
C	-1.289601000	2.380215000	-0.177278000
H	-1.025300000	2.177543000	0.870713000
H	-0.423852000	2.114877000	-0.798707000
H	-1.472353000	3.460707000	-0.282214000
C	-3.735781000	2.149041000	0.265482000
H	-4.680006000	1.629780000	0.060381000
H	-3.522692000	2.057311000	1.337313000
H	-3.875811000	3.215673000	0.029951000
C	-2.857867000	1.890367000	-2.074049000
H	-2.894606000	2.978733000	-2.233861000
H	-2.072555000	1.485839000	-2.729643000
H	-3.828199000	1.476870000	-2.382453000
C	-3.288631000	-2.717225000	-0.331141000

H	-2.244406000	-3.053005000	-0.419949000
H	-3.555894000	-2.686597000	0.732597000
H	-3.924347000	-3.463326000	-0.831721000
C	-4.957111000	-0.888446000	-0.742489000
H	-5.129569000	-0.701964000	0.325665000
H	-5.203663000	0.016655000	-1.315947000
H	-5.642337000	-1.684570000	-1.073291000
C	-3.294663000	-1.503249000	-2.519064000
H	-3.422809000	-0.557027000	-3.060359000
H	-2.299027000	-1.905116000	-2.750499000
H	-4.041035000	-2.213374000	-2.907159000
S	-0.385609000	-0.629189000	1.926710000
C	-2.017409000	-0.457160000	1.499049000
S	-3.336472000	-0.487084000	2.490766000
C	-0.622654000	-0.605816000	-0.984261000

Activation of C₂H₂

TS-1 (C₂H₂) : E= -1260.107729

C	0.215133000	-0.486677000	-0.759144000
H	0.131623000	-1.491126000	-1.195628000
H	0.242892000	0.220709000	-1.601085000
P	1.769213000	-0.329126000	0.203898000
H	0.524542000	-0.303764000	1.604855000
B	-1.099929000	-0.077853000	0.157715000
C	2.822987000	1.016188000	-0.599870000
C	2.623181000	-2.013077000	0.180802000
C	1.544852000	-3.062157000	0.497982000
H	0.954623000	-2.796486000	1.388150000
H	0.852302000	-3.211565000	-0.341105000
H	2.039402000	-4.026945000	0.693190000
C	3.654486000	-2.053437000	1.318211000
H	4.469520000	-1.332740000	1.178792000
H	3.177245000	-1.847885000	2.288000000
H	4.101717000	-3.059505000	1.366194000
C	3.283120000	-2.364415000	-1.153186000
H	3.634166000	-3.409194000	-1.122610000
H	2.575509000	-2.271712000	-1.991040000
H	4.154855000	-1.728516000	-1.361201000
C	2.141240000	2.347679000	-0.251699000
H	1.123288000	2.415013000	-0.663483000
H	2.073098000	2.494526000	0.835953000
H	2.734728000	3.172718000	-0.677808000
C	4.229221000	1.012042000	0.008510000
H	4.197687000	1.038546000	1.108301000
H	4.814968000	0.136686000	-0.306057000
H	4.767738000	1.909965000	-0.333887000
C	2.920319000	0.893576000	-2.124554000
H	3.401289000	-0.038838000	-2.445652000
H	1.933624000	0.958114000	-2.603571000
H	3.526006000	1.731692000	-2.506989000
C	-1.232519000	1.527893000	0.268171000
C	-1.560656000	2.218328000	-0.915260000
C	-0.973865000	2.308295000	1.402267000
H	-1.788885000	1.646160000	-1.820542000
H	-0.732363000	1.820667000	2.349450000
C	-1.604981000	3.609102000	-0.970793000
C	-1.009725000	3.705123000	1.357633000
H	-1.862289000	4.110358000	-1.906096000
H	-0.792817000	4.281204000	2.259581000
C	-1.318215000	4.362346000	0.170040000

H	-1.344084000	5.452715000	0.132204000
C	-4.876517000	-0.953594000	-0.497154000
C	-4.820807000	-2.315492000	-0.786651000
C	-3.706116000	-0.250719000	-0.203972000
H	-5.733417000	-2.868453000	-1.016816000
H	-3.768818000	0.816036000	0.025074000
C	-3.586511000	-2.966589000	-0.778927000
C	-2.450990000	-0.878209000	-0.198015000
H	-3.531042000	-4.034567000	-0.999376000
C	-2.425845000	-2.252412000	-0.490598000
H	-1.471866000	-2.787389000	-0.478883000
H	-5.836766000	-0.433899000	-0.497465000
C	-0.638783000	-0.613147000	1.863983000
C	-1.206280000	-1.080519000	2.847268000
H	-1.743412000	-1.497133000	3.682236000

TS-2a (C2H2) : E= -1874.917356

C	1.712597000	-0.222249000	-0.778532000
H	1.745908000	-1.139745000	-1.386047000
H	1.628920000	0.627192000	-1.473831000
P	3.293068000	-0.022427000	0.139030000
H	2.066830000	0.018121000	1.598876000
B	0.390498000	-0.187257000	0.186986000
C	-0.797340000	-1.263676000	-0.023567000
C	-0.443918000	1.192907000	0.236337000
C	4.338957000	1.208314000	-0.843923000
C	4.093032000	-1.732639000	0.198729000
C	-1.752639000	0.897506000	0.032971000
C	-1.970481000	-0.587436000	-0.080901000
C	-0.638357000	-2.732659000	-0.034621000
C	-0.069652000	-3.385853000	-1.140042000
C	-1.005666000	-3.508000000	1.074970000
C	0.134054000	-4.764560000	-1.132587000
H	0.198642000	-2.798508000	-2.021732000
C	-0.796020000	-4.886012000	1.086619000
H	-1.470979000	-3.012199000	1.929953000
C	-0.221749000	-5.519651000	-0.014999000
H	0.571597000	-5.252829000	-2.005380000
H	-1.088545000	-5.471179000	1.960511000
H	-0.060440000	-6.598673000	-0.006179000
C	-3.318829000	-1.203068000	-0.152150000
C	-3.594560000	-2.240339000	-1.054254000
C	-4.343214000	-0.775034000	0.706643000
C	-4.854296000	-2.834185000	-1.094641000
H	-2.809200000	-2.577888000	-1.732115000
C	-5.600684000	-1.372161000	0.669496000
H	-4.147378000	0.037501000	1.409285000
C	-5.862012000	-2.403204000	-0.232898000
H	-5.049266000	-3.637668000	-1.806954000
H	-6.382800000	-1.026627000	1.347614000
H	-6.849240000	-2.866848000	-0.266892000
C	0.138884000	2.548203000	0.316416000
C	0.893468000	2.938560000	1.434692000
C	-0.010721000	3.467037000	-0.735858000
C	1.467566000	4.206723000	1.504222000
H	1.011402000	2.238928000	2.264767000
C	0.577629000	4.728322000	-0.673109000
H	-0.601731000	3.177471000	-1.607577000
C	1.319688000	5.104368000	0.447690000
H	2.041433000	4.493150000	2.387889000
H	0.452987000	5.425834000	-1.503336000

H	1.775923000	6.094241000	0.498737000
C	-2.847991000	1.886629000	-0.114949000
C	-2.967934000	2.960392000	0.779225000
C	-3.777086000	1.778915000	-1.160836000
C	-3.983688000	3.901763000	0.629790000
H	-2.253205000	3.049389000	1.599320000
C	-4.789403000	2.723525000	-1.313224000
H	-3.701830000	0.943366000	-1.859722000
C	-4.897300000	3.787502000	-0.417758000
H	-4.062928000	4.728925000	1.337183000
H	-5.501182000	2.625686000	-2.134551000
H	-5.693060000	4.524918000	-0.535018000
C	3.021499000	-2.698665000	0.730191000
H	2.673030000	-2.408270000	1.731183000
H	2.143700000	-2.770276000	0.073890000
H	3.461435000	-3.706113000	0.805832000
C	5.244264000	-1.718999000	1.214361000
H	6.094939000	-1.108401000	0.888987000
H	4.904549000	-1.344917000	2.191823000
H	5.608829000	-2.749277000	1.355282000
C	4.591619000	-2.228467000	-1.159891000
H	4.914517000	-3.278332000	-1.066732000
H	3.801416000	-2.189742000	-1.925350000
H	5.454280000	-1.647797000	-1.516218000
C	3.737391000	2.589151000	-0.546799000
H	2.672919000	2.655897000	-0.820788000
H	3.821035000	2.840188000	0.519764000
H	4.282608000	3.352358000	-1.125505000
C	5.789871000	1.194916000	-0.353361000
H	5.852625000	1.286824000	0.741644000
H	6.322170000	0.284559000	-0.662256000
H	6.321358000	2.053410000	-0.794184000
C	4.305398000	0.963030000	-2.356807000
H	4.735165000	-0.006652000	-2.636938000
H	3.284655000	1.018346000	-2.758083000
H	4.898905000	1.748047000	-2.853671000
C	0.957288000	-0.387696000	1.898938000
C	0.478728000	-0.809676000	2.950894000
H	0.031149000	-1.180952000	3.857253000

TS-2b (C2H2) : E= -3857.605507

C	-2.317083000	1.245505000	-0.794286000
H	-1.988040000	2.034964000	-1.484895000
H	-2.631736000	0.392300000	-1.416584000
P	-3.808533000	1.781370000	0.153242000
H	-2.626859000	1.252363000	1.650977000
B	-1.084168000	0.723700000	0.142385000
C	0.446924000	1.245128000	-0.031416000
C	-0.831977000	-0.878266000	0.169176000
C	-5.299897000	1.028899000	-0.728514000
C	-3.843599000	3.669454000	0.082941000
C	0.495737000	-1.102384000	0.029327000
C	1.261670000	0.168982000	-0.050525000
C	0.971585000	2.618599000	0.063581000
C	0.700281000	3.586379000	-0.903294000
C	1.774413000	3.012174000	1.138384000
C	1.167056000	4.891873000	-0.800464000
C	2.261205000	4.310121000	1.264780000
C	1.957078000	5.253942000	0.288111000
C	2.737706000	0.209448000	-0.090866000
C	3.419239000	0.887659000	-1.103256000

C	3.501112000	-0.435861000	0.882860000
C	4.809639000	0.916209000	-1.152679000
C	4.891540000	-0.429798000	0.848635000
C	5.546060000	0.250554000	-0.175961000
C	-1.828294000	-1.961712000	0.119090000
C	-2.832744000	-2.094650000	1.080930000
C	-1.836535000	-2.897349000	-0.924317000
C	-3.787997000	-3.102811000	1.027987000
C	-2.780380000	-3.918153000	-0.998228000
C	-3.760344000	-4.023646000	-0.014832000
C	1.157524000	-2.420429000	-0.041038000
C	0.961806000	-3.387378000	0.947130000
C	2.015673000	-2.737780000	-1.095563000
C	1.596679000	-4.624458000	0.890760000
C	2.666853000	-3.964250000	-1.168610000
C	2.453735000	-4.910717000	-0.168784000
C	-2.406409000	4.152711000	0.329422000
H	-1.947732000	3.683625000	1.213766000
H	-1.767435000	3.958869000	-0.540934000
H	-2.420891000	5.241919000	0.494964000
C	-4.722624000	4.163937000	1.240802000
H	-5.766043000	3.835519000	1.147502000
H	-4.338647000	3.807002000	2.207905000
H	-4.717767000	5.265469000	1.256215000
C	-4.331023000	4.256837000	-1.242570000
H	-4.188787000	5.349792000	-1.225154000
H	-3.763389000	3.861367000	-2.098268000
H	-5.400020000	4.067567000	-1.411427000
C	-5.234244000	-0.474716000	-0.422898000
H	-4.350811000	-0.942889000	-0.884118000
H	-5.206806000	-0.669804000	0.659898000
H	-6.125228000	-0.970228000	-0.840514000
C	-6.590788000	1.592272000	-0.124847000
H	-6.602438000	1.493238000	0.971324000
H	-6.742114000	2.649648000	-0.382953000
H	-7.449739000	1.029583000	-0.523508000
C	-5.297901000	1.219237000	-2.249104000
H	-5.424721000	2.267403000	-2.542314000
H	-4.371593000	0.843169000	-2.706548000
H	-6.136262000	0.648501000	-2.681116000
C	-1.466306000	1.161870000	1.869525000
C	-0.701532000	1.348833000	2.815159000
H	0.013531000	1.487440000	3.610012000
F	0.170573000	-3.138581000	1.979264000
F	1.403267000	-5.523016000	1.840946000
F	3.060392000	-6.080204000	-0.226395000
F	3.470383000	-4.244176000	-2.179660000
F	2.206247000	-1.862727000	-2.073446000
F	2.896024000	-1.058102000	1.887083000
F	5.593823000	-1.047703000	1.782276000
F	6.864526000	0.269642000	-0.217311000
F	5.434794000	1.559982000	-2.123063000
F	2.746605000	1.515127000	-2.055830000
F	-0.949616000	-2.817590000	-1.906933000
F	-2.759605000	-4.778328000	-2.001595000
F	-4.667894000	-4.978975000	-0.082599000
F	-4.745227000	-3.161865000	1.938921000
F	-2.931613000	-1.208257000	2.064201000
F	-0.044687000	3.276178000	-1.958504000
F	0.866191000	5.786219000	-1.725304000
F	2.405830000	6.490323000	0.398662000

F	3.006815000	4.651057000	2.302666000
F	2.079763000	2.141724000	2.098392000

TS-3 (C2H2) : E= -1336.177277

H	-0.924251000	-0.639916000	-1.692631000
H	-1.179707000	-2.086401000	-0.693263000
C	1.331798000	0.479942000	0.129654000
C	1.771116000	-0.773494000	-0.033855000
C	-3.882900000	-1.541783000	0.072456000
C	-2.908655000	1.347821000	-0.708163000
C	1.798029000	1.863741000	0.173505000
C	2.703569000	2.364024000	-0.776494000
C	1.331451000	2.730694000	1.175121000
C	3.127146000	3.690167000	-0.724698000
H	3.064830000	1.698649000	-1.563645000
C	1.770269000	4.050583000	1.236428000
H	0.626346000	2.343514000	1.914803000
C	2.666404000	4.537082000	0.283717000
H	3.825568000	4.065701000	-1.474858000
H	1.407759000	4.707186000	2.029376000
H	3.003936000	5.573823000	0.326439000
C	2.996401000	-1.542342000	-0.221007000
C	2.922761000	-2.929317000	-0.418319000
C	4.262361000	-0.933555000	-0.185121000
C	4.078367000	-3.687451000	-0.589846000
H	1.937857000	-3.400166000	-0.433447000
C	5.417385000	-1.691677000	-0.350823000
H	4.326326000	0.143146000	-0.015086000
C	5.328613000	-3.070015000	-0.557729000
H	4.005898000	-4.765173000	-0.745945000
H	6.394860000	-1.207360000	-0.316638000
H	6.235853000	-3.662147000	-0.689396000
C	-1.580870000	2.102629000	-0.857791000
H	-1.080981000	2.243268000	0.110864000
H	-0.871938000	1.585043000	-1.518933000
H	-1.784239000	3.097515000	-1.284973000
C	-3.836552000	2.181397000	0.185755000
H	-4.821928000	1.716733000	0.319899000
H	-3.390462000	2.339644000	1.178497000
H	-3.991525000	3.168375000	-0.278875000
C	-3.542504000	1.142085000	-2.085727000
H	-3.647629000	2.119496000	-2.584470000
H	-2.920214000	0.501400000	-2.728370000
H	-4.545988000	0.698642000	-2.014230000
C	-3.476516000	-2.624144000	1.085924000
H	-2.493027000	-3.059655000	0.852535000
H	-3.429215000	-2.219957000	2.107642000
H	-4.218827000	-3.438066000	1.067449000
C	-5.216207000	-0.930005000	0.511677000
H	-5.126310000	-0.406320000	1.475621000
H	-5.610479000	-0.224798000	-0.234078000
H	-5.960564000	-1.733352000	0.632013000
C	-4.030915000	-2.180665000	-1.312574000
H	-4.341560000	-1.455451000	-2.075634000
H	-3.095188000	-2.651014000	-1.645727000
H	-4.801640000	-2.967603000	-1.264588000
B	0.269297000	-0.636899000	0.242693000
C	-1.045992000	-0.994093000	-0.658628000
P	-2.500085000	-0.268446000	0.159722000
H	0.414144000	-1.821761000	3.959070000
C	0.066248000	-1.415378000	3.025247000

C	-0.291359000	-0.945503000	1.947459000
H	-1.409594000	-0.436282000	1.594285000

add-1 (C2H2) : E= -1260.159839

C	0.027513000	-0.591140000	-0.741512000
H	-0.077457000	-1.637027000	-1.056798000
H	-0.087320000	0.048760000	-1.628319000
P	1.666516000	-0.364829000	-0.062159000
H	1.543176000	0.269381000	1.189999000
B	-1.159649000	-0.152696000	0.407228000
C	2.702700000	0.851565000	-1.018303000
C	2.524206000	-1.983422000	0.342574000
C	1.470413000	-3.089066000	0.512408000
H	0.672673000	-2.804317000	1.211095000
H	1.017999000	-3.367092000	-0.449918000
H	1.980616000	-3.980874000	0.908059000
C	3.265938000	-1.783720000	1.671495000
H	4.008424000	-0.974195000	1.619661000
H	2.554502000	-1.558307000	2.479812000
H	3.797128000	-2.712735000	1.929437000
C	3.492550000	-2.416370000	-0.763883000
H	3.890197000	-3.408318000	-0.499647000
H	2.984689000	-2.512842000	-1.734864000
H	4.347512000	-1.737066000	-0.877308000
C	1.900749000	2.163518000	-1.042634000
H	0.977107000	2.071110000	-1.628999000
H	1.617774000	2.513307000	-0.037769000
H	2.526053000	2.936992000	-1.514718000
C	4.027867000	1.094169000	-0.286734000
H	3.859994000	1.434894000	0.746291000
H	4.671490000	0.204462000	-0.262017000
H	4.579568000	1.888825000	-0.812063000
C	2.936887000	0.390707000	-2.461080000
H	3.621745000	-0.462605000	-2.531455000
H	1.991576000	0.125549000	-2.957714000
H	3.383189000	1.224597000	-3.024561000
C	-1.113057000	1.477017000	0.496315000
C	-1.480245000	2.254522000	-0.618509000
C	-0.637356000	2.176287000	1.616104000
H	-1.872183000	1.751184000	-1.509321000
H	-0.367224000	1.611883000	2.512935000
C	-1.362339000	3.642819000	-0.627809000
C	-0.507939000	3.569074000	1.620182000
H	-1.658979000	4.211806000	-1.511828000
H	-0.132662000	4.078248000	2.510755000
C	-0.863653000	4.308606000	0.494565000
H	-0.766812000	5.395911000	0.493354000
C	-4.958662000	-0.582263000	-0.649271000
C	-5.026983000	-1.939836000	-0.952255000
C	-3.753366000	-0.013559000	-0.230072000
H	-5.966867000	-2.386949000	-1.281654000
H	-3.730547000	1.051139000	0.013941000
C	-3.880261000	-2.723887000	-0.818887000
C	-2.580339000	-0.771909000	-0.105596000
H	-3.920978000	-3.793390000	-1.036734000
C	-2.685533000	-2.142192000	-0.400186000
H	-1.805963000	-2.784444000	-0.280785000
H	-5.851436000	0.041270000	-0.733299000
C	-0.784478000	-0.792379000	1.829040000
C	-0.496919000	-1.241416000	2.925857000
H	-0.292630000	-1.645992000	3.899807000

add-2a (C2H2) : E= -1874.973325

C	1.549762000	-0.139959000	-0.692224000
H	1.587613000	-1.098943000	-1.232950000
H	1.301152000	0.650022000	-1.416528000
P	3.202510000	0.162568000	-0.085533000
H	3.136239000	0.777437000	1.179376000
B	0.344968000	-0.173917000	0.493256000
C	-0.754848000	-1.320611000	0.147519000
C	-0.598678000	1.144602000	0.385009000
C	4.102201000	1.416301000	-1.129171000
C	4.126944000	-1.432883000	0.209823000
C	-1.871957000	0.752567000	0.122836000
C	-1.969474000	-0.740082000	-0.004897000
C	-0.399658000	-2.752876000	0.108170000
C	-0.085092000	-3.386912000	-1.105415000
C	-0.222588000	-3.479604000	1.296889000
C	0.393428000	-4.697107000	-1.132687000
H	-0.215160000	-2.834016000	-2.039704000
C	0.253215000	-4.788814000	1.270004000
H	-0.450591000	-2.992308000	2.246480000
C	0.569636000	-5.402483000	0.056914000
H	0.626914000	-5.170072000	-2.088690000
H	0.379345000	-5.335796000	2.206439000
H	0.943066000	-6.427665000	0.039036000
C	-3.265268000	-1.448162000	-0.162869000
C	-3.445703000	-2.445268000	-1.131134000
C	-4.342543000	-1.139333000	0.682677000
C	-4.660972000	-3.118956000	-1.246570000
H	-2.623021000	-2.687404000	-1.804239000
C	-5.555438000	-1.812917000	0.569437000
H	-4.219004000	-0.361341000	1.438730000
C	-5.720134000	-2.806147000	-0.396840000
H	-4.780769000	-3.891503000	-2.008257000
H	-6.378724000	-1.560663000	1.239971000
H	-6.672079000	-3.332000000	-0.487770000
C	-0.097782000	2.530545000	0.423674000
C	0.734355000	2.964445000	1.471322000
C	-0.370501000	3.435397000	-0.619127000
C	1.256625000	4.257358000	1.483894000
H	0.945881000	2.273539000	2.289808000
C	0.167936000	4.720054000	-0.614275000
H	-1.018242000	3.113774000	-1.437730000
C	0.984626000	5.139307000	0.437860000
H	1.883640000	4.578524000	2.318612000
H	-0.056869000	5.402907000	-1.435981000
H	1.397196000	6.149540000	0.445397000
C	-3.032785000	1.663534000	-0.040492000
C	-3.247873000	2.694681000	0.886049000
C	-3.927356000	1.534104000	-1.113549000
C	-4.313292000	3.578814000	0.738732000
H	-2.563941000	2.793049000	1.731071000
C	-4.992740000	2.420199000	-1.262482000
H	-3.783361000	0.728836000	-1.836929000
C	-5.189513000	3.446259000	-0.338149000
H	-4.462614000	4.373031000	1.472288000
H	-5.677015000	2.306397000	-2.105093000
H	-6.026145000	4.137233000	-0.454007000
C	3.133958000	-2.510295000	0.675992000
H	2.570311000	-2.201750000	1.565158000
H	2.410523000	-2.783823000	-0.105226000

H	3.713059000	-3.413933000	0.922862000
C	5.162900000	-1.199049000	1.317503000
H	5.907882000	-0.436677000	1.053990000
H	4.669267000	-0.903535000	2.255207000
H	5.698234000	-2.142668000	1.502700000
C	4.796829000	-1.913939000	-1.082004000
H	5.240712000	-2.902809000	-0.891300000
H	4.067298000	-2.034709000	-1.897337000
H	5.600731000	-1.246809000	-1.420282000
C	3.360750000	2.744867000	-0.903633000
H	2.286092000	2.687409000	-1.135937000
H	3.454960000	3.091272000	0.135080000
H	3.806252000	3.508666000	-1.559587000
C	5.556245000	1.583570000	-0.676103000
H	5.624162000	1.820770000	0.396386000
H	6.169061000	0.694977000	-0.880220000
H	5.998763000	2.426459000	-1.229064000
C	4.034524000	1.038032000	-2.613470000
H	4.574326000	0.109600000	-2.839616000
H	2.996151000	0.930688000	-2.957807000
H	4.497211000	1.846575000	-3.200076000
C	0.902553000	-0.349831000	1.977746000
C	1.316433000	-0.455489000	3.120496000
H	1.646635000	-0.554719000	4.137721000

add-2b (C2H2) : E= -3857.660065

C	-2.286743000	1.097314000	-0.822388000
H	-1.961305000	1.924045000	-1.469056000
H	-2.487939000	0.236296000	-1.477661000
P	-3.835511000	1.590355000	-0.064024000
H	-3.888848000	1.066853000	1.241237000
B	-1.090022000	0.684158000	0.289848000
C	0.417191000	1.243262000	-0.017944000
C	-0.767060000	-0.919910000	0.221094000
C	-5.303021000	0.800475000	-0.894740000
C	-3.949851000	3.442382000	0.147898000
C	0.566993000	-1.095576000	0.059595000
C	1.276591000	0.201043000	-0.043601000
C	0.884816000	2.637689000	0.077058000
C	0.550028000	3.599063000	-0.874497000
C	1.667623000	3.065591000	1.155258000
C	0.928075000	4.931062000	-0.758173000
C	2.067882000	4.392874000	1.292624000
C	1.697055000	5.329298000	0.331927000
C	2.748486000	0.313025000	-0.112977000
C	3.371662000	1.029199000	-1.137082000
C	3.567821000	-0.287027000	0.844579000
C	4.756212000	1.143134000	-1.211491000
C	4.955131000	-0.195553000	0.784392000
C	5.549422000	0.524147000	-0.249210000
C	-1.724137000	-2.035714000	0.163883000
C	-2.789374000	-2.155568000	1.063056000
C	-1.665442000	-3.008564000	-0.847538000
C	-3.715140000	-3.190353000	0.996809000
C	-2.577765000	-4.057548000	-0.930907000
C	-3.610107000	-4.152060000	-0.002243000
C	1.285646000	-2.385411000	0.002058000
C	1.134122000	-3.349271000	1.001106000
C	2.159574000	-2.678052000	-1.046686000
C	1.826788000	-4.556039000	0.961740000
C	2.869261000	-3.872558000	-1.102074000

C	2.699798000	-4.815340000	-0.090873000
C	-2.534612000	4.019763000	0.308599000
H	-1.966698000	3.532521000	1.112719000
H	-1.966803000	3.944179000	-0.627372000
H	-2.635120000	5.089241000	0.550179000
C	-4.761106000	3.721745000	1.419788000
H	-5.782258000	3.320111000	1.367190000
H	-4.259032000	3.297295000	2.301778000
H	-4.834293000	4.810735000	1.560688000
C	-4.591419000	4.099833000	-1.079698000
H	-4.547310000	5.190947000	-0.944213000
H	-4.039447000	3.862023000	-2.001491000
H	-5.645461000	3.824924000	-1.214502000
C	-5.154555000	-0.709566000	-0.646011000
H	-4.235212000	-1.118785000	-1.091139000
H	-5.161084000	-0.950611000	0.427700000
H	-6.007436000	-1.226429000	-1.112020000
C	-6.611593000	1.269640000	-0.248473000
H	-6.614659000	1.091056000	0.837462000
H	-6.819931000	2.331840000	-0.431598000
H	-7.441717000	0.690727000	-0.681123000
C	-5.298925000	1.067815000	-2.403854000
H	-5.471160000	2.123628000	-2.645726000
H	-4.353578000	0.752093000	-2.868951000
H	-6.108023000	0.482433000	-2.866678000
C	-1.383425000	1.167418000	1.779667000
C	-1.551047000	1.568485000	2.917348000
H	-1.674933000	1.892279000	3.934203000
F	0.324777000	-3.131742000	2.025829000
F	1.670085000	-5.452354000	1.921900000
F	3.359887000	-5.957646000	-0.134664000
F	3.685744000	-4.128046000	-2.110415000
F	2.307319000	-1.813180000	-2.041684000
F	3.025047000	-0.949838000	1.855984000
F	5.710116000	-0.771306000	1.704507000
F	6.864059000	0.623689000	-0.315197000
F	5.323271000	1.823306000	-2.193970000
F	2.647749000	1.613876000	-2.080623000
F	-0.746618000	-2.939255000	-1.800857000
F	-2.484389000	-4.948990000	-1.903042000
F	-4.494598000	-5.129048000	-0.084635000
F	-4.734322000	-3.221792000	1.843486000
F	-2.992120000	-1.225305000	1.988675000
F	2.041013000	2.208231000	2.091671000
F	-0.186963000	3.259117000	-1.932789000
F	0.557337000	5.816208000	-1.670386000
F	2.063744000	6.592385000	0.458876000
F	2.798407000	4.771199000	2.328601000

add-3 (C2H2) : E= -1336.222176

H	0.616201000	0.960811000	-1.462221000
H	1.103247000	2.268295000	-0.346517000
P	2.393306000	0.308830000	-0.011879000
B	-0.326225000	0.791258000	0.652429000
C	-1.309033000	-0.425142000	0.376359000
C	-1.819848000	0.778108000	0.158813000
C	3.843871000	1.468918000	0.140698000
C	2.646871000	-1.176265000	-1.098617000
C	-1.639818000	-1.845437000	0.412507000
C	-2.412467000	-2.451667000	-0.592599000
C	-1.139793000	-2.656154000	1.446709000

C	-2.677258000	-3.819588000	-0.562483000
H	-2.792276000	-1.833214000	-1.408989000
C	-1.419154000	-4.019576000	1.484324000
H	-0.532801000	-2.186441000	2.224940000
C	-2.186007000	-4.609117000	0.477253000
H	-3.274242000	-4.273604000	-1.355921000
H	-1.034763000	-4.630584000	2.303380000
H	-2.398281000	-5.679096000	0.502786000
C	-3.067669000	1.461809000	-0.163696000
C	-3.088837000	2.860072000	-0.279410000
C	-4.269023000	0.757072000	-0.356134000
C	-4.267150000	3.534520000	-0.591378000
H	-2.158276000	3.406258000	-0.112665000
C	-5.447134000	1.430326000	-0.664177000
H	-4.266032000	-0.329363000	-0.247864000
C	-5.449687000	2.821631000	-0.787461000
H	-4.265594000	4.622628000	-0.678388000
H	-6.372544000	0.869369000	-0.807463000
H	-6.373939000	3.348696000	-1.030468000
C	1.282596000	-1.871067000	-1.228745000
H	0.898938000	-2.209346000	-0.256115000
H	0.514175000	-1.226867000	-1.677820000
H	1.409178000	-2.756449000	-1.870931000
C	3.625561000	-2.159505000	-0.442464000
H	4.646363000	-1.765837000	-0.370019000
H	3.286929000	-2.452220000	0.562339000
H	3.662591000	-3.072202000	-1.056872000
C	3.152429000	-0.749279000	-2.480370000
H	3.156749000	-1.629515000	-3.141162000
H	2.500042000	0.008899000	-2.939100000
H	4.178817000	-0.356489000	-2.443085000
C	3.532189000	2.330694000	1.375890000
H	2.556034000	2.832048000	1.305365000
H	3.520762000	1.728592000	2.295727000
H	4.313102000	3.100775000	1.472504000
C	5.162257000	0.723715000	0.364213000
H	5.097568000	0.009868000	1.199375000
H	5.491321000	0.186106000	-0.536115000
H	5.942728000	1.458988000	0.614349000
C	3.940093000	2.362423000	-1.101109000
H	4.177509000	1.793360000	-2.009819000
H	3.010103000	2.920955000	-1.274530000
H	4.746153000	3.095864000	-0.944778000
C	0.894227000	1.190812000	-0.423466000
H	0.851185000	1.745631000	4.223017000
C	0.534857000	1.482007000	3.231143000
C	0.120765000	1.193813000	2.120079000
H	2.263560000	-0.223391000	1.287827000

Activation of CH₄

TS-1 (CH₄) : E= -1223.270765

C	0.150770000	-0.545154000	-0.784797000
H	0.056741000	-1.565447000	-1.180284000
H	0.144619000	0.133820000	-1.649357000
P	1.684022000	-0.359892000	0.186278000
H	0.514864000	-0.257069000	1.416732000
B	-1.076430000	-0.122106000	0.260463000
C	2.751199000	1.016277000	-0.542644000
C	2.595833000	-2.012268000	0.233820000
C	1.550380000	-3.109343000	0.484967000

H	0.933081000	-2.894772000	1.369041000
H	0.885933000	-3.257832000	-0.376526000
H	2.076914000	-4.059553000	0.665666000
C	3.561013000	-2.012942000	1.428822000
H	4.368474000	-1.278498000	1.325232000
H	3.025738000	-1.805203000	2.367464000
H	4.024876000	-3.008427000	1.517456000
C	3.341571000	-2.333670000	-1.063265000
H	3.739745000	-3.360016000	-1.007971000
H	2.673324000	-2.278653000	-1.936100000
H	4.191454000	-1.657971000	-1.230495000
C	2.051403000	2.343226000	-0.216022000
H	1.053397000	2.414955000	-0.671916000
H	1.935752000	2.486535000	0.867732000
H	2.665700000	3.168481000	-0.610753000
C	4.134429000	1.023457000	0.116292000
H	4.062969000	1.050037000	1.214170000
H	4.741708000	0.156011000	-0.176776000
H	4.674082000	1.927905000	-0.206040000
C	2.898046000	0.900096000	-2.064071000
H	3.402485000	-0.023311000	-2.375006000
H	1.924355000	0.952043000	-2.570183000
H	3.501858000	1.749209000	-2.423950000
C	-1.231319000	1.488261000	0.291496000
C	-1.609439000	2.145605000	-0.895492000
C	-0.958212000	2.303619000	1.397589000
H	-1.852240000	1.546498000	-1.779386000
H	-0.666621000	1.850385000	2.348555000
C	-1.687403000	3.532971000	-0.981690000
C	-1.027143000	3.698459000	1.325349000
H	-1.984379000	4.006761000	-1.919678000
H	-0.795460000	4.300051000	2.206847000
C	-1.385040000	4.320044000	0.132896000
H	-1.437565000	5.408389000	0.070775000
C	-4.883510000	-1.028530000	-0.271919000
C	-4.830954000	-2.399934000	-0.513127000
C	-3.708572000	-0.310931000	-0.037700000
H	-5.747340000	-2.963568000	-0.697542000
H	-3.772965000	0.763720000	0.152227000
C	-3.594147000	-3.044929000	-0.514459000
C	-2.449103000	-0.930275000	-0.043259000
H	-3.538576000	-4.120171000	-0.696367000
C	-2.429761000	-2.314571000	-0.284245000
H	-1.473184000	-2.846622000	-0.282284000
H	-5.845648000	-0.512238000	-0.264189000
C	-0.710507000	-0.667984000	2.011292000
H	-1.691043000	-0.252839000	2.289974000
H	-0.074633000	-0.369125000	2.867919000
H	-0.773800000	-1.763480000	2.019524000

TS-2a (CH4) : E= -1838.078858

C	-1.662211000	0.202920000	-0.795734000
H	-1.678323000	1.137520000	-1.377043000
H	-1.534862000	-0.625988000	-1.508367000
P	-3.226922000	-0.035278000	0.117208000
H	-2.071827000	-0.096581000	1.386915000
B	-0.431611000	0.158684000	0.306915000
C	0.709113000	1.295869000	0.114842000
C	0.488711000	-1.176472000	0.269781000
C	-4.223794000	-1.389027000	-0.743139000
C	-4.149737000	1.609141000	0.150851000

C	1.779827000	-0.805846000	0.074024000
C	1.914709000	0.689077000	-0.003515000
C	0.454778000	2.752952000	0.126348000
C	0.018014000	3.420163000	-1.030276000
C	0.561895000	3.492650000	1.313504000
C	-0.310048000	4.774610000	-0.998434000
H	-0.053569000	2.861844000	-1.967364000
C	0.229127000	4.846271000	1.347914000
H	0.917290000	2.991618000	2.216626000
C	-0.213931000	5.491683000	0.194033000
H	-0.640992000	5.274324000	-1.910903000
H	0.322232000	5.402156000	2.282753000
H	-0.472271000	6.551458000	0.221132000
C	3.225325000	1.378258000	-0.115172000
C	3.425286000	2.402472000	-1.051004000
C	4.289046000	1.030708000	0.731566000
C	4.649225000	3.063561000	-1.135892000
H	2.609442000	2.674957000	-1.721444000
C	5.510704000	1.694086000	0.650048000
H	4.152041000	0.230104000	1.461272000
C	5.696016000	2.712668000	-0.285210000
H	4.785342000	3.855895000	-1.873936000
H	6.324832000	1.412360000	1.319895000
H	6.654967000	3.229232000	-0.352075000
C	0.006783000	-2.571801000	0.324839000
C	-0.670385000	-3.053785000	1.456392000
C	0.180574000	-3.444615000	-0.762133000
C	-1.151267000	-4.360933000	1.504630000
H	-0.802577000	-2.393914000	2.316210000
C	-0.314009000	-4.746469000	-0.721037000
H	0.716123000	-3.085739000	-1.643770000
C	-0.983533000	-5.210832000	0.411877000
H	-1.664246000	-4.717311000	2.400166000
H	-0.171240000	-5.406934000	-1.578311000
H	-1.365289000	-6.232415000	0.445240000
C	2.930735000	-1.733456000	-0.067557000
C	3.103342000	-2.789097000	0.839432000
C	3.859913000	-1.589204000	-1.108830000
C	4.166439000	-3.678872000	0.707388000
H	2.389795000	-2.905861000	1.656938000
C	4.921334000	-2.481782000	-1.243667000
H	3.746409000	-0.766852000	-1.818178000
C	5.079169000	-3.529264000	-0.336186000
H	4.283832000	-4.491876000	1.425824000
H	5.632937000	-2.356022000	-2.061428000
H	5.913142000	-4.225232000	-0.440242000
C	-3.160374000	2.675438000	0.645700000
H	-2.857369000	2.488442000	1.684953000
H	-2.254936000	2.749108000	0.028941000
H	-3.661180000	3.656184000	0.620178000
C	-5.298131000	1.547308000	1.168307000
H	-6.126410000	0.907235000	0.844512000
H	-4.943969000	1.188291000	2.146563000
H	-5.699735000	2.563383000	1.309743000
C	-4.676907000	2.013272000	-1.227683000
H	-5.088696000	3.033920000	-1.172409000
H	-3.876847000	2.015903000	-1.983828000
H	-5.482995000	1.349928000	-1.571093000
C	-3.541284000	-2.713341000	-0.377505000
H	-2.487656000	-2.742629000	-0.693217000
H	-3.572117000	-2.897806000	0.705430000

H	-4.066529000	-3.539275000	-0.883824000
C	-5.667527000	-1.425041000	-0.232129000
H	-5.715358000	-1.442305000	0.867169000
H	-6.257941000	-0.573464000	-0.597625000
H	-6.148571000	-2.343736000	-0.603438000
C	-4.218807000	-1.232489000	-2.268222000
H	-4.678426000	-0.293055000	-2.599835000
H	-3.201604000	-1.283231000	-2.678899000
H	-4.794935000	-2.062691000	-2.708352000
C	-0.952523000	0.381585000	2.081862000
H	0.103418000	0.178547000	2.322528000
H	-1.481850000	-0.224703000	2.841927000
H	-1.171170000	1.436769000	2.287913000

TS-2b (CH4) : E= -3820.769971

C	2.209201000	1.388937000	0.894076000
H	1.780574000	2.114004000	1.598959000
H	2.625620000	0.567139000	1.497962000
P	3.562233000	2.100802000	-0.118472000
H	2.478084000	1.453531000	-1.335088000
B	1.086901000	0.784377000	-0.150102000
C	-0.475132000	1.206957000	0.034151000
C	0.923374000	-0.839373000	-0.115853000
C	5.204341000	1.433994000	0.516015000
C	3.482404000	3.982110000	-0.028308000
C	-0.389748000	-1.138636000	0.020724000
C	-1.226353000	0.086492000	0.067336000
C	-1.089972000	2.544257000	-0.063506000
C	-0.971948000	3.491531000	0.952876000
C	-1.828848000	2.913760000	-1.191167000
C	-1.530609000	4.760454000	0.851213000
C	-2.403834000	4.176009000	-1.317699000
C	-2.253615000	5.102587000	-0.289391000
C	-2.703407000	0.041618000	0.043941000
C	-3.481206000	0.676188000	1.012506000
C	-3.367213000	-0.626468000	-0.986261000
C	-4.872075000	0.644599000	0.962419000
C	-4.755182000	-0.678806000	-1.052914000
C	-5.508372000	-0.037086000	-0.072602000
C	1.972688000	-1.872069000	-0.087638000
C	2.949652000	-1.943660000	-1.081919000
C	2.060730000	-2.822207000	0.938353000
C	3.963074000	-2.892779000	-1.074990000
C	3.063688000	-3.788660000	0.967900000
C	4.018416000	-3.827130000	-0.044996000
C	-0.986881000	-2.486811000	0.107140000
C	-0.742897000	-3.462486000	-0.860654000
C	-1.842466000	-2.819423000	1.159158000
C	-1.325796000	-4.724185000	-0.785938000
C	-2.443206000	-4.070244000	1.250118000
C	-2.180575000	-5.025809000	0.271280000
C	2.000100000	4.380225000	-0.050801000
H	1.446048000	3.899864000	-0.871269000
H	1.503164000	4.134770000	0.895954000
H	1.928550000	5.470288000	-0.192913000
C	4.155402000	4.543296000	-1.289372000
H	5.220919000	4.285333000	-1.350014000
H	3.661590000	4.172644000	-2.199800000
H	4.076801000	5.642022000	-1.282884000
C	4.119424000	4.578191000	1.228920000
H	3.915662000	5.660874000	1.251724000

H	3.697944000	4.139734000	2.145815000
H	5.209910000	4.448465000	1.245090000
C	5.201516000	-0.064343000	0.181626000
H	4.409123000	-0.596874000	0.728975000
H	5.067916000	-0.244374000	-0.895508000
H	6.164746000	-0.503670000	0.486238000
C	6.367873000	2.098821000	-0.227035000
H	6.249454000	2.021192000	-1.318564000
H	6.481025000	3.158714000	0.039046000
H	7.304465000	1.587847000	0.046132000
C	5.371523000	1.592180000	2.031291000
H	5.477384000	2.638651000	2.339026000
H	4.525224000	1.153575000	2.579624000
H	6.282912000	1.057748000	2.344889000
C	1.283860000	1.259894000	-1.948848000
H	0.870050000	2.260658000	-2.129731000
H	0.518613000	0.499221000	-2.167528000
H	2.023122000	1.048747000	-2.744480000
F	2.962198000	-1.042348000	-2.060322000
F	4.890086000	-2.885591000	-2.018343000
F	4.979380000	-4.730758000	-0.017579000
F	3.120467000	-4.663308000	1.957248000
F	1.196368000	-2.809046000	1.943328000
F	0.043979000	-3.198526000	-1.893494000
F	-2.085754000	-1.931439000	2.113414000
F	-3.247517000	-4.362822000	2.257129000
F	-2.742373000	-6.217004000	0.343554000
F	-1.086918000	-5.631180000	-1.717318000
F	-2.663487000	-1.214050000	-1.945467000
F	-5.360605000	-1.310863000	-2.043400000
F	-6.826185000	-0.071280000	-0.127019000
F	-5.593465000	1.250590000	1.889262000
F	-2.903759000	1.320183000	2.015432000
F	-1.984303000	2.052603000	-2.189786000
F	-3.086493000	4.498735000	-2.403105000
F	-2.790611000	6.303976000	-0.395524000
F	-1.376867000	5.641893000	1.825136000
F	-0.287977000	3.200724000	2.054522000

TS-3 (CH4) : E= -1299.333835

H	1.097242000	2.175184000	0.704671000
H	0.780204000	0.705073000	1.651601000
C	-1.763513000	0.810980000	-0.114446000
C	-1.305697000	-0.433881000	-0.259176000
C	2.836913000	-1.261465000	0.762992000
C	3.892792000	1.519000000	-0.234863000
C	-2.997287000	1.568094000	0.077106000
C	-4.260992000	0.954719000	0.026935000
C	-2.934189000	2.952719000	0.296479000
C	-5.420705000	1.704325000	0.199523000
H	-4.319488000	-0.119427000	-0.160266000
C	-4.094191000	3.702342000	0.476263000
H	-1.952335000	3.429735000	0.324817000
C	-5.341151000	3.079693000	0.429053000
H	-6.395327000	1.215156000	0.152946000
H	-4.027310000	4.777741000	0.650245000
H	-6.252099000	3.664760000	0.566306000
C	-1.768288000	-1.821382000	-0.253477000
C	-2.687225000	-2.282590000	0.704074000
C	-1.286930000	-2.733767000	-1.206755000
C	-3.109428000	-3.610199000	0.705377000

H	-3.061301000	-1.583296000	1.455200000
C	-1.722080000	-4.056270000	-1.215532000
H	-0.570436000	-2.381298000	-1.952304000
C	-2.632515000	-4.501454000	-0.256526000
H	-3.818767000	-3.952732000	1.461099000
H	-1.345864000	-4.746825000	-1.972600000
H	-2.968270000	-5.539673000	-0.257782000
C	3.335363000	2.910814000	-0.566592000
H	2.658279000	2.891028000	-1.433174000
H	2.797823000	3.351913000	0.283530000
H	4.176554000	3.577850000	-0.812611000
C	4.795507000	1.077560000	-1.396268000
H	5.225305000	0.079768000	-1.239410000
H	4.239134000	1.064975000	-2.345181000
H	5.629492000	1.790232000	-1.499291000
C	4.698983000	1.610887000	1.062616000
H	5.452287000	2.409636000	0.963537000
H	4.056380000	1.857884000	1.920889000
H	5.236375000	0.678198000	1.283836000
C	1.634239000	-2.185452000	0.527854000
H	0.705139000	-1.768549000	0.940977000
H	1.467201000	-2.367754000	-0.543387000
H	1.823857000	-3.154190000	1.017273000
C	4.087836000	-1.909232000	0.160402000
H	4.001838000	-2.023470000	-0.930800000
H	5.000678000	-1.338762000	0.384121000
H	4.211857000	-2.913572000	0.595535000
C	3.022155000	-1.070088000	2.272454000
H	3.896233000	-0.455012000	2.518470000
H	2.135411000	-0.615660000	2.734811000
H	3.167259000	-2.059086000	2.736794000
B	-0.244632000	0.699728000	-0.394266000
P	2.432171000	0.334326000	-0.143117000
H	0.477834000	0.269758000	-2.940963000
C	0.319806000	1.038047000	-2.165299000
H	-0.732236000	1.335418000	-2.287579000
H	0.912357000	1.928893000	-2.429133000
C	0.976046000	1.084660000	0.639483000
H	1.382598000	0.414221000	-1.454168000

add-1 (CH4) : E= -1223.325285

C	0.101613000	-0.878114000	-0.457564000
H	0.121193000	-1.975353000	-0.530556000
H	-0.097297000	-0.470329000	-1.460604000
P	1.719343000	-0.325287000	0.048418000
H	1.601956000	0.539124000	1.155784000
B	-1.134434000	-0.367413000	0.606684000
C	2.514315000	0.770108000	-1.235599000
C	2.816769000	-1.702322000	0.679708000
C	1.943247000	-2.731034000	1.412663000
H	1.373972000	-2.280123000	2.234942000
H	1.232909000	-3.230989000	0.740930000
H	2.608479000	-3.500897000	1.833063000
C	3.827130000	-1.126054000	1.681419000
H	4.498106000	-0.383027000	1.233122000
H	3.317883000	-0.663835000	2.539902000
H	4.448760000	-1.949058000	2.066086000
C	3.537479000	-2.399308000	-0.479378000
H	4.070268000	-3.277055000	-0.082668000
H	2.831078000	-2.756002000	-1.244313000
H	4.280288000	-1.748593000	-0.959754000

C	1.592660000	1.993722000	-1.368105000
H	0.607053000	1.724197000	-1.769330000
H	1.425508000	2.510128000	-0.410203000
H	2.062099000	2.702150000	-2.068121000
C	3.902241000	1.232387000	-0.781742000
H	3.871568000	1.708901000	0.209862000
H	4.632135000	0.411316000	-0.759236000
H	4.271453000	1.982309000	-1.497863000
C	2.597029000	0.065356000	-2.594840000
H	3.311348000	-0.767039000	-2.602982000
H	1.615915000	-0.311254000	-2.917198000
H	2.931261000	0.799867000	-3.343703000
C	-1.133981000	1.271871000	0.585058000
C	-1.689293000	1.976051000	-0.500326000
C	-0.556769000	2.056395000	1.597789000
H	-2.185253000	1.408073000	-1.294832000
H	-0.152569000	1.566544000	2.489119000
C	-1.636749000	3.365366000	-0.594229000
C	-0.494704000	3.452120000	1.520736000
H	-2.081164000	3.872128000	-1.453919000
H	-0.038200000	4.024054000	2.332049000
C	-1.026388000	4.113317000	0.415860000
H	-0.985783000	5.202245000	0.350165000
C	-4.997170000	-0.938506000	0.193215000
C	-5.096481000	-1.859506000	-0.852464000
C	-3.747485000	-0.489625000	0.611469000
H	-6.073170000	-2.213757000	-1.187690000
H	-3.691103000	0.242794000	1.423080000
C	-3.932522000	-2.314945000	-1.463798000
C	-2.549501000	-0.933461000	0.018942000
H	-3.992639000	-3.031855000	-2.285927000
C	-2.684899000	-1.854571000	-1.029659000
H	-1.795865000	-2.236705000	-1.540212000
H	-5.901669000	-0.567210000	0.680211000
C	-0.896534000	-0.955070000	2.115137000
H	-1.701733000	-0.604422000	2.782104000
H	0.050221000	-0.637529000	2.594895000
H	-0.925018000	-2.057495000	2.138349000

add-2a (CH4) : E= -1838.137711

C	1.581140000	0.776806000	0.512567000
H	1.650235000	1.861739000	0.684819000
H	1.290833000	0.301643000	1.461775000
P	3.236681000	0.234899000	0.112738000
H	3.220020000	-0.652314000	-0.982117000
B	0.374429000	0.463135000	-0.629299000
C	-0.941426000	1.318076000	-0.189835000
C	-0.244892000	-1.047115000	-0.493098000
C	3.958049000	-0.804086000	1.482511000
C	4.326766000	1.641913000	-0.456302000
C	-1.568652000	-0.947033000	-0.185075000
C	-1.993007000	0.476948000	-0.025002000
C	-1.015803000	2.793703000	-0.193129000
C	-0.424099000	3.558515000	0.826327000
C	-1.641084000	3.480128000	-1.247342000
C	-0.458896000	4.952784000	0.797361000
H	0.037146000	3.045291000	1.673976000
C	-1.673765000	4.872425000	-1.279178000
H	-2.111843000	2.899665000	-2.043612000
C	-1.081223000	5.616713000	-0.258740000
H	-0.004902000	5.523329000	1.610301000

H	-2.171725000	5.381740000	-2.106558000
H	-1.111023000	6.707139000	-0.282911000
C	-3.403995000	0.885733000	0.195425000
C	-3.734129000	1.847067000	1.161255000
C	-4.440729000	0.336516000	-0.574973000
C	-5.055199000	2.248061000	1.350809000
H	-2.938734000	2.280048000	1.770253000
C	-5.760884000	0.738153000	-0.387745000
H	-4.204105000	-0.415568000	-1.330175000
C	-6.074761000	1.694829000	0.577516000
H	-5.288246000	2.996870000	2.110052000
H	-6.550383000	0.299241000	-1.000368000
H	-7.109871000	2.006723000	0.726605000
C	0.474763000	-2.328192000	-0.641453000
C	1.407996000	-2.514588000	-1.678211000
C	0.300227000	-3.391629000	0.266730000
C	2.134744000	-3.700157000	-1.800733000
H	1.538701000	-1.718755000	-2.413800000
C	1.025600000	-4.572970000	0.148433000
H	-0.413897000	-3.273419000	1.083889000
C	1.952418000	-4.735508000	-0.884358000
H	2.842520000	-3.818622000	-2.624006000
H	0.868961000	-5.375485000	0.871883000
H	2.519332000	-5.663247000	-0.977027000
C	-2.523218000	-2.070359000	0.002382000
C	-2.656823000	-3.082862000	-0.958258000
C	-3.318270000	-2.136570000	1.156165000
C	-3.550236000	-4.134765000	-0.766107000
H	-2.045220000	-3.036369000	-1.861864000
C	-4.209408000	-3.189053000	1.350812000
H	-3.235102000	-1.345109000	1.904193000
C	-4.329031000	-4.193047000	0.389889000
H	-3.642849000	-4.912608000	-1.526284000
H	-4.818914000	-3.221799000	2.255645000
H	-5.032158000	-5.014287000	0.538257000
C	3.484757000	2.607533000	-1.303167000
H	3.072777000	2.118210000	-2.193992000
H	2.648914000	3.051547000	-0.744421000
H	4.142973000	3.425498000	-1.634263000
C	5.459028000	1.090262000	-1.332581000
H	6.115499000	0.394293000	-0.796098000
H	5.061009000	0.581229000	-2.222656000
H	6.076168000	1.933411000	-1.679273000
C	4.894494000	2.397430000	0.750475000
H	5.416109000	3.295116000	0.385504000
H	4.101990000	2.732059000	1.437180000
H	5.621433000	1.796227000	1.313571000
C	3.065234000	-2.052755000	1.548207000
H	2.019864000	-1.802089000	1.776420000
H	3.075477000	-2.625908000	0.608855000
H	3.438748000	-2.705526000	2.352504000
C	5.395178000	-1.228956000	1.169709000
H	5.472942000	-1.720892000	0.188081000
H	6.097966000	-0.384952000	1.201899000
H	5.717274000	-1.956643000	1.930340000
C	3.890376000	-0.070940000	2.827578000
H	4.561355000	0.795218000	2.877388000
H	2.869030000	0.264042000	3.057378000
H	4.193289000	-0.774722000	3.617923000
C	0.762047000	0.865082000	-2.170349000
H	-0.034872000	0.516591000	-2.847451000

H	1.705256000	0.425560000	-2.547537000
H	0.835942000	1.958174000	-2.299951000
add-2b (CH4) : E= -3820.828832			
C	1.614254000	2.161915000	0.509184000
H	1.188296000	3.176278000	0.519160000
H	1.520666000	1.770419000	1.532841000
P	3.360049000	2.342305000	0.150156000
H	3.754876000	1.398935000	-0.821366000
B	0.742433000	1.190530000	-0.536563000
C	-0.845701000	1.236342000	-0.162683000
C	0.982724000	-0.425532000	-0.329716000
C	4.381155000	1.906121000	1.647687000
C	3.780064000	3.986512000	-0.626441000
C	-0.224589000	-1.013983000	-0.123861000
C	-1.318718000	-0.024404000	-0.050076000
C	-1.737436000	2.407935000	-0.217613000
C	-1.666413000	3.427185000	0.733827000
C	-2.693895000	2.555238000	-1.228253000
C	-2.489354000	4.547589000	0.688099000
C	-3.530547000	3.666876000	-1.296414000
C	-3.426939000	4.667391000	-0.333721000
C	-2.741949000	-0.405604000	0.064981000
C	-3.551024000	0.085027000	1.090523000
C	-3.329817000	-1.262004000	-0.867449000
C	-4.893574000	-0.267282000	1.192218000
C	-4.667303000	-1.634649000	-0.781962000
C	-5.450807000	-1.131928000	0.253474000
C	2.209700000	-1.244281000	-0.317803000
C	3.178582000	-1.177238000	-1.323716000
C	2.484717000	-2.137882000	0.729989000
C	4.340575000	-1.944678000	-1.307888000
C	3.630689000	-2.926461000	0.766025000
C	4.564973000	-2.834946000	-0.262423000
C	-0.483621000	-2.465638000	-0.001332000
C	-0.077815000	-3.368154000	-0.985829000
C	-1.156617000	-2.982960000	1.106598000
C	-0.323650000	-4.733544000	-0.872169000
C	-1.421688000	-4.341918000	1.238409000
C	-1.001187000	-5.219924000	0.242372000
C	2.665257000	4.357953000	-1.614234000
H	2.561062000	3.618503000	-2.417626000
H	1.687808000	4.468766000	-1.125232000
H	2.927281000	5.325157000	-2.069341000
C	5.097144000	3.868061000	-1.405076000
H	5.956367000	3.639106000	-0.763655000
H	5.029989000	3.100787000	-2.190375000
H	5.296494000	4.831314000	-1.898842000
C	3.875043000	5.070256000	0.453145000
H	3.984478000	6.046770000	-0.041931000
H	2.966976000	5.112445000	1.073932000
H	4.745545000	4.930517000	1.108062000
C	4.134511000	0.409199000	1.889138000
H	3.071652000	0.179687000	2.057346000
H	4.493456000	-0.197360000	1.044399000
H	4.690367000	0.102969000	2.788466000
C	5.875342000	2.131633000	1.398598000
H	6.224916000	1.618337000	0.489951000
H	6.128117000	3.198010000	1.325169000
H	6.436166000	1.716978000	2.249983000
C	3.915552000	2.697320000	2.877076000
H	4.118842000	3.771669000	2.792804000

H	2.843949000	2.559598000	3.075920000
H	4.465025000	2.322501000	3.753893000
C	0.824570000	1.630960000	-2.111968000
H	0.237189000	0.928124000	-2.723105000
H	1.844488000	1.628798000	-2.527722000
H	0.394334000	2.635282000	-2.269514000
F	3.024113000	-0.344706000	-2.347459000
F	5.223137000	-1.840872000	-2.288797000
F	5.658229000	-3.576345000	-0.239470000
F	3.852461000	-3.740410000	1.784572000
F	1.678553000	-2.203407000	1.783628000
F	0.554603000	-2.939077000	-2.067987000
F	-1.538561000	-2.171019000	2.083364000
F	-2.050664000	-4.807678000	2.304351000
F	-1.240752000	-6.513218000	0.357887000
F	0.070395000	-5.568365000	-1.819539000
F	-2.608129000	-1.727476000	-1.878068000
F	-5.203650000	-2.442629000	-1.681238000
F	-6.723021000	-1.472910000	0.346563000
F	-5.641405000	0.201838000	2.177354000
F	-3.046655000	0.897844000	2.008495000
F	-2.821256000	1.624730000	-2.164320000
F	-4.419350000	3.782107000	-2.269455000
F	-4.215814000	5.726293000	-0.389797000
F	-2.393637000	5.491582000	1.611867000
F	-0.804650000	3.335516000	1.743934000

add-3 (CH4) : E= -1299.386682

H	-1.159672000	-2.139985000	0.368173000
H	-0.546524000	-0.754096000	1.303604000
P	-2.387038000	-0.164070000	-0.075331000
B	0.325636000	-0.749201000	-0.787991000
C	1.817589000	-0.849330000	-0.303028000
C	1.385879000	0.399335000	-0.441648000
C	-3.133991000	0.544294000	1.490249000
C	-3.561526000	-1.238629000	-1.054146000
C	3.025002000	-1.584043000	0.061998000
C	4.124320000	-0.943791000	0.662897000
C	3.107922000	-2.965681000	-0.171115000
C	5.265891000	-1.660554000	1.007970000
H	4.064820000	0.129112000	0.858688000
C	4.254174000	-3.682453000	0.166142000
H	2.251239000	-3.463348000	-0.630107000
C	5.337667000	-3.033052000	0.757528000
H	6.108199000	-1.147651000	1.476556000
H	4.302644000	-4.755473000	-0.029400000
H	6.234592000	-3.594088000	1.025909000
C	1.914457000	1.762343000	-0.425451000
C	1.236672000	2.815961000	0.212691000
C	3.126769000	2.065954000	-1.073969000
C	1.749343000	4.112030000	0.214768000
H	0.302994000	2.602557000	0.737999000
C	3.633141000	3.362116000	-1.083078000
H	3.664064000	1.258633000	-1.576357000
C	2.948827000	4.393917000	-0.437136000
H	1.208522000	4.908401000	0.730316000
H	4.573124000	3.570776000	-1.597810000
H	3.348428000	5.409140000	-0.442049000
C	-2.728552000	-1.990277000	-2.105729000
H	-2.194142000	-1.307117000	-2.779396000
H	-1.977370000	-2.650103000	-1.652542000

H	-3.415425000	-2.603995000	-2.708932000
C	-4.611736000	-0.390395000	-1.783676000
H	-5.249097000	0.185085000	-1.100594000
H	-4.147923000	0.302712000	-2.499505000
H	-5.264191000	-1.066294000	-2.357812000
C	-4.247016000	-2.256412000	-0.136643000
H	-4.815184000	-2.964788000	-0.758713000
H	-3.518452000	-2.837152000	0.448571000
H	-4.955504000	-1.779322000	0.554545000
C	-2.175631000	1.659994000	1.941516000
H	-1.138927000	1.302264000	2.037179000
H	-2.185998000	2.515734000	1.251830000
H	-2.497696000	2.021809000	2.929793000
C	-4.526885000	1.140163000	1.266263000
H	-4.540692000	1.874664000	0.447204000
H	-5.279097000	0.366740000	1.058066000
H	-4.838127000	1.664304000	2.183367000
C	-3.190726000	-0.524348000	2.590041000
H	-3.886062000	-1.339171000	2.353625000
H	-2.201533000	-0.959802000	2.786354000
H	-3.538962000	-0.048887000	3.520039000
C	-0.893209000	-1.072133000	0.309492000
C	-1.998452000	1.253268000	-1.138483000
H	-2.852209000	1.938813000	-1.219116000
H	-1.714834000	0.867287000	-2.126016000
H	-1.113203000	1.763723000	-0.737839000
H	-0.009992000	-0.973096000	-1.950435000

Activation of SiH₄

TS-1 (SiH₄): E= -1474.600396

C	0.232770000	-0.368487000	-0.868324000
H	0.233807000	-1.374824000	-1.305859000
H	0.241067000	0.340881000	-1.711210000
P	1.776656000	-0.166957000	0.114733000
B	-1.149517000	-0.130784000	0.007671000
C	2.520336000	1.512542000	-0.294978000
C	2.979564000	-1.596663000	-0.214639000
C	2.200556000	-2.872758000	-0.567117000
H	1.428963000	-3.109694000	0.177182000
H	1.731486000	-2.804241000	-1.558519000
H	2.913347000	-3.711887000	-0.597303000
C	3.744203000	-1.831147000	1.096666000
H	4.290785000	-0.934805000	1.423083000
H	3.061119000	-2.135264000	1.904760000
H	4.477505000	-2.641148000	0.955872000
C	3.967753000	-1.326743000	-1.353309000
H	4.572463000	-2.234352000	-1.511263000
H	3.450923000	-1.102215000	-2.297342000
H	4.660466000	-0.506015000	-1.125793000
C	1.462267000	2.563030000	0.080758000
H	0.581998000	2.514428000	-0.574985000
H	1.115988000	2.461591000	1.117714000
H	1.913181000	3.561283000	-0.037034000
C	3.758532000	1.723677000	0.583958000
H	3.512728000	1.611518000	1.651262000
H	4.574935000	1.029487000	0.339016000
H	4.137473000	2.746764000	0.432651000
C	2.862781000	1.702913000	-1.777217000
H	3.741511000	1.131435000	-2.094028000
H	2.016223000	1.436316000	-2.427468000

H	3.080480000	2.769348000	-1.948604000
C	-1.703807000	1.373332000	0.012118000
C	-1.982897000	1.990442000	-1.219797000
C	-1.972152000	2.112664000	1.171683000
H	-1.810939000	1.438897000	-2.149758000
H	-1.781008000	1.664819000	2.150849000
C	-2.483719000	3.289494000	-1.292818000
C	-2.467195000	3.416386000	1.111073000
H	-2.691148000	3.740564000	-2.265296000
H	-2.657611000	3.968323000	2.033535000
C	-2.719106000	4.012726000	-0.122950000
H	-3.103624000	5.032774000	-0.174515000
C	-4.591959000	-1.985119000	-0.204553000
C	-4.211259000	-3.320334000	-0.330126000
C	-3.622500000	-0.988068000	-0.101364000
H	-4.967509000	-4.103390000	-0.410477000
H	-3.937467000	0.053242000	0.000863000
C	-2.855889000	-3.647875000	-0.355401000
C	-2.250418000	-1.288787000	-0.131634000
H	-2.547077000	-4.690575000	-0.450882000
C	-1.894954000	-2.641978000	-0.263645000
H	-0.838466000	-2.923130000	-0.286825000
H	-5.650646000	-1.719069000	-0.185588000
H	-0.921796000	-0.290415000	1.431515000
Si	0.486225000	-0.509330000	2.165720000
H	0.512125000	-1.921268000	1.591012000
H	0.519116000	-0.959381000	3.614173000
H	0.592753000	0.973406000	2.459526000

TS-2a(SiH4): E= -2089.406486

C	-1.565959000	-0.129455000	-0.545063000
H	-1.372977000	0.505621000	-1.422482000
H	-1.511862000	-1.171296000	-0.895046000
P	-3.325343000	0.093051000	0.005458000
B	-0.264389000	0.044986000	0.495658000
C	0.775414000	1.252185000	0.248054000
C	0.704671000	-1.239925000	0.450922000
C	-4.235409000	-1.451875000	-0.580520000
C	-4.008075000	1.682925000	-0.750911000
C	1.945767000	-0.803515000	0.122536000
C	1.999789000	0.699500000	0.054627000
C	0.467537000	2.697108000	0.353789000
C	0.347551000	3.516936000	-0.777329000
C	0.214093000	3.269922000	1.610050000
C	-0.010768000	4.859435000	-0.660620000
H	0.516434000	3.083355000	-1.765849000
C	-0.144052000	4.610637000	1.730756000
H	0.304385000	2.647061000	2.503316000
C	-0.261514000	5.411412000	0.594272000
H	-0.096247000	5.476762000	-1.556911000
H	-0.329122000	5.034434000	2.719486000
H	-0.541617000	6.461751000	0.687763000
C	3.291495000	1.426169000	-0.050343000
C	3.514768000	2.420067000	-1.011506000
C	4.331732000	1.112211000	0.837672000
C	4.734989000	3.092068000	-1.074246000
H	2.729020000	2.654566000	-1.728896000
C	5.548535000	1.785251000	0.779076000
H	4.177231000	0.326471000	1.580356000
C	5.754516000	2.779934000	-0.177928000
H	4.889109000	3.861654000	-1.832550000

H	6.342937000	1.530223000	1.482380000
H	6.709551000	3.305469000	-0.227427000
C	0.237691000	-2.643038000	0.483129000
C	-0.228397000	-3.218629000	1.675685000
C	0.164291000	-3.406213000	-0.693096000
C	-0.752424000	-4.509379000	1.693093000
H	-0.175578000	-2.637604000	2.599182000
C	-0.369429000	-4.694995000	-0.678969000
H	0.537872000	-2.973928000	-1.624469000
C	-0.832788000	-5.250424000	0.513140000
H	-1.105295000	-4.938041000	2.632938000
H	-0.417871000	-5.270498000	-1.605246000
H	-1.248694000	-6.259074000	0.524866000
C	3.106407000	-1.660547000	-0.220811000
C	3.413852000	-2.806277000	0.527430000
C	3.909414000	-1.351555000	-1.329869000
C	4.489949000	-3.618748000	0.175306000
H	2.801280000	-3.054547000	1.395923000
C	4.980432000	-2.166723000	-1.685011000
H	3.686861000	-0.460504000	-1.919589000
C	5.276412000	-3.302966000	-0.932136000
H	4.717503000	-4.503627000	0.772176000
H	5.589876000	-1.910307000	-2.553202000
H	6.120178000	-3.938480000	-1.205985000
C	-2.906528000	2.752465000	-0.746418000
H	-2.450182000	2.910686000	0.240749000
H	-2.102017000	2.510112000	-1.452305000
H	-3.349572000	3.708425000	-1.069486000
C	-5.160726000	2.150810000	0.148267000
H	-5.979285000	1.419305000	0.195337000
H	-4.806336000	2.337977000	1.172866000
H	-5.572159000	3.093574000	-0.246307000
C	-4.489022000	1.517792000	-2.195263000
H	-4.802285000	2.504175000	-2.574321000
H	-3.684957000	1.151091000	-2.850502000
H	-5.349997000	0.842233000	-2.283525000
C	-3.717572000	-2.619813000	0.275370000
H	-2.631828000	-2.774816000	0.173727000
H	-3.944191000	-2.475218000	1.340974000
H	-4.216461000	-3.543412000	-0.059255000
C	-5.736174000	-1.286798000	-0.314764000
H	-5.930525000	-1.020584000	0.735456000
H	-6.197817000	-0.525438000	-0.958413000
H	-6.242918000	-2.243399000	-0.517850000
C	-3.986378000	-1.789403000	-2.054786000
H	-4.377093000	-1.028127000	-2.739520000
H	-2.917088000	-1.935774000	-2.264663000
H	-4.495128000	-2.739621000	-2.284978000
H	-0.485274000	0.202720000	1.819208000
Si	-2.128114000	0.213949000	2.162125000
H	-2.329703000	0.295620000	3.654634000
H	-2.139052000	-1.266972000	1.982843000
H	-2.147978000	1.672727000	1.833194000

TS-2b(SiH4): E= -4072.093681

C	2.133117000	-1.263437000	-0.588429000
H	1.666875000	-2.054528000	-1.189460000
H	2.353690000	-0.451868000	-1.295682000
C	-0.580200000	-1.191437000	0.185438000
C	0.694878000	0.931805000	0.312164000
C	5.089658000	-0.761071000	-0.620590000

C	3.900450000	-3.665890000	-0.800050000
C	-0.608315000	1.155768000	0.042650000
C	-1.382064000	-0.117404000	0.021478000
C	-1.087570000	-2.565850000	0.352115000
C	-0.839556000	-3.565851000	-0.587350000
C	-1.828732000	-2.925165000	1.481123000
C	-1.255757000	-4.878771000	-0.401114000
C	-2.265055000	-4.231385000	1.689304000
C	-1.974334000	-5.212008000	0.744933000
C	-2.854669000	-0.157342000	-0.084392000
C	-3.501202000	-0.945908000	-1.038000000
C	-3.651375000	0.591029000	0.784443000
C	-4.889391000	-0.990644000	-1.125593000
C	-5.040356000	0.565998000	0.711833000
C	-5.659339000	-0.230976000	-0.247798000
C	1.745753000	1.965684000	0.351924000
C	2.256469000	2.432319000	1.565950000
C	2.331100000	2.451105000	-0.816739000
C	3.303718000	3.346615000	1.617605000
C	3.391810000	3.352975000	-0.792647000
C	3.874553000	3.805900000	0.431395000
C	-1.235692000	2.463404000	-0.239834000
C	-1.121629000	3.542340000	0.639005000
C	-1.994102000	2.650987000	-1.397607000
C	-1.728167000	4.766626000	0.373602000
C	-2.613040000	3.863913000	-1.681528000
C	-2.475969000	4.925654000	-0.790322000
C	2.664885000	-4.487174000	-0.393755000
H	2.617499000	-4.642449000	0.692454000
H	1.722471000	-4.039898000	-0.731462000
H	2.742432000	-5.476579000	-0.871368000
C	5.126295000	-4.410584000	-0.250256000
H	6.076688000	-4.004486000	-0.611879000
H	5.138229000	-4.402250000	0.849969000
H	5.073268000	-5.461111000	-0.576221000
C	3.962579000	-3.574265000	-2.326287000
H	3.939436000	-4.591140000	-2.750260000
H	3.102294000	-3.024578000	-2.738084000
H	4.887025000	-3.092372000	-2.673635000
C	5.166300000	0.393296000	0.388176000
H	4.207143000	0.920237000	0.472883000
H	5.459223000	0.045776000	1.389734000
H	5.919208000	1.118841000	0.038860000
C	6.456043000	-1.455099000	-0.647777000
H	6.676797000	-1.969358000	0.299399000
H	6.539310000	-2.176537000	-1.471405000
H	7.231859000	-0.689318000	-0.802562000
C	4.784926000	-0.173183000	-2.004542000
H	4.551384000	-0.938731000	-2.755856000
H	3.956588000	0.548219000	-1.976885000
H	5.673153000	0.379932000	-2.350010000
F	1.751894000	1.982554000	2.703142000
F	3.771391000	3.771625000	2.778255000
F	4.884971000	4.655141000	0.470576000
F	3.955022000	3.755513000	-1.919509000
F	1.915192000	2.007588000	-1.999271000
F	-0.445923000	3.413640000	1.770201000
F	-2.126933000	1.658031000	-2.267465000
F	-3.314405000	4.019998000	-2.790107000
F	-3.054512000	6.081771000	-1.051025000
F	-1.609806000	5.772395000	1.222323000

F	-3.082420000	1.337484000	1.721348000
F	-5.772162000	1.273598000	1.554105000
F	-6.975607000	-0.270223000	-0.323126000
F	-5.481782000	-1.741551000	-2.037403000
F	-2.797616000	-1.665892000	-1.899030000
F	-2.115946000	-2.013926000	2.399390000
F	-2.946960000	-4.546226000	2.777205000
F	-2.374717000	-6.455252000	0.935516000
F	-0.975047000	-5.805661000	-1.301218000
F	-0.181613000	-3.274134000	-1.706329000
H	3.089874000	-0.227119000	1.930939000
Si	2.429231000	-1.547582000	2.103521000
H	2.451763000	-1.706089000	3.594561000
H	1.860516000	-2.856558000	1.670782000
H	0.954920000	-0.832097000	1.721717000
B	0.929417000	-0.659549000	0.401343000
P	3.764582000	-1.962143000	0.012538000

TS-3(SiH4): E= -1550.668153

H	-0.903993000	-0.014727000	-1.716425000
H	-1.008146000	-1.661353000	-1.066347000
C	1.582820000	0.564668000	0.061431000
C	1.817659000	-0.760195000	0.042464000
C	-3.848185000	-1.335781000	-0.639095000
C	-2.879135000	1.580725000	-0.015653000
C	2.278881000	1.846444000	-0.043578000
C	3.329051000	2.019121000	-0.960493000
C	1.898335000	2.936814000	0.753837000
C	3.978848000	3.245196000	-1.074475000
H	3.620118000	1.178841000	-1.594647000
C	2.563163000	4.156788000	0.652694000
H	1.083994000	2.809583000	1.469078000
C	3.602288000	4.316871000	-0.263986000
H	4.786061000	3.365450000	-1.799050000
H	2.265625000	4.990676000	1.290825000
H	4.116217000	5.275633000	-0.348848000
C	2.891908000	-1.745250000	-0.007909000
C	2.569360000	-3.109735000	-0.060107000
C	4.245699000	-1.371325000	0.024137000
C	3.570729000	-4.076423000	-0.096884000
H	1.515147000	-3.394927000	-0.062867000
C	5.246177000	-2.338051000	-0.007914000
H	4.502301000	-0.311988000	0.086778000
C	4.911463000	-3.692176000	-0.073129000
H	3.306874000	-5.134506000	-0.138404000
H	6.294624000	-2.036394000	0.020672000
H	5.697941000	-4.448303000	-0.099976000
C	-1.554928000	2.310856000	0.257200000
H	-1.125156000	2.011016000	1.223386000
H	-0.803258000	2.121228000	-0.521245000
H	-1.753807000	3.393936000	0.287715000
C	-3.885148000	1.970131000	1.076532000
H	-4.870342000	1.510038000	0.927778000
H	-3.512402000	1.689996000	2.072564000
H	-4.021495000	3.063128000	1.060507000
C	-3.397851000	1.988342000	-1.396665000
H	-3.472335000	3.086910000	-1.436120000
H	-2.715130000	1.672597000	-2.199730000
H	-4.397373000	1.581565000	-1.603463000
C	-3.595362000	-2.775921000	-0.167142000
H	-2.604440000	-3.145917000	-0.465771000

H	-3.673624000	-2.868507000	0.925540000
H	-4.354765000	-3.430204000	-0.623958000
C	-5.234969000	-0.905871000	-0.149985000
H	-5.286870000	-0.876890000	0.949070000
H	-5.529619000	0.077453000	-0.541051000
H	-5.977735000	-1.638696000	-0.502508000
C	-3.790627000	-1.303049000	-2.170912000
H	-4.017276000	-0.310987000	-2.580707000
H	-2.806612000	-1.617821000	-2.546401000
H	-4.538698000	-2.007954000	-2.567870000
H	-0.067918000	-0.497216000	1.603008000
H	-1.334470000	-2.240045000	1.402688000
Si	-1.499411000	-0.932521000	2.187986000
H	-1.664671000	0.481542000	2.755995000
H	-1.938258000	-1.622732000	3.469806000
B	0.360232000	-0.345388000	0.125620000
C	-0.958264000	-0.598736000	-0.783497000
P	-2.511427000	-0.253924000	0.124590000

add-1 (SiH4): E= -1474.650702

C	-0.054416000	-0.676380000	-0.576964000
H	-0.148433000	-1.762251000	-0.703972000
H	-0.141328000	-0.228730000	-1.576676000
P	1.613268000	-0.382812000	0.048339000
B	-1.269206000	-0.159179000	0.462759000
C	2.411485000	1.111702000	-0.791037000
C	2.604778000	-1.976437000	-0.146039000
C	1.743714000	-3.127457000	0.406117000
H	1.370170000	-2.925312000	1.421141000
H	0.885637000	-3.361176000	-0.235945000
H	2.373057000	-4.029295000	0.454674000
C	3.910870000	-1.950871000	0.659739000
H	4.584793000	-1.136407000	0.373565000
H	3.718851000	-1.880881000	1.741070000
H	4.441747000	-2.900038000	0.487245000
C	2.881401000	-2.231838000	-1.631537000
H	3.325488000	-3.233238000	-1.745408000
H	1.953070000	-2.208226000	-2.222003000
H	3.586622000	-1.504415000	-2.056254000
C	1.893531000	2.379070000	-0.090913000
H	0.796603000	2.420565000	-0.041115000
H	2.301950000	2.477485000	0.926758000
H	2.237085000	3.252654000	-0.666884000
C	3.938666000	1.089464000	-0.669410000
H	4.266984000	1.024777000	0.378099000
H	4.400399000	0.272345000	-1.239565000
H	4.324829000	2.036590000	-1.076977000
C	2.000766000	1.160537000	-2.268483000
H	2.215449000	0.225500000	-2.805101000
H	0.932930000	1.394783000	-2.374780000
H	2.566622000	1.968636000	-2.757379000
C	-1.493149000	1.438891000	0.302343000
C	-1.613645000	2.039174000	-0.965606000
C	-1.560111000	2.304791000	1.404911000
H	-1.607797000	1.404163000	-1.858909000
H	-1.504231000	1.878021000	2.410642000
C	-1.750122000	3.417777000	-1.129933000
C	-1.689442000	3.688116000	1.259937000
H	-1.840408000	3.844363000	-2.131619000
H	-1.725904000	4.328752000	2.143883000
C	-1.772807000	4.253427000	-0.011929000

H	-1.869588000	5.334015000	-0.132171000
C	-4.879348000	-1.344398000	-0.674227000
C	-4.825507000	-2.713523000	-0.424353000
C	-3.777818000	-0.531888000	-0.390953000
H	-5.684612000	-3.350352000	-0.644177000
H	-3.848135000	0.541295000	-0.587460000
C	-3.660842000	-3.260177000	0.118365000
C	-2.590414000	-1.052126000	0.144375000
H	-3.608077000	-4.330275000	0.331892000
C	-2.571705000	-2.436552000	0.394306000
H	-1.672093000	-2.881194000	0.836007000
H	-5.787277000	-0.902706000	-1.091133000
H	-0.889888000	-0.421445000	1.620302000
Si	1.593657000	0.083776000	2.290910000
H	1.255560000	-1.149693000	3.034950000
H	3.015392000	0.437019000	2.573417000
H	0.735039000	1.242078000	2.590000000

add-2a (SiH4): E= -2089.465367

C	1.461158000	0.126978000	0.671747000
H	1.439419000	1.017851000	1.321504000
H	1.310696000	-0.751817000	1.316587000
P	3.142534000	0.013187000	0.024261000
B	0.243138000	0.173133000	-0.476932000
C	-0.873222000	1.315903000	-0.189948000
C	-0.706004000	-1.143968000	-0.392047000
C	4.088240000	-1.298709000	0.984804000
C	3.941869000	1.712327000	0.042927000
C	-1.989865000	-0.753371000	-0.182757000
C	-2.096825000	0.738051000	-0.091347000
C	-0.558292000	2.758367000	-0.151386000
C	-0.303704000	3.408919000	1.067842000
C	-0.368282000	3.488078000	-1.335707000
C	0.132474000	4.733560000	1.103810000
H	-0.444998000	2.855107000	1.999881000
C	0.065835000	4.811488000	-1.302030000
H	-0.556880000	2.992848000	-2.290395000
C	0.325464000	5.439942000	-0.082707000
H	0.321020000	5.216806000	2.064681000
H	0.202906000	5.358951000	-2.236771000
H	0.666626000	6.476184000	-0.058339000
C	-3.401204000	1.442894000	-0.006830000
C	-3.628905000	2.456005000	0.935073000
C	-4.444560000	1.107843000	-0.884303000
C	-4.853416000	3.119836000	0.992796000
H	-2.836181000	2.716022000	1.636546000
C	-5.667488000	1.770993000	-0.828781000
H	-4.287637000	0.314170000	-1.617643000
C	-5.877641000	2.780980000	0.110959000
H	-5.007851000	3.903693000	1.736569000
H	-6.463799000	1.496133000	-1.522677000
H	-6.837376000	3.298394000	0.157631000
C	-0.228043000	-2.538521000	-0.299746000
C	0.330332000	-3.214263000	-1.396598000
C	-0.260855000	-3.211949000	0.934560000
C	0.853327000	-4.500292000	-1.264248000
H	0.325000000	-2.720073000	-2.370352000
C	0.262447000	-4.497342000	1.070418000
H	-0.719085000	-2.709646000	1.789980000
C	0.831578000	-5.144786000	-0.026632000
H	1.273970000	-5.006737000	-2.135569000

H	0.220627000	-4.998962000	2.039269000
H	1.240742000	-6.150976000	0.078155000
C	-3.140533000	-1.671696000	0.007946000
C	-3.312223000	-2.772372000	-0.844400000
C	-4.069032000	-1.484051000	1.044066000
C	-4.366905000	-3.663700000	-0.663809000
H	-2.605508000	-2.919210000	-1.662553000
C	-5.123390000	-2.376448000	1.226894000
H	-3.959735000	-0.625804000	1.710289000
C	-5.276987000	-3.470035000	0.374565000
H	-4.480411000	-4.511603000	-1.341617000
H	-5.833338000	-2.214810000	2.040020000
H	-6.105244000	-4.166230000	0.516742000
C	2.910892000	2.689924000	-0.542383000
H	2.556422000	2.381920000	-1.536912000
H	2.031549000	2.805734000	0.103535000
H	3.386105000	3.678425000	-0.641762000
C	5.200480000	1.744044000	-0.834219000
H	5.970676000	1.031760000	-0.514769000
H	4.966248000	1.557918000	-1.893050000
H	5.633196000	2.754670000	-0.775581000
C	4.284147000	2.134884000	1.475248000
H	4.600623000	3.189365000	1.461111000
H	3.414108000	2.061696000	2.144756000
H	5.109529000	1.544015000	1.897728000
C	3.522217000	-2.649838000	0.514797000
H	2.424628000	-2.703416000	0.592107000
H	3.805355000	-2.877395000	-0.524857000
H	3.938710000	-3.447616000	1.149241000
C	5.593886000	-1.251141000	0.712063000
H	5.825354000	-1.298169000	-0.361863000
H	6.060591000	-0.350887000	1.135928000
H	6.062586000	-2.124194000	1.192255000
C	3.833172000	-1.145599000	2.490218000
H	4.183694000	-0.181626000	2.881344000
H	2.770445000	-1.258687000	2.741105000
H	4.384001000	-1.941492000	3.015193000
H	0.713986000	0.342141000	-1.615920000
Si	3.187719000	-0.627259000	-2.173902000
H	4.598890000	-1.050039000	-2.396235000
H	2.281293000	-1.766873000	-2.386512000
H	2.896432000	0.543020000	-3.028518000

add-2b(SiH4): E= -4072.157799

C	-1.942470000	1.397685000	-0.701058000
H	-1.467421000	2.108448000	-1.392544000
H	-2.261241000	0.539066000	-1.310319000
P	-3.448078000	2.192526000	-0.096893000
B	-0.889335000	0.868510000	0.484463000
C	0.695437000	1.185581000	0.241220000
C	-0.817186000	-0.757877000	0.420329000
C	-4.897467000	1.627090000	-1.150184000
C	-3.183694000	4.047583000	-0.064937000
C	0.453420000	-1.147736000	0.182244000
C	1.367487000	0.014598000	0.128234000
C	1.437432000	2.461205000	0.319394000
C	1.287650000	3.469645000	-0.633532000
C	2.365191000	2.703234000	1.339115000
C	1.987475000	4.668573000	-0.577258000
C	3.085405000	3.893185000	1.418221000
C	2.897198000	4.879951000	0.454840000

C	2.832305000	-0.141760000	0.010182000
C	3.564377000	0.497729000	-0.992109000
C	3.536293000	-0.952450000	0.902723000
C	4.944473000	0.352095000	-1.094999000
C	4.913925000	-1.123377000	0.812232000
C	5.619473000	-0.464508000	-0.191540000
C	-1.947556000	-1.702247000	0.343531000
C	-2.680667000	-2.084987000	1.468575000
C	-2.347214000	-2.243244000	-0.882481000
C	-3.785392000	-2.926879000	1.380431000
C	-3.442252000	-3.096394000	-0.997778000
C	-4.164335000	-3.439940000	0.141924000
C	0.900535000	-2.533087000	-0.071720000
C	0.623988000	-3.569113000	0.822973000
C	1.615750000	-2.855888000	-1.227330000
C	1.039572000	-4.875012000	0.580885000
C	2.047148000	-4.152826000	-1.487210000
C	1.755032000	-5.165997000	-0.577809000
C	-1.824362000	4.274350000	0.613118000
H	-1.782175000	3.851485000	1.626836000
H	-1.013449000	3.833838000	0.024985000
H	-1.647424000	5.358680000	0.683241000
C	-4.272130000	4.756615000	0.750454000
H	-5.275010000	4.644290000	0.321029000
H	-4.296088000	4.413486000	1.796117000
H	-4.038457000	5.832146000	0.771626000
C	-3.132225000	4.605333000	-1.491308000
H	-2.859220000	5.670582000	-1.440981000
H	-2.368052000	4.099932000	-2.100495000
H	-4.103532000	4.533786000	-2.000544000
C	-5.227067000	0.199847000	-0.678512000
H	-4.333950000	-0.443411000	-0.637991000
H	-5.704643000	0.195342000	0.313593000
H	-5.935259000	-0.256604000	-1.387101000
C	-6.131407000	2.515695000	-0.971638000
H	-6.416817000	2.627906000	0.084498000
H	-5.986716000	3.513794000	-1.408002000
H	-6.977264000	2.044863000	-1.496115000
C	-4.491360000	1.586606000	-2.630284000
H	-4.152192000	2.562435000	-3.002194000
H	-3.699583000	0.849648000	-2.819683000
H	-5.370791000	1.288388000	-3.221511000
H	-1.214049000	1.279115000	1.603816000
Si	-3.925032000	1.602397000	2.064272000
H	-5.362215000	1.948411000	2.228470000
H	-3.717874000	0.154883000	2.232552000
H	-3.108577000	2.428684000	2.977093000
F	-2.334767000	-1.635944000	2.664880000
F	-4.470984000	-3.249906000	2.465116000
F	-5.208878000	-4.243849000	0.048792000
F	-3.804660000	-3.573385000	-2.177972000
F	-1.698787000	-1.913871000	-1.995184000
F	-0.037934000	-3.325549000	1.944751000
F	0.769073000	-5.838098000	1.445817000
F	2.151934000	-6.402356000	-0.815817000
F	2.711357000	-4.433168000	-2.596120000
F	1.883009000	-1.914689000	-2.123112000
F	2.889301000	-1.571880000	1.880809000
F	5.556967000	-1.891422000	1.675209000
F	6.927843000	-0.612764000	-0.286872000
F	5.618014000	0.969107000	-2.052080000

F	2.950815000	1.258127000	-1.887873000
F	2.579762000	1.790832000	2.276198000
F	3.947766000	4.092526000	2.401267000
F	3.571137000	6.014423000	0.523737000
F	1.798558000	5.603322000	-1.496396000
F	0.435319000	3.304892000	-1.647233000

add-3 (SiH4): E= -1550.711102

H	0.929914000	-1.931936000	-0.874086000
H	0.510390000	-0.336004000	-1.544864000
P	2.346468000	-0.226403000	-0.010080000
B	-0.385172000	-0.607477000	0.544382000
C	-1.905791000	-0.804065000	0.210226000
C	-1.531448000	0.467901000	0.295795000
C	3.225756000	0.733583000	-1.367133000
C	3.367848000	-1.630246000	0.706022000
C	-3.069038000	-1.637609000	-0.074843000
C	-4.233754000	-1.109761000	-0.661180000
C	-3.035644000	-3.011138000	0.213329000
C	-5.326347000	-1.926259000	-0.937074000
H	-4.263427000	-0.045980000	-0.906592000
C	-4.132632000	-3.827329000	-0.053461000
H	-2.126547000	-3.422866000	0.656653000
C	-5.282407000	-3.288111000	-0.630495000
H	-6.220519000	-1.499455000	-1.395502000
H	-4.090346000	-4.892073000	0.184309000
H	-6.140821000	-3.926744000	-0.846156000
C	-2.099366000	1.812950000	0.269141000
C	-1.376299000	2.902377000	-0.245904000
C	-3.385457000	2.065172000	0.782441000
C	-1.921278000	4.184340000	-0.272755000
H	-0.372120000	2.726676000	-0.637531000
C	-3.924900000	3.347938000	0.770310000
H	-3.952672000	1.231160000	1.201370000
C	-3.198436000	4.414609000	0.237168000
H	-1.343642000	5.011252000	-0.690683000
H	-4.922603000	3.518130000	1.179870000
H	-3.623931000	5.419241000	0.223365000
C	2.422905000	-2.505701000	1.544866000
H	1.943106000	-1.940494000	2.354745000
H	1.623999000	-2.955345000	0.940458000
H	3.019155000	-3.316895000	1.991052000
C	4.476667000	-1.093584000	1.620700000
H	5.181976000	-0.434184000	1.100126000
H	4.065270000	-0.553386000	2.486272000
H	5.046927000	-1.949148000	2.014808000
C	3.973666000	-2.478677000	-0.417140000
H	4.420288000	-3.381509000	0.027682000
H	3.212590000	-2.805070000	-1.141589000
H	4.770563000	-1.946863000	-0.956054000
C	2.396107000	2.012896000	-1.566253000
H	1.342452000	1.787623000	-1.790455000
H	2.432672000	2.675110000	-0.687365000
H	2.807300000	2.574403000	-2.419232000
C	4.660858000	1.111332000	-0.990976000
H	4.714453000	1.636953000	-0.026609000
H	5.320066000	0.233027000	-0.952170000
H	5.060271000	1.788212000	-1.762458000
C	3.219799000	-0.060858000	-2.679861000
H	3.823602000	-0.974771000	-2.622348000
H	2.201525000	-0.336306000	-2.985822000

H	3.648571000	0.573377000	-3.471525000
C	0.780423000	-0.869507000	-0.621939000
Si	1.944185000	1.229350000	1.723768000
H	3.187652000	2.054276000	1.774201000
H	1.841328000	0.480877000	2.993137000
H	0.784166000	2.085328000	1.412557000
H	0.071250000	-0.785604000	1.681077000

Additional calculations replacing the P'Bu₂ fragment by PPh₂

1-pph2: E= -1330.469690

H	-0.819371000	-0.505361000	-1.790065000
H	-0.174272000	-2.162423000	-1.532385000
P	-1.141958000	-1.284575000	0.512718000
B	1.220374000	-0.541183000	-0.874102000
C	1.455277000	0.995651000	-1.110705000
C	2.289963000	1.736441000	-0.253860000
C	0.781872000	1.699317000	-2.125728000
C	2.431446000	3.116340000	-0.392275000
C	0.940570000	3.072952000	-2.289553000
C	1.760589000	3.786343000	-1.414557000
C	2.389171000	-1.460825000	-0.372715000
C	3.735470000	-1.124529000	-0.612446000
C	2.132615000	-2.674611000	0.293883000
C	4.776278000	-1.956709000	-0.205466000
C	3.168556000	-3.499420000	0.725812000
C	4.493327000	-3.142136000	0.472877000
H	1.876313000	4.865654000	-1.530288000
H	0.417648000	3.591875000	-3.094908000
H	3.066088000	3.672026000	0.300368000
H	2.813559000	1.224906000	0.557565000
H	0.123066000	1.159739000	-2.810722000
H	1.100141000	-2.972583000	0.494300000
H	2.943515000	-4.427241000	1.254191000
H	5.307109000	-3.791861000	0.800440000
H	5.811184000	-1.680894000	-0.415120000
H	3.968158000	-0.198654000	-1.143296000
C	-0.832127000	0.396111000	1.214777000
C	0.013836000	0.488541000	2.324448000
C	-1.330422000	1.572550000	0.637484000
C	0.365358000	1.735292000	2.847356000
H	0.405970000	-0.425911000	2.777125000
C	-0.979029000	2.814951000	1.155879000
C	-0.130050000	2.897632000	2.262797000
H	1.026669000	1.794013000	3.713473000
H	0.145878000	3.873562000	2.666049000
C	-2.893170000	-1.111603000	-0.036119000
C	-3.847644000	-0.650770000	0.883556000
C	-3.326947000	-1.524235000	-1.301043000
C	-5.194306000	-0.585340000	0.538283000
H	-3.528203000	-0.327173000	1.877733000
C	-4.678720000	-1.465125000	-1.644579000
H	-2.607663000	-1.897656000	-2.032818000
C	-5.615474000	-0.993001000	-0.728849000
H	-5.920570000	-0.213275000	1.263029000
H	-4.998056000	-1.789145000	-2.636608000
H	-6.671391000	-0.943046000	-0.998768000
H	-1.362827000	3.725307000	0.692231000
H	-1.991003000	1.513866000	-0.231574000
C	-0.223847000	-1.142348000	-1.119292000

2a-pph2: E= -1945.268879

C	1.646936000	1.009760000	-0.991952000
H	2.229165000	0.317640000	-1.618037000
H	1.683934000	2.032240000	-1.404757000
P	2.471880000	1.131060000	0.686724000
B	0.163913000	0.575625000	-0.774949000
C	-0.437845000	-0.894814000	-0.786972000
C	-1.055947000	1.521043000	-0.399759000
C	-2.114075000	0.697506000	-0.189042000
C	-1.734462000	-0.767731000	-0.403079000
C	0.283510000	-2.154775000	-1.056804000
C	1.159267000	-2.233652000	-2.152354000
C	0.123104000	-3.296512000	-0.255727000
C	1.839636000	-3.413258000	-2.447313000
H	1.286471000	-1.360992000	-2.796441000
C	0.799140000	-4.476163000	-0.552664000
H	-0.533816000	-3.250196000	0.614468000
C	1.660063000	-4.541451000	-1.648519000
H	2.507148000	-3.451783000	-3.309901000
H	0.661839000	-5.350148000	0.086925000
H	2.189874000	-5.467475000	-1.878038000
C	-2.714214000	-1.857214000	-0.197391000
C	-2.910030000	-2.835342000	-1.183683000
C	-3.465467000	-1.927236000	0.984659000
C	-3.832511000	-3.859599000	-0.989426000
H	-2.326840000	-2.784614000	-2.105159000
C	-4.379488000	-2.959723000	1.182109000
H	-3.329797000	-1.164532000	1.753994000
C	-4.567674000	-3.926450000	0.194943000
H	-3.978203000	-4.611261000	-1.766814000
H	-4.953294000	-3.004106000	2.109004000
H	-5.290709000	-4.729502000	0.346104000
C	-1.094129000	2.999250000	-0.425493000
C	-0.103526000	3.755291000	0.219741000
C	-2.102779000	3.684259000	-1.124960000
C	-0.131102000	5.149109000	0.183965000
H	0.685269000	3.241859000	0.774289000
C	-2.125817000	5.074847000	-1.164770000
H	-2.874231000	3.111031000	-1.642827000
C	-1.141421000	5.814642000	-0.507522000
H	0.643936000	5.715921000	0.702756000
H	-2.917794000	5.586273000	-1.714702000
H	-1.161314000	6.905118000	-0.537942000
C	-3.487126000	1.111901000	0.174062000
C	-3.689534000	2.028923000	1.216399000
C	-4.603069000	0.614283000	-0.515007000
C	-4.974466000	2.439417000	1.559260000
H	-2.823433000	2.419316000	1.754112000
C	-5.887365000	1.036452000	-0.178731000
H	-4.461613000	-0.106231000	-1.322642000
C	-6.077013000	1.946408000	0.860746000
H	-5.115874000	3.151119000	2.373990000
H	-6.745339000	0.647149000	-0.728911000
H	-7.084184000	2.270076000	1.128063000
C	2.491745000	-0.638852000	1.213096000
C	1.685922000	-1.004876000	2.295941000
C	3.294216000	-1.610796000	0.599277000
C	1.689897000	-2.318483000	2.770537000
H	1.061812000	-0.249279000	2.780121000
C	3.305427000	-2.917354000	1.077853000

H	3.927305000	-1.336607000	-0.248761000
C	2.507797000	-3.270525000	2.168761000
H	1.062110000	-2.591819000	3.620364000
H	3.932940000	-3.667263000	0.593430000
H	2.520241000	-4.295907000	2.542926000
C	4.237925000	1.345602000	0.198318000
C	5.211514000	1.147724000	1.190187000
C	4.648399000	1.766553000	-1.070096000
C	6.559811000	1.349694000	0.913615000
H	4.905939000	0.820780000	2.187903000
C	6.001628000	1.978262000	-1.344721000
H	3.914907000	1.931915000	-1.860606000
C	6.959848000	1.768328000	-0.357325000
H	7.303902000	1.183811000	1.694434000
H	6.304793000	2.305804000	-2.340593000
H	8.016749000	1.930970000	-0.573805000

TS-1-pph2 (H2) : E= -1331.576374

H	-0.257638000	-0.590141000	1.676404000
H	-0.291642000	-2.094302000	0.726609000
H	-1.161068000	-0.752153000	-1.515553000
P	1.111393000	-0.562045000	-0.384798000
H	-0.107503000	-0.672295000	-1.535539000
B	-1.596195000	-0.446787000	-0.228281000
C	-1.669914000	1.162160000	-0.242058000
C	-1.220680000	1.963566000	-1.301055000
C	-2.128314000	1.827118000	0.909693000
C	-1.196851000	3.357206000	-1.211334000
C	-2.113502000	3.217052000	1.010860000
C	-1.637438000	3.989312000	-0.050726000
C	-2.990725000	-1.222035000	-0.066686000
C	-4.198633000	-0.592051000	-0.414137000
C	-3.076221000	-2.548033000	0.388300000
C	-5.424885000	-1.247973000	-0.316748000
C	-4.296831000	-3.214330000	0.493671000
C	-5.478783000	-2.564596000	0.140086000
H	-1.621105000	5.078163000	0.023964000
H	-2.478556000	3.702101000	1.918798000
H	-0.833600000	3.951281000	-2.052358000
H	-0.869882000	1.489344000	-2.223006000
H	-2.507770000	1.235218000	1.749151000
H	-2.166975000	-3.084426000	0.672720000
H	-4.326864000	-4.244541000	0.854301000
H	-6.436822000	-3.081427000	0.221669000
H	-6.343967000	-0.728536000	-0.595373000
H	-4.172801000	0.442281000	-0.767028000
C	1.754603000	1.098278000	-0.033465000
C	2.672212000	1.646943000	-0.940325000
C	1.315838000	1.860805000	1.052689000
C	3.146670000	2.942574000	-0.758315000
H	3.010234000	1.058837000	-1.797644000
C	1.784509000	3.162766000	1.223970000
C	2.698525000	3.704022000	0.321775000
H	3.859685000	3.363395000	-1.468842000
H	3.060320000	4.724465000	0.456447000
C	2.509204000	-1.707151000	-0.142768000
C	3.666978000	-1.344231000	0.555487000
C	2.397301000	-3.000758000	-0.670575000
C	4.695043000	-2.269949000	0.728586000
H	3.764214000	-0.336648000	0.965083000
C	3.424576000	-3.923410000	-0.490646000

H	1.503226000	-3.286088000	-1.231224000
C	4.575303000	-3.558159000	0.208637000
H	5.593614000	-1.982671000	1.276714000
H	3.329519000	-4.928271000	-0.904591000
H	5.381895000	-4.279921000	0.345276000
H	1.423266000	3.757805000	2.063845000
H	0.582890000	1.456173000	1.751424000
C	-0.311751000	-0.994633000	0.655439000

TS-2a-pph2 (H2) : E= -1946.383563

C	1.403863000	0.171112000	0.940313000
H	1.551046000	1.044190000	1.592475000
H	1.442258000	-0.733331000	1.566993000
H	0.514550000	0.439513000	-1.279527000
P	2.756211000	0.035914000	-0.280315000
H	1.446265000	0.020761000	-1.347839000
B	0.050871000	0.177789000	0.029893000
C	-1.162429000	1.208110000	0.196844000
C	-0.718523000	-1.217094000	-0.177974000
C	-2.048164000	-0.973808000	-0.078744000
C	-2.317756000	0.500823000	0.092670000
C	-1.041467000	2.677196000	0.319012000
C	-0.473363000	3.249890000	1.468495000
C	-1.437466000	3.531771000	-0.720760000
C	-0.300071000	4.629727000	1.573369000
H	-0.178585000	2.598033000	2.294442000
C	-1.260986000	4.909970000	-0.618854000
H	-1.886694000	3.097609000	-1.616172000
C	-0.689122000	5.465507000	0.526442000
H	0.135898000	5.054171000	2.479806000
H	-1.574295000	5.556707000	-1.440336000
H	-0.555216000	6.545600000	0.605895000
C	-3.683652000	1.077620000	0.051523000
C	-4.079478000	2.078794000	0.950057000
C	-4.603579000	0.646325000	-0.917065000
C	-5.355711000	2.633633000	0.880542000
H	-3.375530000	2.419475000	1.711217000
C	-5.876568000	1.205258000	-0.989672000
H	-4.312554000	-0.137418000	-1.619192000
C	-6.258388000	2.200144000	-0.090042000
H	-5.647289000	3.409554000	1.590361000
H	-6.575865000	0.858422000	-1.752286000
H	-7.258016000	2.634454000	-0.144245000
C	-0.060582000	-2.532474000	-0.338248000
C	0.551212000	-2.873622000	-1.556917000
C	0.016660000	-3.449763000	0.720316000
C	1.197120000	-4.098477000	-1.719010000
H	0.495877000	-2.170134000	-2.391447000
C	0.675227000	-4.669516000	0.563344000
H	-0.458579000	-3.199019000	1.670949000
C	1.264393000	-5.001427000	-0.656694000
H	1.652315000	-4.348024000	-2.679213000
H	0.719786000	-5.369954000	1.399243000
H	1.768403000	-5.961248000	-0.781820000
C	-3.120858000	-1.997092000	-0.035684000
C	-3.148321000	-3.075909000	-0.930957000
C	-4.123507000	-1.913995000	0.943058000
C	-4.150570000	-4.041540000	-0.849591000
H	-2.377216000	-3.150334000	-1.699617000
C	-5.120045000	-2.881666000	1.027818000
H	-4.116264000	-1.077212000	1.644097000

C	-5.139076000	-3.948537000	0.129251000
H	-4.159396000	-4.872003000	-1.557543000
H	-5.888552000	-2.799614000	1.798185000
H	-5.923518000	-4.704528000	0.191715000
C	3.456996000	1.694638000	-0.532390000
C	4.678198000	1.848191000	-1.207651000
C	2.706376000	2.830972000	-0.205597000
C	5.152137000	3.119517000	-1.516829000
H	5.262730000	0.969008000	-1.489986000
C	3.180529000	4.102601000	-0.530244000
H	1.741231000	2.740206000	0.294766000
C	4.404219000	4.249560000	-1.178252000
H	6.108519000	3.229760000	-2.030287000
H	2.578375000	4.974827000	-0.270135000
H	4.776735000	5.244560000	-1.426476000
C	4.082292000	-1.054241000	0.330625000
C	5.259533000	-0.582642000	0.924456000
C	3.842938000	-2.433469000	0.258071000
C	6.193070000	-1.486845000	1.428703000
H	5.445639000	0.490499000	0.999373000
C	4.776790000	-3.330687000	0.771425000
H	2.920274000	-2.809325000	-0.192798000
C	5.953891000	-2.858998000	1.351922000
H	7.109547000	-1.115359000	1.889707000
H	4.578908000	-4.402109000	0.713217000
H	6.687109000	-3.562743000	1.749252000

add-1-pph2 (H2) : E= -1331.604723

H	-0.187640000	1.029981000	1.448762000
H	-0.254946000	-0.750257000	1.607685000
H	-1.179144000	0.695685000	-1.195257000
P	1.171107000	-0.015228000	-0.159541000
H	0.862004000	-0.781907000	-1.297643000
B	-1.531487000	0.040844000	-0.199059000
C	-2.814194000	0.748076000	0.483898000
C	-3.259587000	2.022071000	0.099643000
C	-3.511704000	0.124641000	1.533614000
C	-4.335499000	2.651823000	0.730909000
C	-4.585077000	0.741019000	2.174047000
C	-5.000961000	2.013087000	1.775171000
C	-1.795973000	-1.486892000	-0.692895000
C	-2.818378000	-1.718833000	-1.633390000
C	-1.066389000	-2.614862000	-0.284668000
C	-3.092840000	-2.986996000	-2.135301000
C	-1.325520000	-3.896864000	-0.783286000
C	-2.341295000	-4.087965000	-1.713929000
H	-5.843631000	2.498439000	2.271384000
H	-5.106377000	0.227575000	2.985226000
H	-4.659835000	3.641816000	0.402169000
H	-2.756507000	2.528755000	-0.730253000
H	-3.208291000	-0.879583000	1.847526000
H	-0.270317000	-2.516595000	0.463405000
H	-0.735759000	-4.747878000	-0.434559000
H	-2.552304000	-5.084593000	-2.105943000
H	-3.896606000	-3.123634000	-2.862005000
H	-3.416829000	-0.867490000	-1.971018000
C	1.689399000	1.635865000	-0.694334000
C	2.971761000	1.820450000	-1.225473000
C	0.807579000	2.717411000	-0.585667000
C	3.371575000	3.086862000	-1.644483000
H	3.663319000	0.978412000	-1.304568000

C	1.219022000	3.981990000	-1.002913000
C	2.496055000	4.166773000	-1.531396000
H	4.370354000	3.229835000	-2.058840000
H	2.811737000	5.158782000	-1.858022000
C	2.629653000	-0.838387000	0.527262000
C	3.384703000	-0.200029000	1.519538000
C	2.952049000	-2.138751000	0.126001000
C	4.462480000	-0.860469000	2.100687000
H	3.132221000	0.816820000	1.831376000
C	4.034278000	-2.795586000	0.712878000
H	2.356192000	-2.642566000	-0.639489000
C	4.786655000	-2.157532000	1.696822000
H	5.051367000	-0.363543000	2.872654000
H	4.287507000	-3.809236000	0.399873000
H	5.631553000	-2.673171000	2.155708000
H	0.532302000	4.824788000	-0.917416000
H	-0.200995000	2.569403000	-0.193428000
C	-0.247550000	0.083824000	0.892445000

add-2a-pph2 (H2) : E= -1946.423038

C	1.207834000	0.131386000	0.712637000
H	1.347509000	1.020653000	1.347084000
H	1.021337000	-0.740889000	1.356141000
H	0.534836000	0.675313000	-1.527460000
P	2.723319000	-0.125225000	-0.164920000
H	2.466611000	-0.892583000	-1.312334000
B	0.023106000	0.294310000	-0.464172000
C	-1.171105000	1.279547000	-0.019355000
C	-0.788015000	-1.098037000	-0.596023000
C	-2.093295000	-0.869805000	-0.293399000
C	-2.334481000	0.581012000	0.004966000
C	-0.963943000	2.729588000	0.174531000
C	-0.523641000	3.233888000	1.410207000
C	-1.061360000	3.623679000	-0.903723000
C	-0.190631000	4.579778000	1.563443000
H	-0.450743000	2.551905000	2.261572000
C	-0.732217000	4.969374000	-0.751123000
H	-1.395999000	3.243109000	-1.870570000
C	-0.290410000	5.454024000	0.481510000
H	0.144815000	4.948000000	2.534996000
H	-0.822368000	5.647670000	-1.601946000
H	-0.034785000	6.508321000	0.599885000
C	-3.689021000	1.156899000	0.196577000
C	-3.948549000	2.076639000	1.222715000
C	-4.741348000	0.807982000	-0.664587000
C	-5.215553000	2.636112000	1.379359000
H	-3.144131000	2.347496000	1.907804000
C	-6.006750000	1.368016000	-0.509824000
H	-4.558768000	0.087147000	-1.464184000
C	-6.249891000	2.284385000	0.513909000
H	-5.395105000	3.349576000	2.185634000
H	-6.810027000	1.085758000	-1.192641000
H	-7.242863000	2.720219000	0.637242000
C	-0.138889000	-2.413096000	-0.758583000
C	0.664256000	-2.690167000	-1.880712000
C	-0.218294000	-3.395509000	0.245102000
C	1.345825000	-3.901258000	-2.002429000
H	0.728657000	-1.940000000	-2.673348000
C	0.470933000	-4.601769000	0.130261000
H	-0.840535000	-3.197539000	1.120825000
C	1.255878000	-4.862875000	-0.994145000

H	1.946863000	-4.099082000	-2.892382000
H	0.387965000	-5.347337000	0.923389000
H	1.786416000	-5.811899000	-1.088731000
C	-3.146936000	-1.906315000	-0.164023000
C	-3.287344000	-2.923966000	-1.119109000
C	-4.012298000	-1.907209000	0.941408000
C	-4.256433000	-3.914425000	-0.970502000
H	-2.626683000	-2.927275000	-1.988275000
C	-4.979586000	-2.897623000	1.091198000
H	-3.919810000	-1.118211000	1.690463000
C	-5.106436000	-3.905616000	0.135182000
H	-4.352290000	-4.695674000	-1.726746000
H	-5.640241000	-2.881031000	1.959765000
H	-5.867729000	-4.679047000	0.250002000
C	3.434557000	1.451607000	-0.684581000
C	4.734002000	1.493316000	-1.207617000
C	2.671108000	2.621740000	-0.593537000
C	5.270170000	2.707232000	-1.627363000
H	5.330239000	0.580195000	-1.279278000
C	3.217486000	3.832896000	-1.016428000
H	1.647362000	2.600346000	-0.213758000
C	4.511876000	3.875734000	-1.530203000
H	6.282387000	2.741973000	-2.032076000
H	2.613804000	4.738734000	-0.945005000
H	4.934752000	4.825438000	-1.861824000
C	3.964286000	-1.108024000	0.708728000
C	4.985319000	-0.538673000	1.476612000
C	3.791688000	-2.498347000	0.675036000
C	5.845360000	-1.365480000	2.196827000
H	5.112690000	0.545905000	1.507185000
C	4.653778000	-3.316011000	1.401898000
H	2.982884000	-2.945291000	0.086120000
C	5.679945000	-2.750367000	2.158923000
H	6.646008000	-0.925740000	2.793007000
H	4.519652000	-4.398139000	1.374753000
H	6.354710000	-3.392769000	2.726781000

Hydrogenation of formaldehyde

CH₂O: E= -114.333352

O	0.671822000	0.000000000	0.000000000
C	-0.523049000	0.000000000	0.000000000
H	-1.118140000	0.943338000	0.000000000
H	-1.118145000	-0.943335000	0.000000000

TS-1 (CH₂O) E= -1298.412415

C	0.091478000	-0.604691000	-0.994117000
H	0.002425000	-1.665493000	-1.266392000
H	0.136211000	-0.033931000	-1.934777000
H	-0.862789000	-0.586886000	1.196519000
P	1.636357000	-0.415662000	-0.044850000
H	1.289157000	-0.158817000	1.390087000
B	-1.161083000	-0.068503000	-0.083234000
C	-2.578488000	-0.776128000	-0.287330000
C	-3.765575000	-0.106818000	0.059459000
C	-2.705297000	-2.099678000	-0.742700000
C	-5.012754000	-0.720304000	-0.051114000
C	-3.946549000	-2.724353000	-0.855328000
C	-5.107856000	-2.033327000	-0.511044000
C	-1.134914000	1.522526000	0.116198000
C	-1.611943000	2.313137000	-0.944997000

C	-0.592277000	2.194958000	1.224038000
C	-1.535943000	3.704348000	-0.917453000
C	-0.521825000	3.590845000	1.262656000
C	-0.986001000	4.350597000	0.191293000
H	-6.082280000	-2.517048000	-0.600179000
H	-4.009433000	-3.753791000	-1.213385000
H	-5.915427000	-0.171181000	0.223660000
H	-3.706824000	0.922872000	0.421379000
H	-1.812493000	-2.669010000	-1.016549000
H	-0.184494000	1.628164000	2.064907000
H	-0.093962000	4.084549000	2.137531000
H	-0.926223000	5.440035000	0.219484000
H	-1.910216000	4.288815000	-1.760429000
H	-2.055514000	1.822867000	-1.817825000
C	2.762289000	0.910836000	-0.740615000
C	2.420551000	-2.108959000	0.088019000
C	3.727245000	-2.012431000	0.883160000
H	4.090358000	-3.030685000	1.093585000
H	4.517785000	-1.487532000	0.328810000
H	3.569626000	-1.505933000	1.847741000
C	1.417227000	-2.936406000	0.913722000
H	1.269627000	-2.485055000	1.905284000
H	0.438474000	-3.024550000	0.416689000
H	1.821280000	-3.953211000	1.036947000
C	2.653790000	-2.784590000	-1.265688000
H	1.735861000	-2.825922000	-1.870223000
H	3.434348000	-2.290075000	-1.856308000
H	2.977235000	-3.822501000	-1.088619000
C	3.626815000	1.432431000	0.415436000
H	4.261282000	0.650607000	0.853827000
H	4.285424000	2.230546000	0.038628000
H	2.998472000	1.855113000	1.213175000
C	1.915320000	2.072027000	-1.280895000
H	1.260050000	2.511247000	-0.516812000
H	2.605107000	2.856069000	-1.630707000
H	1.293474000	1.773005000	-2.136064000
C	3.634835000	0.371025000	-1.877689000
H	3.027917000	-0.075067000	-2.680395000
H	4.200469000	1.208540000	-2.314994000
H	4.362770000	-0.374786000	-1.530333000
C	-0.616066000	-0.730611000	2.448485000
H	-0.918813000	-1.802782000	2.482709000
H	-1.440723000	-0.077950000	2.809186000
O	0.599690000	-0.416172000	2.730224000

TS-2a (CH2O) E= -1913.224170

C	-1.675096000	0.340804000	-1.080744000
H	-1.763681000	1.297672000	-1.612591000
H	-1.660654000	-0.462930000	-1.830967000
H	-0.637493000	0.565491000	1.143834000
P	-3.133768000	0.141731000	-0.010399000
H	-2.673300000	-0.219897000	1.403594000
C	-4.354708000	-1.106556000	-0.704779000
C	-3.856359000	1.845111000	0.274773000
C	-5.085487000	1.714160000	1.182956000
H	-5.409743000	2.721545000	1.487410000
H	-5.935184000	1.229423000	0.682120000
H	-4.839919000	1.150325000	2.095948000
C	-2.776947000	2.628116000	1.044214000
H	-2.583785000	2.157599000	2.017722000
H	-1.831907000	2.710864000	0.484727000

H	-3.147133000	3.651057000	1.216130000
C	-4.197664000	2.600540000	-1.012459000
H	-3.313013000	2.736723000	-1.651515000
H	-4.987777000	2.116841000	-1.599287000
H	-4.553018000	3.606509000	-0.739001000
C	-5.055526000	-1.752193000	0.498845000
H	-5.588347000	-1.014781000	1.115214000
H	-5.789905000	-2.489428000	0.137912000
H	-4.328114000	-2.274645000	1.137544000
C	-3.586987000	-2.189161000	-1.477101000
H	-2.757431000	-2.619747000	-0.900244000
H	-4.289492000	-3.003554000	-1.713081000
H	-3.193380000	-1.805907000	-2.429271000
C	-5.376545000	-0.476607000	-1.656117000
H	-4.885302000	0.028725000	-2.500965000
H	-6.007853000	-1.278572000	-2.070096000
H	-6.038919000	0.240858000	-1.154159000
C	-0.793633000	0.363378000	2.406375000
H	-0.560429000	1.413041000	2.693083000
H	0.082839000	-0.302118000	2.550900000
O	-1.974451000	-0.093384000	2.660706000
B	-0.310811000	0.229346000	-0.206644000
C	0.900959000	1.265803000	-0.309276000
C	0.435714000	-1.174068000	-0.043275000
C	1.770962000	-0.924341000	-0.088875000
C	2.051250000	0.553166000	-0.184541000
C	0.756483000	2.736296000	-0.311376000
C	0.116519000	3.388381000	-1.378036000
C	1.177560000	3.509607000	0.782032000
C	-0.104020000	4.764846000	-1.349920000
H	-0.189192000	2.804433000	-2.249437000
C	0.951255000	4.884069000	0.813676000
H	1.686002000	3.013819000	1.612198000
C	0.305737000	5.516898000	-0.249461000
H	-0.595280000	5.253597000	-2.193499000
H	1.280784000	5.466878000	1.675695000
H	0.129472000	6.593262000	-0.222809000
C	3.412061000	1.129190000	-0.063439000
C	3.831523000	2.167297000	-0.907823000
C	4.297672000	0.668988000	0.923324000
C	5.096982000	2.732525000	-0.766856000
H	3.152086000	2.528861000	-1.681781000
C	5.560147000	1.238777000	1.067758000
H	3.988594000	-0.143166000	1.584228000
C	5.965036000	2.271769000	0.222630000
H	5.407174000	3.538180000	-1.434316000
H	6.233121000	0.871337000	1.844202000
H	6.956087000	2.714920000	0.333877000
C	-0.206444000	-2.505200000	0.014378000
C	0.012650000	-3.466725000	-0.985288000
C	-0.630920000	-4.702202000	-0.941954000
H	0.699585000	-3.232598000	-1.801520000
H	-0.452366000	-5.433390000	-1.732497000
C	2.850390000	-1.940891000	-0.119865000
C	2.859422000	-3.031459000	0.761497000
C	3.881160000	-1.833803000	-1.065807000
C	3.869984000	-3.988811000	0.694596000
H	2.064004000	-3.122815000	1.503813000
C	4.886515000	-2.793981000	-1.136536000
H	3.888987000	-0.984505000	-1.751966000
C	4.885408000	-3.874673000	-0.254718000

H	3.864358000	-4.830056000	1.389644000
H	5.677177000	-2.695075000	-1.882093000
H	5.675933000	-4.625109000	-0.306200000
C	-1.088737000	-2.821252000	1.063450000
C	-1.715230000	-4.067177000	1.113658000
H	-1.294451000	-2.084769000	1.845361000
C	-1.495346000	-5.009913000	0.109764000
H	-2.384786000	-4.298287000	1.944751000
H	-1.992597000	-5.980500000	0.146880000

MeOH E= -115.519520

O	0.046520000	-0.750159000	0.000000000
C	0.046520000	0.651351000	0.000000000
H	-0.439157000	1.081836000	0.894279000
H	1.093131000	0.983597000	0.000000000
H	-0.439157000	1.081836000	-0.894279000
H	-0.866094000	-1.054105000	0.000000000

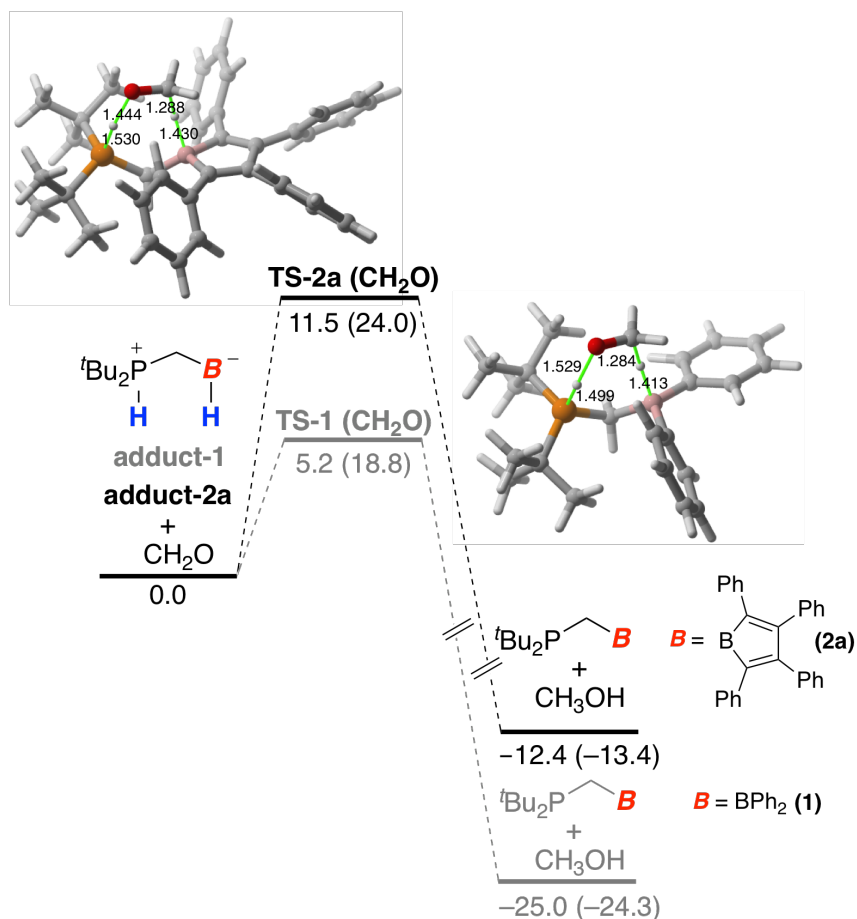


Figure S2. Comparative computed reaction profiles for the hydrogenation reaction of formaldehyde mediated by H₂-adducts derived for FLPs **1** and **2a**. Relative energies (free energies within parentheses) and bond distances are given in kcal/mol and angstroms, respectively. All data have been computed at the PCM(toluene)-M06-2X/def2-TZVPP//M06-2X/def2-SVP level.