Supplementary Information

Theoretical Mechanism for selective catalysis of Double Hydrophosphination of Terminal Arylacetylenes by an Iron Complex

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Full Gaussian 09 Reference

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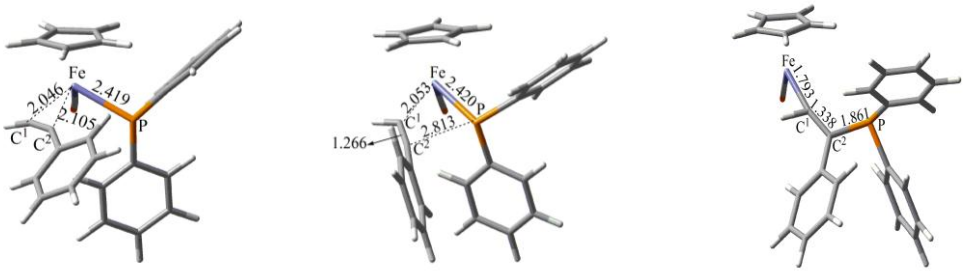
Cartesian coordinates of all structures:

All calculations were carried out using DFT as implemented in Gaussian 09. We chose to use the popular B3LYP functional, which includes Becke's three-parameter hybrid functional combined with the Lee−Yang−Parr correction for correlation. The standard 6-31G(d,p) basis set are used for H, C, O, and P atoms, while the effective core potentials (ECPs) of Hay and Wadt are combined with double-ζvalence basis sets (LanL2DZ) for Fe. Frequencies were analyzed at the same level to characterize the nature of stationary points (energy minima or first order saddle points) and to provide thermodynamic quantities. The intrinsic reaction coordinate (IRC) paths were also traced to verify the profiles that connect each transition state to correct associated local minima.

Solvent effect was calculated by using self-consistent reaction field (SCRF) method based on the integral equation formalism polarizabl continuum model (IEFPCM) model at M06/[LANL2DZ+6-311++G (d, p)] level of theory. Phenylacetylene was choosen as the solvent. For all cited energies, ZPE corrections were taken into consideration. The energies showed in the whole text were all calculated in this level.

Figure S1 Optimized structures of **Int4`**, **TS3`**and **Int5-2**. Bond lengths are in angstroms.



Int4`** **TS3` **Int5-2**

Table 1. Atom coordinates and absolute energy of **Cat-pre** (Energy= -583.389259043 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	-0.11450300	-0.00009600	0.04944400
C	-0.95279400	-0.00050800	1.91135300
H	-0.60721000	-0.89401100	2.43873100
H	-0.60771200	0.89328900	2.43860700
H	-2.04598600	-0.00061800	1.90505100
C	-1.22894700	1.30078000	-0.34831200
C	-1.22994700	-1.29989700	-0.34884100
O	-1.94899800	2.16956900	-0.58895200
O	-1.95088700	-2.16789200	-0.58972500
C	1.54055000	0.70590100	-1.14854200
C	1.54024000	-0.70658400	-1.14851100
C	1.69390400	-1.15183300	0.20958300
C	1.81224200	-0.00033900	1.03070100
C	1.69431000	1.15115600	0.20954600
H	1.42128800	1.34127500	-2.01535000
H	1.42092200	-1.34191300	-2.01534100
H	1.73540100	-2.17965900	0.54156900
H	1.90553900	-0.00031800	2.10734000
H	1.73657900	2.17899800	0.54138700

Table 2. Atom coordinates and absolute energy of **TS** (Energy= -583.364857172 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	-0.03431300	0.07184000	0.12350100
C	-1.69339800	-0.86881400	1.32441700

H	-1.73041700	-1.93856300	1.52727400
H	-0.94854900	-0.41056400	1.99411400
H	-2.65137900	-0.38939600	1.52492500
C	-0.77158000	1.67233500	0.01447300
C	-1.52271600	-0.77816700	-0.34675800
O	-1.20467800	2.73878700	-0.09217600
O	-2.31627400	-1.29385100	-1.06643300
C	1.70233200	0.60059200	-0.93598700
C	1.36206000	-0.74425400	-1.23932100
C	1.40107100	-1.48430100	-0.02121700
C	1.84018500	-0.60114700	1.02069800
C	2.03391600	0.67824100	0.46794200
H	1.75018900	1.41679800	-1.64349000
H	1.05427000	-1.11922800	-2.20507800
H	1.17747900	-2.53635300	0.09103500
H	1.95332400	-0.86419800	2.06441900
H	2.34360800	1.56725900	0.99916500

Table 3. Atom coordinates and absolute energy of **Fe-Cat** (Energy= -583.36497749 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	-0.02891700	0.07743000	0.14575700
C	-1.72668600	-0.88168400	1.29828300
H	-1.75350100	-1.94481400	1.53649800
H	-0.95581400	-0.40556100	1.93551800
H	-2.67386400	-0.39410300	1.53084700
C	-0.76602100	1.67674900	0.02102200
C	-1.53383100	-0.77962600	-0.31782800
O	-1.19753600	2.74269500	-0.09801900
O	-2.29271200	-1.28115900	-1.09025000
C	1.67820300	0.57278000	-0.97097700
C	1.33037800	-0.78007700	-1.22887900
C	1.40035200	-1.48617700	0.00703300
C	1.86750400	-0.57534700	1.01346100
C	2.04893600	0.68748900	0.42074700
H	1.70877600	1.36906500	-1.70174800
H	0.99416100	-1.18008800	-2.17491100
H	1.17917100	-2.53463300	0.15345400
H	2.00933000	-0.81034900	2.06035200
H	2.37256500	1.59037300	0.91927900

Table 4. Atom coordinates and absolute energy of **Ph_2PH** (Energy= -804.977286433 a.u.)

Atom	Coordinates (Angstroms) X	Y	Z
P	-0.04823900	1.66400600	-0.30351900
H	0.01884600	1.72128200	-1.72458100
C	-1.45897500	0.46327100	-0.15260300
C	-2.64161500	0.92922100	0.43864500
C	-1.40531800	-0.86691500	-0.59670500
C	-3.75195100	0.09192700	0.57152900
H	-2.69196300	1.95341000	0.79868200
C	-2.51060900	-1.70514500	-0.45900600
H	-0.49237000	-1.24947100	-1.04353600
C	-3.68752000	-1.22660200	0.12320900
H	-4.66157600	0.46896100	1.03028700
H	-2.45507000	-2.73299500	-0.80669500
H	-4.54744600	-1.88166000	0.22980600
C	1.43345300	0.58378100	-0.07796700
C	2.22504100	0.14530900	-1.15088100
C	1.82304600	0.23672700	1.22670600
C	3.37021200	-0.62176000	-0.92643900
H	1.94654900	0.40390700	-2.16876700
C	2.95733400	-0.54155300	1.45021600
H	1.23356900	0.57928100	2.07343500
C	3.73642900	-0.97092700	0.37334500
H	3.97178300	-0.95050300	-1.76924400
H	3.23911600	-0.80566700	2.46552800
H	4.62498900	-1.57064400	0.54757000

Table 5. Atom coordinates and absolute energy of **HC(O)Me** (Energy= -153.778476165 a.u.)

Atom	Coordinates (Angstroms) X	Y	Z
C	0.23931000	0.41240800	0.00000000
O	1.22753900	-0.28704100	0.00000000
H	0.33231000	1.52200900	0.00000000
C	-1.17247000	-0.13623400	-0.00000100
H	-1.92181000	0.65870500	-0.00008200
H	-1.31589800	-0.77078600	-0.88092600
H	-1.31595200	-0.77064900	0.88101500

Table 6. Atom coordinates and absolute energy of **PhC≡CH** (Energy= -308.22490703 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
C	-1.51237000	-1.20835000	0.00000000
C	-0.12004200	-1.21307100	0.00000000
C	0.59398900	-0.00001000	-0.00000200
C	-0.12003300	1.21306600	-0.00000100
C	-1.51235500	1.20836000	0.00000100
C	-2.21265000	0.00000600	0.00000000
H	-2.05267000	-2.15039800	0.00000100
H	0.42817800	-2.14941500	0.00000000
H	0.42820700	2.14939900	-0.00000100
H	-2.05265300	2.15040900	0.00000100
H	-3.29857600	0.00001600	0.00000100
C	2.02394100	-0.00000600	-0.00000100
C	3.23419400	0.00000100	0.00000200
H	4.29946500	0.00001300	0.00000400

Table 7. Atom coordinates and absolute energy of **Int1** (Energy= -1388.39845082 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	-1.54718200	-0.39247500	0.17852800
P	0.48803800	0.00533800	-0.67053900
H	0.52228000	0.04338500	-2.07917900
C	1.25895700	1.63593400	-0.27653900
C	2.31060900	1.75032300	0.64284700
C	0.73074100	2.79614700	-0.86736800
C	2.83156800	3.00612900	0.96468500
H	2.73513200	0.86177900	1.10015200
C	1.26102300	4.04585900	-0.54679800
H	-0.09923700	2.70677200	-1.56165800
C	2.31026700	4.15516500	0.36987200
H	3.64840900	3.08242900	1.67695800
H	0.85204400	4.93712500	-1.01457400
H	2.71887500	5.13069500	0.61777500
C	1.83586900	-1.20842500	-0.35459700
C	2.97260900	-1.24733600	-1.17923700
C	1.73666100	-2.11619300	0.70829800
C	3.98565300	-2.17541700	-0.94405100
H	3.06537800	-0.54945700	-2.00716300
C	2.75512300	-3.04191200	0.94751900
H	0.85344100	-2.10293600	1.33943400

C	3.87883900	-3.07342400	0.12168900
H	4.85686200	-2.20003000	-1.59234100
H	2.66539800	-3.74186500	1.77327500
H	4.66795700	-3.79751300	0.30308100
C	-1.59978300	-2.01814300	-0.44770900
O	-1.65460600	-3.10972600	-0.83896800
C	-2.33510400	0.31194100	-1.46221700
O	-1.82989400	1.22466800	-2.10405300
C	-3.67277000	-0.25331900	-1.94758600
H	-4.14525300	0.43259700	-2.65806300
H	-3.47840700	-1.20744900	-2.45322300
H	-4.34689600	-0.46757000	-1.11408600
C	-3.14212200	-0.48994900	1.62017500
C	-1.93296000	-0.89181400	2.28185100
C	-1.02861600	0.19038300	2.23067800
C	-1.67098100	1.28095000	1.55246700
C	-2.98260000	0.86392000	1.21048600
H	-4.03088400	-1.09409900	1.50167100
H	-1.74347200	-1.86533900	2.71359800
H	-0.02176000	0.20139700	2.62534600
H	-1.23663400	2.24952600	1.35275700
H	-3.71896800	1.46037700	0.68999800

Table 8. Atom coordinates and absolute energy of **TS1** (Energy= -1388.34468949 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	1.87833200	-0.05203400	-0.21804800
P	-0.76202200	0.05040200	-0.54586200
H	-0.09262700	-0.04684200	0.71164700
C	-1.73523100	1.54757800	-0.06886400
C	-2.48539200	2.22044300	-1.04560000
C	-1.71308800	2.05572800	1.24103200
C	-3.21443300	3.36469000	-0.71812800
H	-2.49810000	1.84926800	-2.06731500
C	-2.42996600	3.20932200	1.56223900
H	-1.13509700	1.54509900	2.00622000
C	-3.18501800	3.86286600	0.58570300
H	-3.79604800	3.87199400	-1.48274700
H	-2.40406500	3.59327400	2.57831100
H	-3.74542800	4.75825000	0.83916900
C	-1.87724700	-1.39298000	-0.26687900
C	-1.91787500	-2.07700100	0.95959200

C	-2.68669600	-1.83842200	-1.32335700
C	-2.75849200	-3.17943100	1.12075000
H	-1.28630800	-1.75097900	1.78057900
C	-3.53816700	-2.93045500	-1.15305400
H	-2.64713800	-1.33250100	-2.28465700
C	-3.57375300	-3.60383900	0.06939200
H	-2.77932700	-3.70418300	2.07185900
H	-4.16354800	-3.26182100	-1.97724900
H	-4.22953400	-4.45998400	0.20007600
C	1.94651400	-1.66092100	-0.92899200
O	2.04902100	-2.70073700	-1.42548600
C	1.94882300	-0.77959500	1.57760600
O	1.02902400	-0.58273900	2.36521600
C	3.15536300	-1.58725300	2.05192700
H	3.19373000	-1.61711100	3.14543200
H	3.04455000	-2.61239000	1.67630100
H	4.09270300	-1.19904400	1.64540000
C	3.83435900	0.62506900	-0.64867900
C	3.05337700	0.93376700	-1.81932000
C	2.02652800	1.80900600	-1.43473700
C	2.17142800	2.08698800	-0.03005100
C	3.31961700	1.40209600	0.43395900
H	4.71393100	-0.00309800	-0.62159400
H	3.19706600	0.51082700	-2.80429500
H	1.23115200	2.17465700	-2.06874800
H	1.52749100	2.72580400	0.55869900
H	3.70204200	1.41750400	1.44501700

Table 9. Atom coordinates and absolute energy of **Int2** (Energy= -1388.35502147 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	1.76852700	-0.07454100	-0.21208700
P	-0.76735500	0.08708200	-0.99732500
H	0.13471100	0.02802000	0.17919300
C	-1.62854300	1.56181200	-0.27147000
C	-2.49405400	2.28058600	-1.11038700
C	-1.43987600	1.99741900	1.05117600
C	-3.17559100	3.40213200	-0.63433300
H	-2.63381900	1.96391600	-2.14124800
C	-2.11369000	3.12704100	1.51893300
H	-0.76577800	1.45256700	1.70709900
C	-2.98421500	3.82826900	0.68090000

H	-3.84642400	3.94685400	-1.29281800
H	-1.96073400	3.45723800	2.54284600
H	-3.50751900	4.70574600	1.05027900
C	-1.78866000	-1.34056300	-0.40457700
C	-1.92181500	-1.70786800	0.94525700
C	-2.47365800	-2.07750700	-1.38254300
C	-2.72910400	-2.78799200	1.30093800
H	-1.38527800	-1.15915400	1.71272400
C	-3.28972400	-3.15203100	-1.02187800
H	-2.36469400	-1.81136700	-2.43085600
C	-3.41763200	-3.50820900	0.32060000
H	-2.82205300	-3.06743900	2.34677100
H	-3.81671800	-3.71245000	-1.78890600
H	-4.04718700	-4.34720600	0.60357200
C	1.82031800	-1.73350500	-0.80123600
O	1.91377600	-2.80964400	-1.21357400
C	1.66108700	-0.66774000	1.64692700
O	0.79015400	-0.25378500	2.39983900
C	2.71222200	-1.62930100	2.19894500
H	2.71835200	-1.60572900	3.29317400
H	2.45528100	-2.64334700	1.86829000
H	3.70720500	-1.40782100	1.80384900
C	3.80248900	0.45170100	-0.50334600
C	3.12037600	0.75259600	-1.73494000
C	2.13141200	1.71279800	-1.45607000
C	2.20117700	2.04193700	-0.05864100
C	3.26569000	1.30066400	0.50994100
H	4.63199600	-0.23228900	-0.38872500
H	3.30216700	0.28182800	-2.69136200
H	1.41149400	2.10555900	-2.16068500
H	1.56036100	2.74040500	0.46070100
H	3.57655300	1.33050000	1.54493100

Table 10. Atom coordinates and absolute energy of **TS2** (Energy= -1388.34850215a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	-1.56326600	0.05272700	-0.11404700
P	0.59314500	-0.08975600	1.10543900
H	-0.69715600	-1.07494500	0.34533000
C	1.40502700	1.44648600	0.44311100
C	1.09302300	2.65086800	1.10117500
C	2.33796200	1.48333800	-0.60598100

C	1.67713300	3.85441600	0.70911500
H	0.38801300	2.64209800	1.92858900
C	2.92989200	2.68824700	-0.99210900
H	2.61672800	0.56549400	-1.11387900
C	2.59875300	3.87786100	-0.34154100
H	1.42220300	4.77234800	1.23162000
H	3.65116600	2.69515600	-1.80494500
H	3.06013200	4.81361400	-0.64357900
C	1.68683200	-1.41928700	0.40602400
C	1.23347100	-2.47191700	-0.40410000
C	3.02963300	-1.44071000	0.83211300
C	2.09303000	-3.50718700	-0.78290400
H	0.20040700	-2.49465100	-0.73721300
C	3.88923100	-2.46568500	0.44296800
H	3.40447000	-0.64711500	1.47332100
C	3.42341000	-3.50529400	-0.36706100
H	1.71738700	-4.31208900	-1.40862400
H	4.92251800	-2.45718500	0.77885300
H	4.09226400	-4.30716100	-0.66607800
C	-2.08846500	0.93712100	1.32168400
O	-2.44889200	1.58582300	2.20695400
C	-2.40612700	-1.65842700	0.55760800
O	-2.73720900	-2.52505800	-0.22418500
C	-2.63965300	-1.84951900	2.05167500
H	-1.77453300	-1.51337500	2.63081500
H	-3.49743200	-1.23965600	2.35811200
H	-2.85739200	-2.90028500	2.26344800
C	-2.68668000	1.38317500	-1.37284300
C	-1.29545800	1.66104100	-1.54964000
C	-0.68721600	0.48001300	-2.05182800
C	-1.68907200	-0.52233900	-2.18558500
C	-2.92913100	0.03821100	-1.76871500
H	-3.42774300	2.07378700	-0.99292300
H	-0.79153000	2.58565500	-1.30927500
H	0.36567100	0.35463000	-2.25744600
H	-1.54043000	-1.54399300	-2.50095100
H	-3.87178100	-0.48547200	-1.71268200

Table 11. Atom coordinates and absolute energy of **Int3** (Energy= -1234.58014913 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	-1.78179300	-0.44665900	-0.01973300

P	0.26224400	-0.01280300	-0.02535700
C	1.68873700	-1.15473500	-0.02359800
C	1.62310900	-2.35488900	0.70582300
C	2.84543700	-0.89109400	-0.78149800
C	2.67689600	-3.26814300	0.67015400
H	0.74709900	-2.56667800	1.31048300
C	3.89810100	-1.80412000	-0.81206100
H	2.91880000	0.03109700	-1.34967200
C	3.81683600	-2.99643800	-0.08820100
H	2.60932400	-4.18889000	1.24268100
H	4.78129600	-1.58672500	-1.40636900
H	4.63808800	-3.70694900	-0.11331600
C	1.01821900	1.65368500	0.01205100
C	2.10991400	1.95417000	0.84792800
C	0.47050600	2.68524400	-0.77091700
C	2.62893200	3.24709900	0.90228800
H	2.55353200	1.17166900	1.45602500
C	0.99119500	3.97855700	-0.71458500
H	-0.35656600	2.46355100	-1.43844300
C	2.07051800	4.26395900	0.12361200
H	3.46931600	3.46179700	1.55661300
H	0.55973600	4.76080600	-1.33303200
H	2.47743800	5.27013400	0.16665300
C	-1.59155000	-2.17930900	-0.25335700
O	-1.57129900	-3.32619800	-0.41714500
C	-3.12675700	0.44716500	1.35303900
C	-2.67113700	1.42685900	0.41533600
C	-3.08119500	1.01082100	-0.88542200
C	-3.75827000	-0.23026200	-0.76474100
C	-3.79296600	-0.57425600	0.63116900
H	-2.94986300	0.45823300	2.41941700
H	-2.11555200	2.32225300	0.65329400
H	-2.86138300	1.51838400	-1.81463800
H	-4.17516800	-0.81217200	-1.57443100
H	-4.23190500	-1.46762900	1.05319200

Table 12. Atom coordinates and absolute energy of **Int4**. (Energy= -1542.82718476 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	-0.51838000	-1.04439200	-0.79852000
C	-1.02193300	0.46631000	-1.56271000
O	-1.41750000	1.39847600	-2.11415900

C	-1.48864600	-0.31845500	0.91064600
C	-2.82160000	0.15882500	1.19304600
C	-3.85334100	0.12601800	0.23940100
C	-3.10633500	0.66629600	2.47842000
C	-5.13092400	0.58256200	0.55953000
H	-3.64270900	-0.25668700	-0.75273900
C	-4.38313300	1.12093300	2.79186800
H	-2.31443400	0.69795700	3.22015700
C	-5.40171100	1.08060500	1.83464300
H	-5.91561100	0.55129300	-0.19090400
H	-4.58531200	1.50933400	3.78597000
H	-6.39708700	1.43774900	2.08174100
C	-0.30502300	-0.62423800	1.19061500
H	0.53256000	-0.80031100	1.83919600
P	1.72042800	-0.13355900	-0.94136400
C	2.76478400	-0.58936800	0.52461900
C	3.76291800	0.28179900	1.00587800
C	2.72220900	-1.88563100	1.07463200
C	4.66515800	-0.12369900	1.98921100
H	3.83799500	1.28665600	0.60413300
C	3.62485500	-2.29224100	2.05845900
H	1.96718100	-2.58574500	0.73310800
C	4.60229200	-1.41200800	2.52416100
H	5.42115000	0.57424900	2.33969500
H	3.55966000	-3.29896800	2.46347600
H	5.30410200	-1.72451200	3.29198900
C	1.61114900	1.71116300	-0.74639900
C	1.87688500	2.49180300	-1.88401200
C	1.26220600	2.37597200	0.44375600
C	1.79393300	3.88551600	-1.84014300
H	2.15735500	1.99892900	-2.81135700
C	1.18415300	3.76742600	0.49172700
H	1.05357800	1.79924200	1.33874600
C	1.44754900	4.52745100	-0.65134200
H	2.00519900	4.46731300	-2.73328100
H	0.91407500	4.26030800	1.42203100
H	1.38472700	5.61143200	-0.61287900
C	-1.76565100	-2.20768000	-2.09886700
C	-1.82922700	-2.78996900	-0.80681100
C	-0.51523600	-3.21170200	-0.45009700
C	0.35535400	-2.90236200	-1.52895300
C	-0.40532500	-2.26355700	-2.54597200
H	-2.59616500	-1.78695100	-2.64966100
H	-2.70890700	-2.85495300	-0.18236500

H	-0.23389900	-3.66938800	0.48767000
H	1.41988400	-3.08381900	-1.56415200
H	-0.02404300	-1.89399400	-3.48716300

Table 13. Atom coordinates and absolute energy of **TS3** (Energy= -1542.81350548 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	-0.75507000	-0.99026900	-0.91580300
C	-1.17327400	0.31482700	-2.01752200
O	-1.52150500	1.11903600	-2.77090900
C	-1.42803800	0.08997800	0.58045100
C	-2.71004400	0.50532900	1.12331200
C	-3.90890700	0.26815100	0.42795200
C	-2.78115000	1.16683900	2.36738200
C	-5.13573400	0.66770900	0.95682300
H	-3.86345200	-0.22588600	-0.53707300
C	-4.00612300	1.56317000	2.89437600
H	-1.86320400	1.36610500	2.91243900
C	-5.19018900	1.31395400	2.19257300
H	-6.04977600	0.47714800	0.40126800
H	-4.04001800	2.06982600	3.85494600
H	-6.14523200	1.62589600	2.60529800
C	-0.16913700	0.11134900	0.84962400
H	0.50863900	0.32191800	1.66484600
P	1.48842600	-0.14025900	-0.74836600
C	2.63684700	-0.78369900	0.55299000
C	4.00333400	-0.46204700	0.42886600
C	2.26312900	-1.68992800	1.55771900
C	4.95163400	-1.01365000	1.28688100
H	4.32422900	0.22780200	-0.34699700
C	3.21711400	-2.25431400	2.41005800
H	1.21801200	-1.95170900	1.68268400
C	4.56313000	-1.91734000	2.28085400
H	5.99798600	-0.74257000	1.17582800
H	2.90139200	-2.95367900	3.17973100
H	5.30414100	-2.35289500	2.94491800
C	1.73271700	1.69104200	-0.64399800
C	1.49626100	2.44396400	-1.80707300
C	2.17896400	2.36386700	0.50646500
C	1.67643200	3.82738400	-1.81388500
H	1.17410100	1.94321400	-2.71524500
C	2.37450700	3.74493200	0.49478800

H	2.39064100	1.80481200	1.41279500
C	2.11741700	4.48259000	-0.66281700
H	1.48261900	4.39062700	-2.72242700
H	2.72471700	4.24607700	1.39325700
H	2.26715300	5.55850400	-0.66951700
C	-2.07343900	-2.34575100	-1.85781700
C	-2.06980600	-2.67711400	-0.47252200
C	-0.75308800	-3.05485200	-0.11803900
C	0.05792000	-2.99465700	-1.29645800
C	-0.75127400	-2.58244600	-2.37613100
H	-2.93385700	-2.03536500	-2.43508400
H	-2.90833000	-2.58142500	0.20245400
H	-0.41645500	-3.33194400	0.87030200
H	1.11833300	-3.20096900	-1.34281800
H	-0.42939700	-2.43262200	-3.39708900

Table 14. Atom coordinates and absolute energy of **Int5** (Energy= -1542.83517927 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	2.22868600	-0.19579400	-0.81803900
C	1.77268700	-1.76076700	-1.47975900
O	1.44762500	-2.75285600	-1.97762200
C	0.86744200	-0.33705200	0.52775700
C	2.01468900	-0.42836200	1.42824500
C	2.96132500	-1.47313300	1.25390000
C	2.35205800	0.62752900	2.32651000
C	4.19851100	-1.43758300	1.93350200
H	2.68179300	-2.37766700	0.72902600
C	3.55293700	0.62916900	3.00680200
H	1.63302900	1.42819200	2.47259300
C	4.49674800	-0.39907200	2.79686600
H	4.89796000	-2.25795900	1.80041500
H	3.77552100	1.42869100	3.70828800
H	5.44178100	-0.38442300	3.33174100
C	-0.44642900	-0.29060300	0.77313700
H	-0.82048400	-0.41542500	1.79379100
P	-1.67367000	-0.08307600	-0.57241000
C	-2.49462400	1.51690500	-0.11168300
C	-3.72216600	1.85144700	-0.71174700
C	-1.88273600	2.46766900	0.71916600
C	-4.32200000	3.08719500	-0.47616900
H	-4.21532400	1.13475100	-1.36374900

C	-2.47986000	3.71024100	0.94991600
H	-0.93529800	2.22944500	1.19393400
C	-3.70168000	4.02407000	0.35545900
H	-5.27398900	3.32185200	-0.94486500
H	-1.99020500	4.43000100	1.60089700
H	-4.16743500	4.98875800	0.53591100
C	-2.95814800	-1.31885000	-0.04911600
C	-3.03869500	-2.51352200	-0.78123500
C	-3.82017000	-1.14405500	1.04604100
C	-3.94842400	-3.51179700	-0.42596100
H	-2.38355300	-2.66006200	-1.63629600
C	-4.73342800	-2.13801100	1.39879100
H	-3.78326500	-0.22231200	1.61956400
C	-4.79878400	-3.32495400	0.66439900
H	-3.99661100	-4.43027900	-1.00454800
H	-5.39483900	-1.98671100	2.24781700
H	-5.51153500	-4.09752800	0.93948200
C	3.91207900	0.97689100	-1.47596600
C	2.98295700	1.82149800	-0.78131900
C	1.74740600	1.78746400	-1.47585900
C	1.88486200	0.89217300	-2.57341500
C	3.24968300	0.42231600	-2.59135100
H	4.93137300	0.77562300	-1.17569900
H	3.19057400	2.37285000	0.12448600
H	0.83506400	2.28758900	-1.18329700
H	1.11258900	0.64046300	-3.28632000
H	3.67364000	-0.26706700	-3.30847600

Table 15. Atom coordinates and absolute energy of **Int5`** (Energy= -1542.86696384 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	-0.75090600	-0.15324300	1.23104200
C	-0.87543900	-1.89460900	1.23542400
O	-1.00907700	-3.04682300	1.26289600
C	-1.42328100	-0.10376700	-0.64774700
C	-2.81042200	-0.09152100	-1.14890300
C	-3.82869500	-0.79167900	-0.47636500
C	-3.15998100	0.62489000	-2.31102000
C	-5.13577500	-0.80210700	-0.96106000
H	-3.57676100	-1.33987500	0.42566600
C	-4.46973400	0.62933900	-2.78667000
H	-2.39374900	1.19259600	-2.83130100

C	-5.46320000	-0.08895200	-2.11640500
H	-5.90216700	-1.36275200	-0.43266000
H	-4.71719900	1.19548100	-3.68073600
H	-6.48432000	-0.08623600	-2.48718400
C	-0.33168300	-0.05356800	-1.45666000
H	-0.27965800	-0.05635700	-2.54657300
P	0.98264000	-0.04677800	-0.24196900
C	1.98242600	1.49110300	-0.41436700
C	3.27833000	1.57573100	0.11856400
C	1.42575800	2.62448700	-1.02679100
C	4.00091300	2.76684900	0.03768700
H	3.73106800	0.70557300	0.58540300
C	2.15155900	3.81372700	-1.10919500
H	0.42488700	2.56758700	-1.44468000
C	3.43997000	3.88861300	-0.57612500
H	5.00440400	2.81648700	0.45106300
H	1.71129100	4.68075300	-1.59387800
H	4.00466600	4.81419300	-0.64137400
C	2.21395200	-1.37877900	-0.54366900
C	2.44318700	-2.35226000	0.43756200
C	2.91705900	-1.45343800	-1.75810500
C	3.35713600	-3.38441600	0.21080200
H	1.90040700	-2.30246800	1.37626100
C	3.82319900	-2.48734700	-1.98574800
H	2.75810100	-0.69996600	-2.52471900
C	4.04470300	-3.45447600	-1.00055300
H	3.52623500	-4.13371700	0.97876900
H	4.35753400	-2.53967300	-2.93014100
H	4.75133000	-4.25988200	-1.17965900
C	-2.15841700	0.26885200	2.78980200
C	-2.10919300	1.37911700	1.90621700
C	-0.78512300	1.89427900	1.90712500
C	-0.01501000	1.11416500	2.83246600
C	-0.85489800	0.12172600	3.38186800
H	-3.02827200	-0.33491300	3.00762300
H	-2.92358300	1.72290500	1.28422100
H	-0.42273400	2.73082800	1.32732600
H	1.03671300	1.24729700	3.04665000
H	-0.56567000	-0.63302600	4.10038400

Table 16. Atom coordinates and absolute energy of **Int6** (Energy= -1542.8348128 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z

Fe	-2.59412300	0.30151500	-0.70909900
C	-2.27749100	1.98465000	-1.10358800
O	-2.06226900	3.07178500	-1.43759700
C	-0.80624400	0.12026900	-0.01506800
C	-1.52705000	-0.04399600	1.24020400
C	-2.39072800	0.99268100	1.68804000
C	-1.60765600	-1.30757700	1.90258800
C	-3.30600100	0.75569100	2.73941500
H	-2.23496500	2.01115200	1.35648400
C	-2.48445300	-1.50813900	2.94738500
H	-0.94764400	-2.10279800	1.57074800
C	-3.35863200	-0.47747500	3.36014700
H	-3.93880300	1.56971100	3.08118000
H	-2.50497500	-2.46687500	3.45841000
H	-4.04929200	-0.64999500	4.18030100
C	0.48385300	0.06529400	-0.35532100
H	0.76043400	0.14453100	-1.40825200
P	1.84758900	-0.12562900	0.86600900
C	2.81250200	-1.50259100	0.07376200
C	2.82357300	-2.74641900	0.72312600
C	3.49198200	-1.37977800	-1.14988600
C	3.48583300	-3.84222900	0.16427500
H	2.31404200	-2.85251600	1.67773400
C	4.15637800	-2.47160900	-1.70839800
H	3.51036100	-0.42119900	-1.66047700
C	4.15322700	-3.70631900	-1.05332600
H	3.48623400	-4.79712200	0.68296200
H	4.67876700	-2.35986100	-2.65484700
H	4.67328100	-4.55528800	-1.48844500
C	2.90587100	1.34125100	0.45348300
C	2.36659100	2.51073100	-0.10344000
C	4.26425200	1.34088100	0.81752400
C	3.16325800	3.64105200	-0.30295500
H	1.31843500	2.53792300	-0.38680000
C	5.05984900	2.46732300	0.61411500
H	4.70533400	0.44927800	1.25569800
C	4.51195100	3.62356200	0.05219300
H	2.72625700	4.53466400	-0.74077600
H	6.10912600	2.44317600	0.89613600
H	5.13145800	4.50209400	-0.10468500
C	-4.49668700	-0.69195400	-0.89777600
C	-3.44826000	-1.67009800	-0.85795300
C	-2.58501500	-1.44068700	-1.95910900

C	-3.06279500	-0.29878700	-2.66108100
C	-4.27760800	0.14007300	-2.01600400
H	-5.29354500	-0.58905200	-0.17406500
H	-3.33017100	-2.43496800	-0.10439000
H	-1.67693200	-1.98351200	-2.18005300
H	-2.62304700	0.13400500	-3.54880800
H	-4.88583200	0.98257400	-2.31492700

Table 17. Atom coordinates and absolute energy of **Int7** (Energy= -2347.86450751 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	1.43033000	1.19920000	-0.96733800
P	1.95396700	-0.61454100	0.22966000
H	1.36224300	-0.66039500	1.50984100
C	3.72116700	-0.88222000	0.68970400
C	4.73982500	-0.19202600	0.02053200
C	4.06526300	-1.78254000	1.71166400
C	6.07894600	-0.40034400	0.36061800
H	4.48132500	0.51557700	-0.76078100
C	5.40045500	-1.98453400	2.05511400
H	3.28730700	-2.32928700	2.23790800
C	6.41027200	-1.29449200	1.37795900
H	6.85967000	0.14176600	-0.16513500
H	5.65420800	-2.67880500	2.85099400
H	7.45066100	-1.45218900	1.64725600
C	1.44574100	-2.28134000	-0.37789700
C	2.20340000	-2.94003500	-1.35915300
C	0.28276500	-2.89718800	0.10869900
C	1.79946500	-4.18045500	-1.85253400
H	3.12713900	-2.49809500	-1.72173500
C	-0.11901200	-4.13954200	-0.38757600
H	-0.31377300	-2.41566300	0.87676300
C	0.63410600	-4.78149400	-1.37116300
H	2.39929900	-4.68039600	-2.60772800
H	-1.01867100	-4.60514700	0.00449500
H	0.32133100	-5.74838700	-1.75453600
C	2.30663900	2.26179200	0.12091500
O	2.91786700	2.98515000	0.78492000
C	-0.28422000	1.39192500	0.06640000
C	-0.49747700	2.63892000	0.85096800
C	-0.51636500	2.61389800	2.25666600
C	-0.64772400	3.88600600	0.21671000

C	-0.68647000	3.78418200	2.99825800
H	-0.39835400	1.66490200	2.77163000
C	-0.83320200	5.05258000	0.95585500
H	-0.63401700	3.93356300	-0.86792900
C	-0.84838800	5.00969100	2.35235500
H	-0.69875700	3.73431200	4.08381600
H	-0.96487600	6.00019100	0.43985400
H	-0.98456700	5.92068400	2.92799700
C	-1.24840600	0.44961300	-0.01363200
H	-1.05937300	-0.45645700	-0.59076100
P	-2.97443000	0.62678700	0.62095100
C	-3.89996400	0.02735600	-0.87636800
C	-4.75096600	0.93852400	-1.52031600
C	-3.75986500	-1.25842300	-1.42776700
C	-5.43876000	0.58232500	-2.68358800
H	-4.87499700	1.93427600	-1.10245600
C	-4.44731200	-1.61770600	-2.58689100
H	-3.11553300	-1.98612100	-0.94221000
C	-5.28802700	-0.69683600	-3.21898000
H	-6.09416000	1.30208800	-3.16653600
H	-4.32867500	-2.61676300	-2.99834900
H	-5.82371000	-0.97802700	-4.12153800
C	-3.12999200	-0.83671500	1.75499600
C	-2.07759800	-1.18694800	2.61770200
C	-4.34937000	-1.52279900	1.89380500
C	-2.22922300	-2.19621900	3.57130100
H	-1.12978100	-0.66150100	2.53959500
C	-4.50187200	-2.53256500	2.84454300
H	-5.18559900	-1.27049100	1.24816900
C	-3.44234100	-2.87644200	3.68720000
H	-1.39807900	-2.44912300	4.22477000
H	-5.45294600	-3.05220300	2.92728100
H	-3.56283300	-3.66199400	4.42779200
C	1.35260000	2.54338400	-2.65335700
C	0.26548300	1.63518800	-2.75064300
C	0.78625900	0.31833300	-2.84609600
C	2.21655800	0.41811600	-2.85119500
C	2.56764600	1.78198200	-2.73497500
H	1.28336400	3.61784500	-2.55904400
H	-0.78187000	1.89142500	-2.69384700
H	0.21092200	-0.59275700	-2.92329000
H	2.90747600	-0.40952700	-2.93022700
H	3.57086600	2.18493600	-2.69876600

Table 18. Atom coordinates and absolute energy of **Int7`** (Energy= -2347.85782385 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	-1.11333700	-1.06318600	-1.04914900
P	-1.95535500	0.61285500	0.16985300
H	-1.55632300	0.61102800	1.52269100
C	-3.78590000	0.67897900	0.40064600
C	-4.64412300	0.13318200	-0.56302100
C	-4.33970200	1.29670800	1.53336900
C	-6.02953500	0.21039200	-0.40369900
H	-4.22667100	-0.36352400	-1.43343600
C	-5.72227100	1.36523500	1.69654200
H	-3.68845800	1.72677400	2.28964000
C	-6.56991600	0.82427600	0.72610000
H	-6.68393300	-0.21767700	-1.15761400
H	-6.13852500	1.83916200	2.58082700
H	-7.64715200	0.87714300	0.85462200
C	-1.56853300	2.37061200	-0.23157100
C	-2.22947000	3.02292300	-1.28360000
C	-0.62110700	3.08025800	0.51887500
C	-1.94482200	4.35484300	-1.58242400
H	-2.99204600	2.50087400	-1.85438700
C	-0.34277600	4.41628500	0.22184800
H	-0.09657200	2.59560200	1.33668100
C	-0.99976200	5.05547400	-0.82967200
H	-2.46865000	4.84791500	-2.39633100
H	0.38492600	4.95668700	0.82019700
H	-0.78313200	6.09506000	-1.05745900
C	-2.25675700	-2.21433200	-0.36669500
O	-3.06486000	-2.97237500	-0.03576300
C	0.25474500	-1.33246400	0.41953800
C	-0.05938000	-2.38459100	1.43893500
C	-0.29910400	-2.04604900	2.78291900
C	-0.08817500	-3.74881800	1.09375700
C	-0.57291000	-3.02730700	3.73853600
H	-0.25950700	-1.00099500	3.07819700
C	-0.34058200	-4.73010600	2.05017300
H	0.09455700	-4.03423100	0.06126900
C	-0.59261800	-4.37460900	3.37816700
H	-0.76296600	-2.73611000	4.76846400
H	-0.34391500	-5.77702200	1.75792400
H	-0.80076500	-5.13944800	4.12090000

C	1.43283100	-0.70189000	0.65888600
H	1.99842100	-1.03177800	1.53699200
P	2.28866700	0.59874700	-0.30727400
C	3.17907400	1.50483300	1.05643900
C	3.02368100	2.89608100	1.14174200
C	4.00889500	0.86822200	1.99485100
C	3.66358400	3.63191800	2.14366200
H	2.40154800	3.40521600	0.41122600
C	4.64568500	1.59848300	2.99755200
H	4.17101900	-0.20427100	1.93253700
C	4.47229500	2.98343400	3.07645100
H	3.53444300	4.71017100	2.19094600
H	5.28391900	1.08888600	3.71452000
H	4.97179000	3.55194100	3.85611300
C	3.73075000	-0.34911000	-1.01508500
C	3.86052900	-1.74376200	-0.93683700
C	4.71059500	0.37230200	-1.72031900
C	4.94037600	-2.39675700	-1.53992900
H	3.11451900	-2.32052100	-0.39787800
C	5.79208900	-0.27658200	-2.31281800
H	4.62654800	1.45362700	-1.80161800
C	5.91012700	-1.66695900	-2.22637100
H	5.02352600	-3.47802600	-1.46572900
H	6.54096200	0.30116600	-2.84813000
H	6.74960400	-2.17453700	-2.69322100
C	-0.57303400	-2.25459600	-2.75865500
C	0.42954000	-1.26647400	-2.56812200
C	-0.16814600	0.01403700	-2.69204700
C	-1.55425200	-0.18348100	-2.99878800
C	-1.80377800	-1.57381300	-3.04843200
H	-0.42969200	-3.32558200	-2.73001600
H	1.46278700	-1.46361100	-2.32528800
H	0.33540200	0.96132900	-2.57578600
H	-2.28173700	0.59772600	-3.16967100
H	-2.75684600	-2.04583900	-3.24732300

Table 19. Atom coordinates and absolute energy of **TS4** (Energy= -2347.798495809 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	1.06200900	-0.95717700	1.25278000
P	2.30512200	0.42764600	-0.10619000
H	0.87062400	-0.14357300	-0.62584600

C	3.99740000	0.00324000	-0.66524000
C	4.77767200	-0.95013900	0.00778000
C	4.53136700	0.62661900	-1.80884700
C	6.05440200	-1.27842700	-0.45336200
H	4.38493500	-1.43279300	0.89623900
C	5.80949000	0.30523500	-2.26106600
H	3.93967400	1.36507300	-2.34211400
C	6.57319300	-0.65204800	-1.58673800
H	6.64395800	-2.02046300	0.07774800
H	6.20735600	0.79551800	-3.14520000
H	7.56639100	-0.90749800	-1.94490300
C	2.34214700	2.20440000	0.33504900
C	3.49301000	2.79563300	0.88664700
C	1.20270000	3.00781200	0.14970400
C	3.50022600	4.14518600	1.24203100
H	4.38951300	2.19992500	1.03085000
C	1.20930800	4.35307300	0.51824600
H	0.30926900	2.58711300	-0.30048000
C	2.35817500	4.92872600	1.06522000
H	4.40132700	4.58308700	1.66302900
H	0.31713500	4.95332600	0.36174800
H	2.36547400	5.97821000	1.34484100
C	1.82480900	-2.43083900	0.65823700
O	2.33538900	-3.43134400	0.38651400
C	-0.37348900	-0.89819000	-0.37884900
C	-0.51349800	-2.14514100	-1.17273800
C	0.32109400	-2.39176800	-2.27795500
C	-1.45934000	-3.12515100	-0.82264400
C	0.20376200	-3.57022800	-3.01313600
H	1.05765000	-1.64716800	-2.56760500
C	-1.56919700	-4.30773500	-1.55503300
H	-2.10539500	-2.95621100	0.03371900
C	-0.73953600	-4.53575500	-2.65399200
H	0.85230900	-3.73514000	-3.86921500
H	-2.30763300	-5.05119600	-1.26670600
H	-0.82615900	-5.45580700	-3.22475200
C	-1.35040400	0.03956100	-0.34194500
H	-1.16930300	0.95150600	0.22925300
P	-2.96044800	-0.01222600	-1.25797400
C	-4.12928100	-0.48862000	0.10705500
C	-4.99986400	-1.56299400	-0.12836900
C	-4.16435500	0.14001600	1.36476900
C	-5.88062900	-2.00273600	0.86390000
H	-4.98219100	-2.05899000	-1.09501600

C	-5.04148700	-0.29875900	2.35693600
H	-3.51330600	0.98675100	1.56292400
C	-5.90086900	-1.37324800	2.10837200
H	-6.54892700	-2.83539900	0.66284800
H	-5.05761900	0.19874700	3.32291900
H	-6.58362400	-1.71402400	2.88160300
C	-3.25275700	1.81100400	-1.41455100
C	-2.24279300	2.59524400	-2.00125200
C	-4.46942400	2.43137600	-1.09027600
C	-2.43142200	3.95911000	-2.22731900
H	-1.30182900	2.13380600	-2.29164100
C	-4.66046200	3.79507400	-1.32301800
H	-5.27153900	1.85075500	-0.64564800
C	-3.64235600	4.56560800	-1.88632500
H	-1.63436000	4.54521600	-2.67687700
H	-5.60884800	4.25570500	-1.05951100
H	-3.79284000	5.62656400	-2.06430100
C	0.31764900	-1.88202800	3.06863000
C	-0.53141500	-0.80521300	2.72305700
C	0.24073100	0.39451200	2.71310100
C	1.57449700	0.05134700	3.09314900
C	1.63345200	-1.34611500	3.30434600
H	0.02990700	-2.92167900	3.14280600
H	-1.57421700	-0.88764600	2.45241200
H	-0.11490200	1.39030500	2.49117000
H	2.40609400	0.73892500	3.15706400
H	2.51056900	-1.91274800	3.58526600

Table 20. Atom coordinates and absolute energy of **TS4`** (Energy= -2347.79116652 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	-0.94942100	-0.82929100	-1.42601700
P	-1.91631700	0.77143500	-0.05707400
H	-0.64483700	-0.12470100	0.45217300
C	-3.60235200	0.52677900	0.62200600
C	-4.63514800	-0.02997000	-0.14975100
C	-3.88192200	0.90677300	1.94724100
C	-5.91104800	-0.20652400	0.38889900
H	-4.43742800	-0.32527500	-1.17521700
C	-5.15766100	0.73281500	2.48370400
H	-3.09391100	1.34099600	2.55585400
C	-6.17429500	0.17327500	1.70588800

H	-6.69813500	-0.64079400	-0.22108800
H	-5.35666000	1.02956000	3.50969200
H	-7.16645900	0.03278900	2.12537700
C	-1.79055700	2.55092700	-0.47047300
C	-2.93860500	3.35067300	-0.61196600
C	-0.52992700	3.14962200	-0.65149700
C	-2.82605400	4.70719300	-0.92183200
H	-3.92328500	2.91556800	-0.47587400
C	-0.42544000	4.50410000	-0.96489800
H	0.37150300	2.55494700	-0.53609300
C	-1.57164100	5.29120700	-1.10156500
H	-3.72654400	5.30674600	-1.02555500
H	0.55845200	4.94688800	-1.09579400
H	-1.48739300	6.34683400	-1.34301200
C	-2.15882200	-2.05775000	-1.04675700
O	-2.96949700	-2.87487600	-0.94876200
C	0.25690900	-1.29651800	0.35163000
C	-0.21678800	-2.53134800	1.04380200
C	-1.25974400	-2.48883000	1.98662900
C	0.38660200	-3.77354500	0.78000600
C	-1.67798700	-3.64634500	2.64189600
H	-1.73893800	-1.54137300	2.21522900
C	-0.03823500	-4.93216500	1.43079500
H	1.18800000	-3.82591300	0.04789400
C	-1.07226300	-4.87426700	2.36663200
H	-2.48030900	-3.58730900	3.37238300
H	0.44189800	-5.88128000	1.20732600
H	-1.40318100	-5.77523500	2.87504000
C	1.51600100	-0.89683900	0.66652700
H	2.07466900	-1.48690300	1.40160700
P	2.36015600	0.63901100	0.11980900
C	3.07955500	1.18562300	1.74222700
C	2.44226600	2.24751200	2.40330700
C	4.19979300	0.59226100	2.34536800
C	2.90463100	2.69853000	3.64112200
H	1.58119100	2.72642300	1.94392700
C	4.66569900	1.04647800	3.57956500
H	4.71576500	-0.22174500	1.84454400
C	4.01832500	2.09917600	4.23100100
H	2.39916600	3.52108700	4.13949400
H	5.53543100	0.57875600	4.03309400
H	4.38344100	2.45237400	5.19135500
C	3.86222000	-0.02189500	-0.74549700
C	4.12415700	-1.38732300	-0.93851500

C	4.76248200	0.91259300	-1.28774900
C	5.25306700	-1.80545900	-1.64950500
H	3.44536900	-2.13046500	-0.53092400
C	5.89442200	0.49604800	-1.98605800
H	4.57408600	1.97602100	-1.16067200
C	6.14217000	-0.86675200	-2.17225100
H	5.43779400	-2.86729800	-1.78848600
H	6.57938000	1.23480600	-2.39296800
H	7.01958700	-1.19233700	-2.72360600
C	-0.29218600	-1.83871500	-3.22606400
C	0.75197600	-0.99967300	-2.76942600
C	0.28300700	0.34626200	-2.76132500
C	-1.06072700	0.33661800	-3.24588200
C	-1.42290000	-1.00018100	-3.53107300
H	-0.24758100	-2.91350000	-3.33539700
H	1.72597100	-1.32889900	-2.43828900
H	0.84923100	1.21701000	-2.46988500
H	-1.70520300	1.20013200	-3.33168900
H	-2.38163300	-1.33622400	-3.90187800

Table 21. Atom coordinates and absolute energy of **2-Z** (Energy= -1113.25996786 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
C	1.67100400	-1.20539400	1.35648200
C	2.86604000	-0.90007900	0.55806900
C	2.91893200	0.10894200	-0.42143800
C	4.03250700	-1.65247800	0.79625700
C	4.08241700	0.32573700	-1.15769100
H	2.06229500	0.75150800	-0.58520700
C	5.19311700	-1.43726000	0.05910800
H	4.01559700	-2.42419200	1.56168100
C	5.22072200	-0.44794500	-0.92647100
H	4.10199800	1.11204500	-1.90658500
H	6.07709200	-2.03707300	0.25545800
H	6.12634100	-0.27270400	-1.49975900
C	0.36426200	-1.00212500	1.08814100
H	-0.34368600	-1.33465500	1.84612000
P	-0.39218000	-0.39144500	-0.47223300
C	-2.10759500	-1.06364900	-0.24448700
C	-3.04824300	-0.52835800	0.64958700
C	-2.46615300	-2.18581400	-1.00607300
C	-4.31091700	-1.10570100	0.78163800

H	-2.79394400	0.34874700	1.23735000
C	-3.72813800	-2.76783600	-0.87091400
H	-1.75213700	-2.60308400	-1.71132500
C	-4.65285300	-2.22782900	0.02297800
H	-5.02958700	-0.67909500	1.47596000
H	-3.98953800	-3.63715200	-1.46763500
H	-5.63742000	-2.67515400	0.12569300
C	-0.65658100	1.41605000	-0.13368200
C	-1.30506100	2.17359800	-1.12503700
C	-0.19408700	2.07420700	1.01491000
C	-1.50378700	3.54289500	-0.96182100
H	-1.65775000	1.68587300	-2.03052800
C	-0.38297200	3.44980000	1.17262800
H	0.31701600	1.50881900	1.78807400
C	-1.04092500	4.18670900	0.18876700
H	-2.01250300	4.11007500	-1.73627200
H	-0.01728100	3.94270300	2.06923000
H	-1.18870100	5.25553500	0.31314000
H	1.89477200	-1.70133900	2.30239300

Table 22. Atom coordinates and absolute energy of **2-E** (Energy= -1113.26277922 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
C	1.91013300	0.01021300	-0.87022000
C	3.25967200	-0.01347000	-0.28590700
C	3.50174600	-0.14201200	1.09450400
C	4.36742500	0.09442800	-1.14470600
C	4.80090700	-0.15586400	1.59154000
H	2.66758500	-0.23900900	1.78230200
C	5.66939100	0.08168000	-0.64774300
H	4.19889600	0.19099300	-2.21421100
C	5.89138600	-0.04296900	0.72369300
H	4.96624800	-0.25808100	2.66020500
H	6.50914700	0.16775600	-1.33110800
H	6.90418800	-0.05511800	1.11533500
C	0.73069800	0.00442100	-0.22341400
H	0.69383700	-0.01821800	0.86571400
P	-0.85180000	-0.00283300	-1.14874500
C	-1.70960100	-1.42999000	-0.32454900
C	-2.10629400	-1.43270600	1.02290900
C	-1.93356200	-2.58167900	-1.09277700
C	-2.70513200	-2.55917200	1.58509500

H	-1.95755100	-0.54468500	1.63035800
C	-2.53145700	-3.71169400	-0.53050900
H	-1.63862700	-2.59027800	-2.13868900
C	-2.91753100	-3.70201200	0.80949700
H	-3.00767700	-2.54629200	2.62857100
H	-2.69862300	-4.59511300	-1.14016300
H	-3.38551600	-4.57846900	1.24859800
C	-1.72227300	1.44764800	-0.38861800
C	-3.12642500	1.50661200	-0.39788900
C	-1.01143700	2.56225200	0.08146100
C	-3.79667700	2.63781100	0.06497500
H	-3.70050600	0.65822200	-0.76022000
C	-1.68355600	3.69586200	0.54299400
H	0.07452700	2.54463500	0.08816700
C	-3.07755600	3.73752300	0.53862600
H	-4.88290500	2.66047400	0.05551600
H	-1.11409600	4.54609000	0.90831700
H	-3.60021700	4.61894500	0.89855100
H	1.88914900	0.03935700	-1.95984300

Table 23. Atom coordinates and absolute energy of **Int8** (Energy= -2347.8566437 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	0.13209500	-1.60498600	-0.37182100
C	0.14222400	-1.51329600	1.38906900
O	0.12890600	-1.56826600	2.54204400
P	2.60274800	-1.39172500	-0.27737400
C	3.28053700	-0.23125400	-1.54359700
C	2.68226900	-0.16019200	-2.81932900
C	3.26802800	0.55239700	-3.86586200
C	4.48064500	1.21712600	-3.67377100
C	5.10267600	1.14062900	-2.42600700
C	4.51792800	0.42569900	-1.38091300
C	3.23311700	-0.75644800	1.34261700
C	3.47482500	-1.74471700	2.31783500
C	3.97531700	-1.41788700	3.57704100
C	4.26716400	-0.08832000	3.88860100
C	4.04342800	0.90401100	2.93312900
C	3.52405000	0.57727700	1.67911900
P	-2.40763600	0.46071900	0.78222900
C	-3.74446200	-0.78394500	0.44725100
C	-3.88273200	-1.84686300	1.35349200

C	-4.85579800	-2.83047600	1.15977600
C	-5.71342700	-2.75749400	0.06093400
C	-5.59743800	-1.69539500	-0.84015700
C	-4.62191500	-0.71553800	-0.64731700
C	-3.22282400	2.01419000	0.17068300
C	-4.23111000	2.56067900	0.98501100
C	-4.87870500	3.74176700	0.62854800
C	-4.51871700	4.41210100	-0.54357000
C	-3.51045300	3.88952100	-1.35270200
C	-2.86836400	2.69899300	-1.00035300
C	0.03252100	0.62666400	-0.80174600
C	0.69414400	1.68052200	0.00308800
C	1.50483300	2.59917800	-0.69222300
C	2.05416500	3.70907400	-0.05154100
C	1.81078100	3.92658400	1.30570900
C	1.02766600	3.01305900	2.01441600
C	0.48178500	1.90078100	1.37674200
C	-1.23922800	0.07962100	-0.60772900
H	1.74464100	-0.67767800	-2.99726900
H	2.77423600	0.58753100	-4.83388900
H	4.93746200	1.77680400	-4.48482500
H	6.05470100	1.63914700	-2.26222900
H	5.03554400	0.37100900	-0.42977300
H	3.27846700	-2.78645000	2.07581200
H	4.15006200	-2.20206100	4.30878100
H	4.66825000	0.17058400	4.86466300
H	4.26234000	1.94296600	3.16468200
H	3.35169100	1.36757800	0.95906000
H	-3.22522100	-1.89942700	2.21739200
H	-4.94976700	-3.64622000	1.87132400
H	-6.47479000	-3.51782400	-0.08834500
H	-6.27066500	-1.62755300	-1.69044600
H	-4.54986400	0.11469800	-1.34443300
H	-4.51043500	2.05585100	1.90682400
H	-5.65842300	4.14402700	1.26946100
H	-5.01668500	5.33738800	-0.81898500
H	-3.21930800	4.40683000	-2.26289500
H	-2.08383500	2.31077400	-1.64147400
H	0.39388800	0.60274000	-1.82550400
H	1.69892200	2.44193900	-1.74874000
H	2.66963900	4.40367500	-0.61612400
H	0.84294300	3.16100100	3.07440400
H	-0.11301200	1.20540400	1.95498700
H	-1.73593900	-0.24426700	-1.51760600

H	2.22963800	4.79479700	1.80650700
C	0.46830300	-3.71523400	-0.63635800
C	0.70675800	-3.09752200	-1.90237100
C	-0.48682900	-2.47364000	-2.31992200
C	-1.49238200	-2.73947300	-1.33293200
C	-0.90581800	-3.51840400	-0.30920900
H	1.19993900	-4.24990200	-0.04884700
H	1.65621100	-3.07341000	-2.41644500
H	-0.62397000	-1.90110500	-3.22779600
H	-2.51860000	-2.40658200	-1.35629200
H	-1.40824800	-3.86405600	0.58348600

Table 24. Atom coordinates and absolute energy of **TS5** (Energy= -2347.82760621 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	0.03547600	-1.86103300	-0.14213200
C	0.01998900	-1.54506900	-1.87294200
O	0.07472600	-1.47383300	-3.02721000
P	-2.20999900	-1.10144100	0.27547600
C	-2.81771300	-0.39470300	1.85460000
C	-2.32105700	-0.94075700	3.05658700
C	-2.73286800	-0.45849200	4.29759700
C	-3.66635300	0.57781700	4.37663300
C	-4.17148900	1.12926400	3.19776100
C	-3.74842300	0.65931800	1.95336100
C	-3.39727300	-0.53605700	-1.00036000
C	-4.78072300	-0.69087300	-0.75838700
C	-5.72099000	-0.40016300	-1.74299100
C	-5.31029900	0.03796200	-3.00550200
C	-3.94871100	0.17824200	-3.26647200
C	-3.00354000	-0.10403100	-2.27752200
P	2.30643200	0.56300400	-0.80458900
C	3.71630000	-0.57272600	-0.38841400
C	4.12648100	-1.49302500	-1.36546700
C	5.18211900	-2.37571900	-1.12292500
C	5.85259800	-2.34270800	0.10076800
C	5.46730000	-1.41907600	1.07644400
C	4.41096200	-0.53980900	0.83215300
C	2.91191000	2.12478700	0.00966500
C	3.82516900	2.90484000	-0.72099900
C	4.32759700	4.09799900	-0.20381900
C	3.91238100	4.54591500	1.05269200

C	2.99648000	3.78996200	1.78433800
C	2.50198800	2.58923700	1.26777700
C	-0.26626500	0.66607300	0.49541300
C	-0.78054200	1.79003000	-0.30346300
C	-1.57961400	2.74798400	0.35861900
C	-2.04842700	3.87959500	-0.30302600
C	-1.73571100	4.08630900	-1.64806500
C	-0.95152500	3.14746200	-2.32146300
C	-0.48115000	2.01343000	-1.66364700
C	0.98080400	-0.04096000	0.35115000
H	-1.61061300	-1.76000700	3.01485200
H	-2.33342100	-0.90287500	5.20544400
H	-3.99700000	0.94754900	5.34278800
H	-4.89457400	1.93959500	3.24302600
H	-4.14528000	1.11322400	1.05258100
H	-5.12061500	-1.05322700	0.20682300
H	-6.77831600	-0.52829200	-1.52688400
H	-6.04402400	0.25880300	-3.77539600
H	-3.61175500	0.51441500	-4.24327500
H	-1.95639000	0.02364900	-2.51009800
H	3.61545100	-1.51201800	-2.32466200
H	5.48563400	-3.08095300	-1.89186800
H	6.67752500	-3.02371700	0.29016700
H	5.99484000	-1.37912300	2.02574200
H	4.13276900	0.18664600	1.59048300
H	4.14189900	2.57369600	-1.70733800
H	5.03536000	4.68310000	-0.78479300
H	4.29521100	5.47988700	1.45440600
H	2.66394300	4.13317500	2.76048500
H	1.78966600	2.01581700	1.85237900
H	-0.63837500	0.68783500	1.51444500
H	-1.81720400	2.60393500	1.40758600
H	-2.65274100	4.60449000	0.23495700
H	-0.70121400	3.29765300	-3.36775200
H	0.13148700	1.30417700	-2.20634700
H	1.37568800	-0.32689200	1.32808000
H	-2.09659500	4.97051800	-2.16531200
C	-0.07475300	-4.05926000	-0.37782600
C	-0.53909700	-3.75888400	0.91707000
C	0.49462100	-3.07970600	1.62964700
C	1.62694100	-2.99574500	0.77182700
C	1.27572000	-3.56824700	-0.47681000
H	-0.63774400	-4.54616100	-1.16187600
H	-1.54158100	-3.93853700	1.27834100

H	0.44819900	-2.73596500	2.65323400
H	2.57645200	-2.54151200	1.00836300
H	1.92961500	-3.65607300	-1.33278300

Table 25. Atom coordinates and absolute energy of **Int9** (Energy= -2347.84363415 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	1.39981500	-1.96283300	0.64435300
C	2.22406200	-2.38432900	-0.87412300
O	2.83995900	-2.78930000	-1.76320200
P	-1.98583900	-0.34298100	1.25969400
C	-1.80482300	1.38644300	1.89920500
C	-2.07456000	1.57057000	3.26656900
C	-1.98483800	2.83252600	3.85550000
C	-1.60347300	3.93506400	3.08859800
C	-1.31704400	3.76658300	1.73271300
C	-1.41954400	2.50517500	1.14178100
C	-3.67933400	-0.30596100	0.49667800
C	-4.27079800	0.83516300	-0.06914400
C	-5.54529500	0.77177700	-0.63388300
C	-6.25101400	-0.43366300	-0.64562700
C	-5.67740300	-1.57501700	-0.08423800
C	-4.40537100	-1.50808300	0.48732700
P	1.55089400	0.48024500	-1.45746300
C	3.16245200	0.98828500	-0.68621100
C	4.33656000	0.68268600	-1.39242400
C	5.59465100	1.01319000	-0.88173600
C	5.70126100	1.65828900	0.35107200
C	4.54340200	1.97344600	1.06733400
C	3.28893600	1.64048900	0.55297200
C	0.79157500	2.13358300	-1.89478700
C	1.17875100	3.38969400	-1.39713800
C	0.54348100	4.55951500	-1.82021000
C	-0.50059900	4.50232600	-2.74629600
C	-0.89168400	3.26599300	-3.26236700
C	-0.24157200	2.10076100	-2.85083900
C	-0.90136600	-0.35200100	-0.31812000
C	-1.12365600	-1.67177600	-1.01996800
C	-1.73996200	-1.78890200	-2.26990100
C	-1.85718900	-3.03528200	-2.88999500
C	-1.36312900	-4.18833800	-2.27369700
C	-0.75671300	-4.09093100	-1.02142400

C	-0.64860000	-2.84150100	-0.40491400
C	0.59939000	-0.15825400	0.02636200
H	-2.35760800	0.71418000	3.87379200
H	-2.20448300	2.95236200	4.91285900
H	-1.52458600	4.91749700	3.54581400
H	-1.01071900	4.61391600	1.12591700
H	-1.18651300	2.40432500	0.08780900
H	-3.74024900	1.78233100	-0.05890600
H	-5.98912000	1.66616000	-1.06303800
H	-7.24410500	-0.48030800	-1.08387500
H	-6.22140800	-2.51558500	-0.08328300
H	-3.96997300	-2.39786800	0.93435700
H	4.26006200	0.17205500	-2.34856800
H	6.48923200	0.76484400	-1.44633500
H	6.67783200	1.91582600	0.75163500
H	4.61779000	2.47991200	2.02619100
H	2.40037300	1.89726300	1.12237500
H	1.99190100	3.46184800	-0.68315800
H	0.86988400	5.51964500	-1.42834400
H	-0.99382400	5.41358000	-3.07294300
H	-1.68978500	3.20912500	-3.99783700
H	-0.52383600	1.14817000	-3.29300700
H	-1.28125700	0.45155000	-0.96301600
H	-2.12459400	-0.89996000	-2.76111700
H	-2.33446600	-3.10608600	-3.86342100
H	-0.37586500	-4.97736100	-0.52253500
H	-0.34694200	-2.79308500	0.65780400
H	0.67832900	0.55900900	0.84862500
H	-1.45354400	-5.15266500	-2.76442300
C	1.56223900	-3.33463600	2.34278600
C	1.06170700	-2.06353400	2.78679300
C	2.05269300	-1.09209000	2.50095300
C	3.13965500	-1.73084500	1.84245500
C	2.83982200	-3.13736800	1.77969600
H	1.03602900	-4.27885500	2.40069400
H	0.10310200	-1.88214100	3.25113700
H	1.97227400	-0.03251300	2.69087700
H	4.04369600	-1.25196300	1.49556500
H	3.46565200	-3.90039200	1.33683400

Table 26. Atom coordinates and absolute energy of **Int9`** (Energy= -2347.88049385 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z

Fe	-0.23302400	-1.77570800	-0.53392700
C	-0.15000500	-1.17186800	-2.16677500
O	-0.08636900	-0.87495800	-3.28848500
P	-1.78131700	-0.35322100	0.19275000
C	-2.61789200	-0.68887400	1.80551700
C	-3.99137700	-0.97382000	1.86662200
C	-4.60053800	-1.29147500	3.08244200
C	-3.85021000	-1.32951400	4.25765000
C	-2.48196100	-1.05436200	4.20935900
C	-1.87045200	-0.74416300	2.99483200
C	-3.13368600	0.32986800	-0.84461900
C	-3.81794100	1.50636900	-0.49330200
C	-4.83989500	1.99438600	-1.30498300
C	-5.19670100	1.31148000	-2.47158800
C	-4.52682700	0.14069400	-2.82589300
C	-3.49676700	-0.34626100	-2.01784300
P	2.20630200	0.56730300	-0.66039600
C	3.44440400	-0.81777500	-0.55819000
C	3.68635400	-1.55747400	-1.72732400
C	4.61274600	-2.60289900	-1.74062400
C	5.32613200	-2.91956700	-0.58300700
C	5.11007800	-2.18168400	0.58346000
C	4.17960500	-1.14012300	0.59419600
C	2.98444500	1.78479300	0.52106700
C	3.89830800	2.70688800	-0.01738500
C	4.51781500	3.66379400	0.78623700
C	4.22274300	3.73050600	2.14992700
C	3.30900200	2.83096800	2.70013700
C	2.69816100	1.86812600	1.89244300
C	-0.40922300	0.89086100	0.54579900
C	-0.50140800	2.21811700	-0.17867700
C	-0.66226900	3.38849500	0.58102400
C	-0.78187900	4.63874700	-0.02648800
C	-0.74139700	4.74498500	-1.41681800
C	-0.58113600	3.59187600	-2.18673700
C	-0.46496800	2.34240600	-1.57751100
C	0.76119000	-0.12924100	0.27543600
H	-4.59301700	-0.93775700	0.96450200
H	-5.66538300	-1.50513300	3.10791600
H	-4.32568400	-1.57279400	5.20329700
H	-1.88746500	-1.08270800	5.11820200
H	-0.80217900	-0.55041100	2.97852700
H	-3.54554900	2.04503500	0.40881800

H	-5.35640800	2.90934700	-1.02970000
H	-5.99359900	1.69480800	-3.10255700
H	-4.79966800	-0.39236000	-3.73203900
H	-2.96855300	-1.25252100	-2.29746100
H	3.14462000	-1.30454100	-2.63509800
H	4.78628400	-3.16051200	-2.65734500
H	6.05391200	-3.72624700	-0.59228200
H	5.67175800	-2.41292100	1.48492500
H	4.03572300	-0.56352800	1.50326700
H	4.11997100	2.67530800	-1.08149300
H	5.22376100	4.36368400	0.34699900
H	4.69711900	4.48066100	2.77665000
H	3.07116400	2.87695000	3.76001200
H	1.99324700	1.17345800	2.34043000
H	-0.45173900	1.12499700	1.61435200
H	-0.68250800	3.31892900	1.66599500
H	-0.89929300	5.52716900	0.58790500
H	-0.54546400	3.66075400	-3.27026200
H	-0.33989600	1.46609100	-2.20015900
H	1.09671200	-0.50254600	1.25042000
H	-0.83047800	5.71601300	-1.89570900
C	-0.57484900	-3.84782400	-1.11749600
C	-1.18154200	-3.61330700	0.13582500
C	-0.16319500	-3.21938000	1.06392800
C	1.08016000	-3.23409700	0.37257500
C	0.83491800	-3.59663100	-0.97555000
H	-1.08047800	-4.14225900	-2.02708800
H	-2.23909200	-3.68237700	0.35236100
H	-0.31745300	-2.98583500	2.10716600
H	2.04220500	-2.95881700	0.77885300
H	1.58257800	-3.68120500	-1.75074500

Table 27. Atom coordinates and absolute energy of **Int10** (Energy= -3152.86166668 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	-1.21774600	0.07728700	-1.53537700
P	-2.55615700	-0.74838800	0.11022800
H	-1.95607000	-0.98239900	1.36069600
C	-3.29854800	-2.41433300	-0.17852600
C	-3.66500000	-2.81952800	-1.46967000
C	-3.53066700	-3.28704400	0.89673100
C	-4.26177500	-4.06414700	-1.68180900

H	-3.47239200	-2.16342100	-2.31278600
C	-4.11795000	-4.53410600	0.68329900
H	-3.24764800	-2.99269100	1.90330900
C	-4.48748600	-4.92372300	-0.60640300
H	-4.53966400	-4.36452300	-2.68802000
H	-4.28687900	-5.20131900	1.52377500
H	-4.94414000	-5.89526500	-0.77191300
C	-4.04317900	0.21454800	0.65696900
C	-5.26907900	0.08804600	-0.01406200
C	-3.95901000	1.08873300	1.75129400
C	-6.38010800	0.83145700	0.38760200
H	-5.37086400	-0.61439300	-0.83622900
C	-5.07389600	1.82580400	2.15495100
H	-3.01463400	1.19664300	2.27471100
C	-6.28528900	1.70498800	1.47197000
H	-7.32200100	0.71823600	-0.14181900
H	-4.99456200	2.49231700	3.00949100
H	-7.15120700	2.27984300	1.78757800
C	-0.68333000	-1.50568200	-2.06211600
O	-0.48417200	-2.53281200	-2.56125300
P	2.45251100	-1.20915700	-1.30247000
C	3.18876300	0.31394900	-2.07322900
C	3.21898200	0.35243200	-3.47685900
C	3.74654500	1.45087200	-4.16095700
C	4.25044200	2.54012800	-3.44959900
C	4.22869500	2.52121000	-2.05258600
C	3.70363500	1.41981600	-1.37323800
C	3.93393400	-2.01968700	-0.52184200
C	5.19040400	-1.42065500	-0.33878900
C	6.25170700	-2.13600200	0.22044400
C	6.07847200	-3.46379400	0.61183800
C	4.83758700	-4.07691300	0.42893900
C	3.78273900	-3.36610900	-0.14244800
P	-0.26889800	1.50759300	1.22416400
C	-0.25976100	3.28202600	0.64573600
C	-1.30655300	4.10014900	1.10202800
C	-1.35525700	5.46100100	0.78879100
C	-0.35428800	6.03412300	0.00448700
C	0.69301300	5.23653600	-0.46245300
C	0.73859300	3.87780100	-0.14481900
C	1.03718900	1.66682300	2.56179800
C	2.29862600	2.26740100	2.41217800
C	3.18922400	2.35139600	3.48341900
C	2.83059900	1.84618700	4.73618900

C	1.57657000	1.26014000	4.90796200
C	0.69371500	1.17093800	3.82902900
C	1.54023400	-0.48274100	0.22439800
C	1.20480600	-1.61266400	1.19086500
C	1.88347400	-1.67668600	2.42016300
C	1.65656800	-2.70971500	3.32944900
C	0.74489200	-3.72244700	3.02953500
C	0.07432300	-3.68962500	1.80651800
C	0.30498600	-2.65151800	0.90055200
C	0.42721400	0.51417000	-0.22917400
H	2.82450200	-0.49213500	-4.03621300
H	3.76247300	1.45462100	-5.24741700
H	4.65926000	3.39700500	-3.97765000
H	4.62630600	3.36269500	-1.49109100
H	3.70451000	1.42159400	-0.28717700
H	5.35417700	-0.39298600	-0.64412200
H	7.21633000	-1.65168700	0.34864100
H	6.90502900	-4.01873700	1.04710100
H	4.69178300	-5.11306100	0.72183800
H	2.82752800	-3.86018800	-0.29420300
H	-2.09460100	3.66293500	1.70918900
H	-2.17720500	6.07014400	1.15521100
H	-0.38964900	7.09114300	-0.24382000
H	1.47744200	5.67228300	-1.07576600
H	1.55989400	3.27999600	-0.52995400
H	2.58476900	2.69410400	1.45622000
H	4.16052300	2.81870500	3.34335000
H	3.52195000	1.91637600	5.57141000
H	1.28450700	0.87055300	5.87948600
H	-0.27832000	0.70562800	3.96857400
H	2.30239300	0.10890100	0.74596600
H	2.60185200	-0.90199800	2.66835600
H	2.19802100	-2.72205400	4.27144500
H	-0.62852000	-4.47597400	1.54519900
H	-0.20712300	-2.67569700	-0.05059500
H	0.95715200	1.22244700	-0.86953500
H	0.56718900	-4.53079300	3.73355700
C	-2.05957300	0.35040000	-3.53086600
C	-0.79408500	1.02545600	-3.45187700
C	-0.92027000	2.05219800	-2.48327600
C	-2.21889600	1.99483900	-1.91925400
C	-2.92745700	0.94147200	-2.58548300
H	-2.29711300	-0.47797400	-4.18504000
H	0.08738300	0.80805600	-4.03806100

H	-0.14167400	2.73744300	-2.19066800
H	-2.61254200	2.64506300	-1.15264600
H	-3.95207700	0.65537800	-2.39618100

Table 28. Atom coordinates and absolute energy of **TS6** (Energy= -3152.79511325 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	-1.39463800	0.41516700	-1.70687200
P	-2.70377800	-0.46497200	-0.05123100
H	-1.19342700	-0.18482500	0.26627700
C	-3.43876500	-2.14097200	-0.20396700
C	-3.75714000	-2.70127100	-1.45101600
C	-3.72993300	-2.87611500	0.95946200
C	-4.34377400	-3.96641000	-1.53492800
H	-3.54854300	-2.14476200	-2.35825500
C	-4.32192000	-4.13556900	0.87477500
H	-3.48660600	-2.45811200	1.93150000
C	-4.62724500	-4.68535100	-0.37352400
H	-4.58138100	-4.38622200	-2.50834100
H	-4.54080200	-4.69032600	1.78293100
H	-5.08393600	-5.66888500	-0.43877800
C	-4.08151700	0.56862400	0.59230800
C	-5.40095900	0.31159900	0.17560200
C	-3.85357500	1.63086600	1.48225200
C	-6.45909600	1.09637900	0.63541500
H	-5.60506200	-0.51132500	-0.50280700
C	-4.91517000	2.41741800	1.93225600
H	-2.84185000	1.82957900	1.82298800
C	-6.22082500	2.15551000	1.51326200
H	-7.47098900	0.87838100	0.30450600
H	-4.71964700	3.23212500	2.62465700
H	-7.04496600	2.76643900	1.87050100
C	-0.96460300	-1.15401400	-2.38439500
O	-0.80282700	-2.13865100	-2.97033500
P	2.19596400	-1.15179000	-1.35094600
C	3.28378100	0.29175100	-1.78689500
C	3.36776200	0.61695700	-3.15157000
C	4.17438700	1.66570100	-3.59902500
C	4.91394500	2.41670300	-2.68445800
C	4.84157400	2.11183400	-1.32309600
C	4.03341000	1.06205100	-0.87997600
C	3.42756400	-2.43215100	-0.80224300

C	4.74474600	-2.18253400	-0.38625100
C	5.59301500	-3.23134000	-0.02575300
C	5.14100600	-4.55082000	-0.07156700
C	3.83721600	-4.81659300	-0.49258900
C	2.99520900	-3.76895000	-0.86470800
P	-0.11210600	1.70592500	1.40258700
C	0.42942800	3.37442600	0.78150900
C	-0.31293400	4.47733600	1.23719100
C	0.01870300	5.77970100	0.85744100
C	1.09826300	6.00534700	0.00217500
C	1.84406800	4.92106500	-0.46512600
C	1.51224400	3.62051000	-0.07882900
C	1.11839200	1.43142500	2.77380000
C	2.44441300	1.89595300	2.78110900
C	3.27632700	1.67038000	3.87937000
C	2.79607700	0.98063000	4.99553700
C	1.47792100	0.52295000	5.00824300
C	0.64859500	0.75035100	3.90846800
C	1.39339400	-0.57334600	0.29556900
C	0.99982200	-1.79079600	1.11708300
C	1.70435400	-2.08683900	2.29459600
C	1.41248200	-3.22388500	3.04773200
C	0.40709000	-4.09967400	2.63580400
C	-0.29630800	-3.82705500	1.46204500
C	0.00059400	-2.68788900	0.71153500
C	0.30583100	0.49929700	-0.01010000
H	2.79538800	0.03408400	-3.86857600
H	4.22444500	1.89490800	-4.65990500
H	5.54361300	3.23250500	-3.02831200
H	5.41598700	2.69056500	-0.60465800
H	3.99152900	0.84537300	0.18343700
H	5.12416900	-1.16723800	-0.35518700
H	6.61007400	-3.01466200	0.29039800
H	5.80241000	-5.36561800	0.20984500
H	3.47680600	-5.84039600	-0.54135100
H	1.98769700	-3.98856600	-1.20512300
H	-1.16052000	4.31022700	1.89706100
H	-0.57085100	6.61571400	1.22376600
H	1.35473500	7.01674900	-0.30031200
H	2.68838800	5.08245700	-1.13004200
H	2.10770500	2.79533200	-0.45472500
H	2.82639800	2.45589500	1.93333700
H	4.29810900	2.04071700	3.86714000
H	3.44275000	0.81071500	5.85190600

H	1.09230400	-0.00712100	5.87469300
H	-0.37907700	0.39800600	3.92769000
H	2.19349800	-0.08230300	0.86079200
H	2.48949100	-1.41396000	2.62629300
H	1.97363700	-3.42423200	3.95646200
H	-1.08045900	-4.49808900	1.12432000
H	-0.54382900	-2.50993800	-0.20727800
H	0.70380900	1.13288200	-0.80604400
H	0.17770700	-4.98671200	3.21991400
C	-2.31363100	1.02676600	-3.55423900
C	-0.95081900	1.49161700	-3.55826100
C	-0.80108800	2.38968800	-2.47901100
C	-2.04212100	2.47610500	-1.77951700
C	-2.97904100	1.64914200	-2.46981500
H	-2.75181600	0.33205700	-4.25748800
H	-0.17978400	1.20085400	-4.25817500
H	0.11196400	2.89445600	-2.19940600
H	-2.24648600	3.08563000	-0.91184400
H	-4.00746300	1.48602600	-2.18066200

Table 29. Atom coordinates and absolute energy of **1a** (Energy= -1918.28405363 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
H	-0.86705500	-1.00249200	-1.83018400
P	1.79892600	0.41035700	-1.42637900
C	1.25446200	2.15764600	-1.11491600
C	1.54436300	3.08635000	-2.12900000
C	1.18577000	4.42833500	-2.00146200
C	0.50896300	4.86525300	-0.86169300
C	0.19925100	3.95353400	0.14817700
C	0.57204400	2.61353300	0.02540500
C	3.39002100	0.31914800	-0.47348900
C	3.71336900	1.14391700	0.61498600
C	4.93856800	1.01148900	1.26952600
C	5.86043500	0.05118400	0.84883400
C	5.55326700	-0.77324200	-0.23402600
C	4.33166000	-0.63440100	-0.89335900
P	-2.08640100	-1.31113900	0.25945000
C	-3.66505000	-0.90937800	-0.62634000
C	-4.85212800	-1.40312200	-0.05511000
C	-6.08675600	-1.19040600	-0.66382100
C	-6.16091300	-0.49411200	-1.87275400

C	-4.99269600	-0.01121700	-2.45995600
C	-3.75569100	-0.21351300	-1.84155700
C	-2.12211400	-0.07976300	1.65377000
C	-2.72010300	1.18786000	1.56547200
C	-2.69008600	2.06646800	2.64867200
C	-2.05746600	1.69504500	3.83813900
C	-1.46180200	0.43796400	3.94127500
C	-1.50124300	-0.44445500	2.85896800
C	0.63180900	-0.60682300	-0.30269500
C	1.15211600	-2.02978000	-0.20637300
C	1.68505400	-2.50724200	0.99870500
C	2.17996500	-3.80733100	1.10264500
C	2.15593900	-4.65662200	-0.00359400
C	1.63714200	-4.19232000	-1.21345000
C	1.14325400	-2.89204900	-1.31398400
C	-0.80476900	-0.49974200	-0.85919600
H	2.05364600	2.74987200	-3.02842000
H	1.42557400	5.12930700	-2.79595600
H	0.21929500	5.90759300	-0.76416900
H	-0.33523900	4.28008200	1.03569900
H	0.31663100	1.92869400	0.82731500
H	3.01179100	1.90275100	0.94664800
H	5.17387800	1.66139800	2.10795500
H	6.81462600	-0.04911900	1.35831300
H	6.26657400	-1.51988900	-0.57132400
H	4.10352900	-1.27353800	-1.74153200
H	-4.80473500	-1.96212000	0.87625100
H	-6.99042900	-1.57609400	-0.20036600
H	-7.12137200	-0.33499600	-2.35428700
H	-5.03925300	0.52874700	-3.40163600
H	-2.86439500	0.17865800	-2.31957200
H	-3.22118000	1.48398800	0.64865200
H	-3.16454300	3.04061700	2.56635800
H	-2.03692800	2.37962900	4.68131700
H	-0.97575300	0.13871800	4.86561800
H	-1.05235600	-1.43012500	2.94988400
H	0.65902600	-0.17192500	0.70221000
H	1.71456700	-1.84969000	1.86334100
H	2.58453800	-4.15511900	2.04892200
H	1.61626200	-4.84365300	-2.08266600
H	0.75130500	-2.54413000	-2.26534400
H	-1.06389100	0.55148200	-1.02095900
H	2.53819100	-5.67016900	0.07505500

Table 30. Atom coordinates and absolute energy of **Int4`** (Energy= -1542.82825101 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	0.17273600	-1.32151600	-0.87296300
P	-0.47358300	0.39544400	0.70324100
C	-0.51741700	2.09277000	-0.04762200
C	0.45368800	2.52627300	-0.96824300
C	-1.43306900	3.05044200	0.43273800
C	0.49853100	3.85228000	-1.40112800
H	1.17806800	1.81933000	-1.35469400
C	-1.38753400	4.37476000	-0.00113600
H	-2.19013500	2.75888200	1.15374400
C	-0.42254500	4.78467900	-0.92328600
H	1.25672400	4.15440000	-2.11920800
H	-2.11102100	5.08858100	0.38432800
H	-0.38872800	5.81612100	-1.26254500
C	-2.28983600	0.08419600	0.98097200
C	-2.65743600	-0.50168400	2.20501500
C	-3.31433200	0.37628100	0.06053400
C	-3.99047700	-0.80443900	2.49592200
H	-1.88848800	-0.70671700	2.94636500
C	-4.64645300	0.08084300	0.35004900
H	-3.07006800	0.84754300	-0.88585300
C	-4.99003700	-0.51617600	1.56695700
H	-4.24621000	-1.25484300	3.45131700
H	-5.41955100	0.31766000	-0.37637000
H	-6.02831100	-0.74524600	1.79007000
C	-0.73185400	-0.33835300	-2.01172800
O	-1.32871500	0.23908300	-2.81587500
C	0.88914200	-3.13014900	0.13633300
C	-0.38134500	-2.75801200	0.64327300
C	-1.31236000	-2.76679400	-0.43646700
C	-0.61068500	-3.19038900	-1.61155500
C	0.74402000	-3.39882200	-1.25952600
H	1.80948500	-3.18485500	0.69966700
H	-0.60397700	-2.47640900	1.66199800
H	-2.36137000	-2.51756500	-0.37012300
H	-1.03391000	-3.29310100	-2.60161300
H	1.54265800	-3.66332100	-1.93803400
C	2.11185600	-0.51156700	-0.75528000
C	3.07375600	-0.14894900	0.26327900
C	2.85494700	-0.38554100	1.63064400

C	4.29239100	0.43858600	-0.13701900
C	3.82981800	-0.05122500	2.56980900
H	1.90838000	-0.80630100	1.94593800
C	5.26091500	0.76981600	0.80501400
H	4.46613200	0.62803600	-1.19181900
C	5.03384700	0.52486600	2.16284900
H	3.64413400	-0.23632900	3.62386000
H	6.19426900	1.22119300	0.48082500
H	5.79013700	0.78635400	2.89728600
C	1.78635700	-0.68221300	-1.95687800
H	1.93078500	-0.66719100	-3.02083500

Table 31. Atom coordinates and absolute energy of **TS3`** (Energy= -1542.79012337 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	-1.08657000	-1.47203900	-0.84972200
P	-0.15003600	0.36698600	0.25347600
C	0.50255300	1.73704000	-0.79974300
C	1.14170600	1.47325100	-2.02874400
C	0.52792200	3.06737300	-0.33311100
C	1.75932600	2.48839300	-2.75992800
H	1.15521500	0.46176000	-2.41922000
C	1.13991700	4.08262500	-1.06774000
H	0.06254400	3.31192600	0.61611100
C	1.75981500	3.80224500	-2.28697500
H	2.23127900	2.25095200	-3.71009400
H	1.13312400	5.09882800	-0.68153600
H	2.23409700	4.59408500	-2.85970400
C	-1.42417700	1.23562800	1.28135700
C	-1.39902000	1.08188900	2.67694300
C	-2.46601200	1.99674100	0.71776200
C	-2.38234200	1.65957900	3.48548700
H	-0.59364000	0.51157300	3.13324500
C	-3.44334900	2.58114300	1.52316000
H	-2.50521400	2.13100000	-0.35961400
C	-3.40702100	2.41136100	2.91096500
H	-2.34159300	1.52756800	4.56354500
H	-4.23747100	3.16745400	1.06803100
H	-4.17068500	2.86467700	3.53680900
C	-1.27040500	-0.65641600	-2.37940300
O	-1.46703300	-0.14839100	-3.40277800
C	-2.97643500	-1.59881000	0.17752300

C	-3.06717100	-2.34595700	-1.02672300
C	-2.10028900	-3.39246200	-0.98255500
C	-1.45403500	-3.32049200	0.29137900
C	-1.98370300	-2.22331000	1.00375300
H	-3.55728100	-0.72522100	0.43475700
H	-3.71834800	-2.12191500	-1.86126400
H	-1.91687400	-4.12691000	-1.75449600
H	-0.65362900	-3.96529000	0.62778900
H	-1.68183100	-1.89028200	1.98644300
C	1.77105000	-1.60046000	-0.34107300
C	2.88298500	-1.25727600	0.46025300
C	3.73660800	-0.19148300	0.08596600
C	3.19808000	-2.02808600	1.60470800
C	4.86441500	0.09268500	0.84475900
H	3.48488300	0.40477000	-0.78423700
C	4.32928500	-1.73267200	2.35463800
H	2.54225100	-2.84539400	1.88590100
C	5.16238800	-0.67330200	1.97772300
H	5.51445100	0.91340300	0.55763600
H	4.56666600	-2.32551500	3.23273700
H	6.04575300	-0.44536100	2.56712900
C	0.86966800	-2.03544800	-1.11587100
H	1.01337200	-2.75942700	-1.91418500

Table 32. Atom coordinates and absolute energy of **Int5-2** (Energy= -1542.81706576 a.u.)

	Coordinates (Angstroms)		
Atom	X	Y	Z
Fe	-3.06154800	-0.54683400	-0.15366800
P	0.73468000	0.52617700	-1.05165200
C	2.40525000	-0.21863500	-1.35310600
C	2.46292100	-1.21228300	-2.34524100
C	3.59264100	0.13504300	-0.69360400
C	3.66502600	-1.84864800	-2.65555500
H	1.55739700	-1.48445900	-2.88215100
C	4.79884500	-0.48961300	-1.01463200
H	3.57974800	0.90688500	0.06841000
C	4.83816700	-1.48601900	-1.99165000
H	3.68691600	-2.61752700	-3.42289900
H	5.70855600	-0.20122300	-0.49483500
H	5.77790700	-1.97257400	-2.23758900
C	1.11426200	2.11829000	-0.17955200
C	0.45153800	2.50878400	0.99508900

C	1.96025800	3.05262600	-0.80524100
C	0.64214400	3.78233500	1.53726000
H	-0.21277300	1.80711200	1.49076700
C	2.15564400	4.32099400	-0.25995900
H	2.47343000	2.78456500	-1.72495800
C	1.49682900	4.69243500	0.91479000
H	0.12438500	4.05959300	2.45181200
H	2.82094700	5.02226800	-0.75639800
H	1.64680200	5.68169500	1.33750400
C	-3.01109300	-1.78786800	-1.40861100
O	-3.01272600	-2.55491300	-2.27106400
C	-3.75093400	1.05454800	1.07137300
C	-3.41052500	1.54648400	-0.21507200
C	-4.21920500	0.86691800	-1.17067600
C	-5.12203600	0.00243900	-0.45397900
C	-4.81459600	0.10140500	0.91854800
H	-3.28590600	1.33886200	2.00511800
H	-2.61392100	2.24135400	-0.44009000
H	-4.19105700	1.00861900	-2.24177700
H	-5.86323000	-0.64824000	-0.89699800
H	-5.27798500	-0.46503400	1.71506500
C	0.02268600	-0.56421300	0.27804500
C	0.82135000	-1.30636800	1.29655600
C	1.76723700	-0.66720500	2.11647100
C	0.62530300	-2.68882900	1.46487500
C	2.47711600	-1.38330300	3.07962400
H	1.93219300	0.39953300	2.01160300
C	1.33554400	-3.40406000	2.42892700
H	-0.07940900	-3.20460300	0.81882900
C	2.26503200	-2.75392900	3.24196800
H	3.19742300	-0.86645100	3.70803300
H	1.16842100	-4.47231100	2.53696200
H	2.82201500	-3.30967900	3.99086200
C	-1.30751900	-0.68296000	0.19200100
H	-1.86132700	-1.37426000	0.96949000