

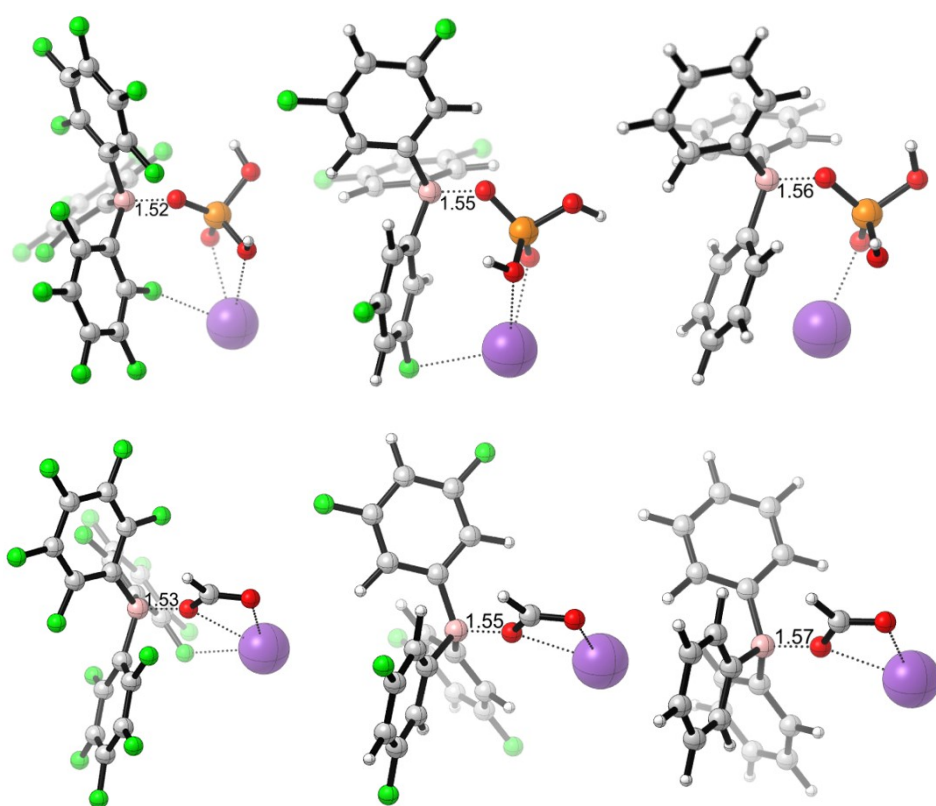
## SUPPORTING INFORMATION FOR

### In Silico Design of Metal-Free Hydrophosphate Catalysts for Hydrogenation of CO<sub>2</sub> to Formate

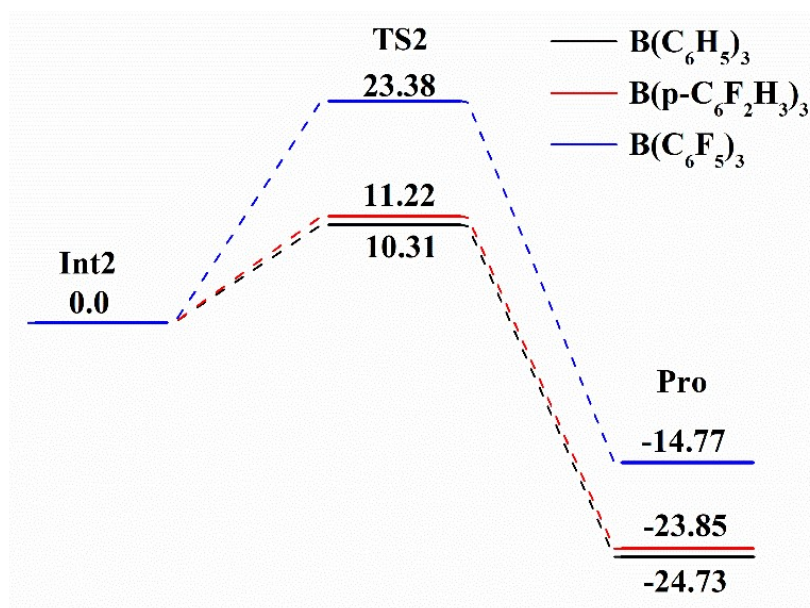
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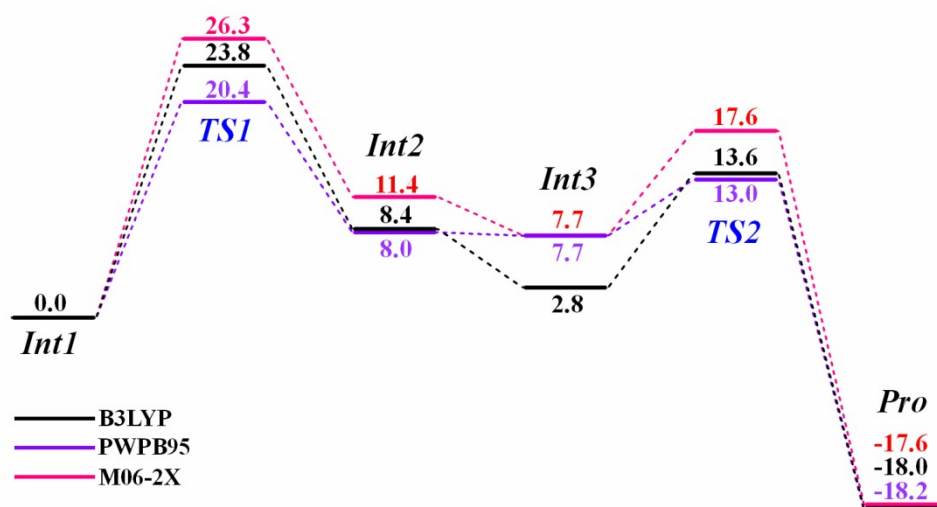


**Figure S1.** The optimized structure of, H: white. C: gray. O: red. B: pink. F: green.K: purple. Solvent is omitted for clarity.



**Figure S2.** The real barrier height of TS2.

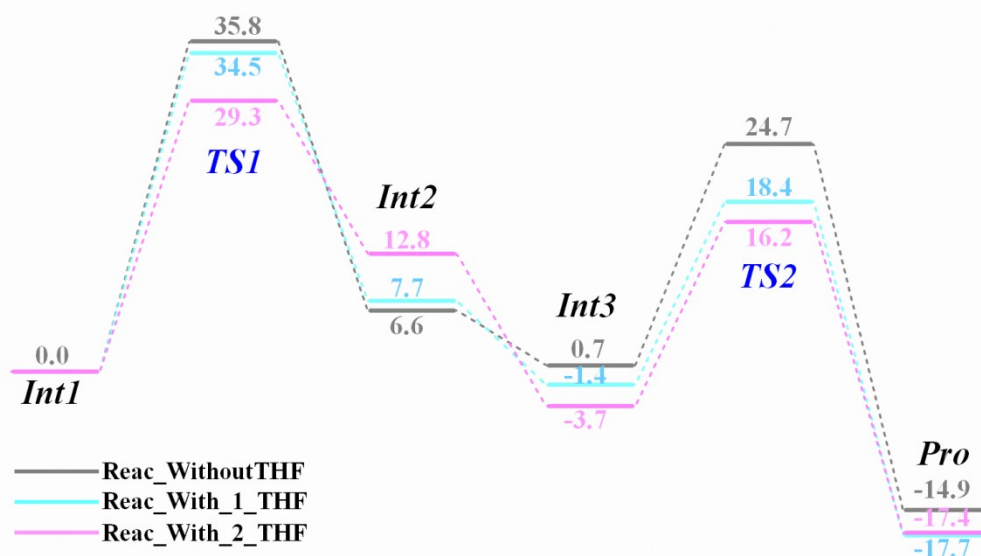
The real barrier height of TS2 can be calculated by subtracting the energy of Int2 from the energy of TS2. Thus, as Figure 2 shown, the real height of B(C<sub>6</sub>H<sub>5</sub>)<sub>3</sub>, B(p-C<sub>6</sub>F<sub>2</sub>H<sub>3</sub>)<sub>3</sub> and B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> are 10.31, 11.22 and 23.38 kcal/mol, respectively.



**Figure S3.** The energy profile (in kcal/mol, Lewis pair is B(C<sub>6</sub>H<sub>5</sub>)-KH<sub>2</sub>PO<sub>4</sub>) for the hydrogenation of CO<sub>2</sub>.

Besides the M06-2X that has been mentioned in our manuscript, B3LYP<sup>[1,2]</sup>-D3(BJ)/6-311g(d,p) and PWPB95<sup>[3]</sup>-D3<sup>[4]</sup>(BJ)/def2-TZVPP are calculated to prove the essential chemistry is not affected by the choice of functional. The calculation of B3LYP-D3(BJ) and PWPB95-D3(BJ) was performed by Gaussian and ORCA<sup>[5]</sup>, respectively. As Fig.S3 shown, the rate-determining step for three functionals is the step of TS1. Beside the B3LYP-D3(BJ), the profile calculated by M06-2X is also consistent with the result of the double hybrid

PWPB95-D3(BJ).



**Figure S4.** The energy profile (in kcal/mol, Lewis pair is  $B(C_6H_5)_3-KH_2PO_4$ ) for the hydrogenation of  $CO_2$ .

- [1] A. D. Becke *J. Chem. Phys.*, 1993, **98**, 5648 —5652  
[2] P. J. Stephens, F. J. Devlin, C. F. Chabalowski and M. J. Frisch, *J. Phys. Chem.*, 1994, **98**, 11623 —11627  
[3] L. Goerigk and S. Grimme, *J. Chem. Theory Comput.*, 2011, **7**, 291 —309  
[4] S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104  
[5] ORCA—an ab initio, density functional and semiempirical program package, V. 4.0.0, F. Neese, MPI für Chemische Energiekonversion, Mülheim A. D. Ruhr, Germany, 2017.

### Cartesians coordinates of the optimized structures

$K_2CO_3$ -BCF(M062x/6-311++G\*\*)

Reactant

C	-3.28903500	1.44765700	-1.39182300
O	-3.73598400	2.00850100	-0.37901000
O	-3.59633400	0.35144100	-1.91295200
K	-4.09777200	-2.02495100	-1.85316400
O	-2.26676300	2.15497600	-2.01991500
B	0.66011600	-0.18487000	-0.62988300
C	-0.62513400	0.09428200	0.37165100
C	1.86199200	0.92217500	-0.51846500
C	1.13246400	-1.70969200	-0.29047300
C	-0.78200300	1.03737300	1.38120000

C	-1.90818200	1.14215000	2.19404500
C	-2.96645900	0.26344000	2.03386400
C	-2.85629000	-0.70075500	1.04793400
C	-1.72189400	-0.75455800	0.25768000
C	1.54941700	-2.06366200	0.98945800
C	1.89500700	-3.35319500	1.36334200
C	1.81537900	-4.37031400	0.41979000
C	1.39512600	-4.07262900	-0.86708500
C	1.06279800	-2.76108900	-1.19432800
C	3.20684300	0.68136400	-0.24326000
C	4.18356900	1.67556900	-0.21961400
C	3.83950500	2.99205300	-0.47987300
C	2.51545600	3.28612700	-0.77213700
C	1.59115000	2.25697800	-0.79344600
F	-1.73044900	-1.72398200	-0.69281700
F	-3.87648800	-1.55567900	0.81683800
F	-4.06453700	0.36795700	2.77412600
F	-2.00015100	2.14330600	3.08352900
F	0.16134400	1.98519000	1.60241400
F	0.63754700	-2.55914300	-2.45490900
F	2.13312500	-5.62280500	0.75323100
F	2.29792700	-3.63124300	2.60656400
F	1.64111400	-1.10967800	1.93445500
F	0.31609400	2.62469600	-1.09345100
F	3.65567000	-0.55699800	0.01023300
F	2.13859000	4.54971500	-1.01805100
F	4.75856200	3.95722000	-0.45442400
F	5.45353600	1.36757400	0.04989900
F	1.29418600	-5.05149700	-1.77504700
H	-1.86887800	1.58135200	-2.68825100
H	0.22299400	-0.13799400	-1.75938200
K	-1.77617000	3.63654600	0.12042700

TS1

C	-2.93535400	0.13389200	-1.71517500
O	-3.75259200	0.72574900	-0.91324400
O	-2.94079600	-1.14791400	-1.82891100
K	-2.89060700	-3.47589100	-1.79813800
O	-2.07168000	0.83399700	-2.38896200
B	0.69304800	0.01414500	0.31757300
C	-0.76472200	-0.15443100	0.87193600
C	1.38186300	1.44041100	0.22594200
C	1.63295800	-1.24925700	0.13143000
C	-1.43499900	0.82307600	1.61831500
C	-2.74425000	0.69467800	2.04531900
C	-3.45929200	-0.45161700	1.72615700
C	-2.82535100	-1.46460000	1.03045600
C	-1.51968900	-1.30067700	0.61664600
C	1.61505200	-2.34526500	0.99323400
C	2.45590600	-3.43997000	0.84447500

C	3.36340900	-3.46463900	-0.20550100
C	3.42610400	-2.39106500	-1.08422700
C	2.57939700	-1.30959800	-0.89285500
C	2.70995000	1.65656800	0.59851400
C	3.33337800	2.89612200	0.52070600
C	2.62502400	3.98708000	0.03994100
C	1.30168600	3.82150500	-0.34620600
C	0.71409800	2.57259700	-0.23931900
F	-0.99332800	-2.33012600	-0.07771500
F	-3.48740100	-2.59476200	0.72890000
F	-4.72052800	-0.58258100	2.10307900
F	-3.33368800	1.67554500	2.73239400
F	-0.80879300	1.95711900	1.97290300
F	2.70346300	-0.29201800	-1.75111200
F	4.17083800	-4.50775300	-0.36550600
F	2.39662200	-4.46525100	1.69504400
F	0.77381200	-2.37827800	2.03465100
F	-0.56797800	2.48736400	-0.61437300
F	3.45783800	0.65531200	1.07847500
F	0.60091500	4.86194400	-0.80634700
F	3.20300400	5.17916800	-0.04425800
F	4.60093800	3.04316500	0.90085600
F	4.30045100	-2.40559500	-2.08893500
H	-0.47255800	0.18158500	-1.91500500
H	0.20966700	-0.10264300	-1.65688300
K	-3.02930400	3.00734100	-1.62966500

Int1

C	-3.34490900	1.17445700	-1.73839500
O	-3.03106400	2.33475500	-1.45109000
O	-4.36538900	0.51979800	-1.46805200
K	-4.39079500	-1.93688300	-1.39701100
O	-2.36893300	0.46284500	-2.53739700
B	0.43233700	-0.02911500	-0.38876300
C	-0.88270100	0.44084500	0.47824900
C	1.76256300	0.88328100	-0.11877800
C	0.88271500	-1.57881600	-0.13787400
C	-1.05758600	1.66790900	1.11147700
C	-2.20592700	2.04516500	1.79989500
C	-3.28538300	1.17716600	1.85866000
C	-3.17822300	-0.04573400	1.21655300
C	-2.00972500	-0.36768400	0.55418200
C	0.59133700	-2.37488200	0.96537200
C	1.05196900	-3.67880800	1.11291500
C	1.85761900	-4.23547300	0.13118500
C	2.19044000	-3.47782400	-0.98355600
C	1.70361800	-2.18192500	-1.08942800
C	2.36366900	0.89857500	1.13876900
C	3.55108600	1.55763200	1.41765600
C	4.19607200	2.25450000	0.40092000
C	3.63730100	2.27805500	-0.86671900
C	2.44626500	1.59547600	-1.09240000

F	-2.03622100	-1.55451100	-0.12485000
F	-4.22049000	-0.89702400	1.18270300
F	-4.40500600	1.51761000	2.48531400
F	-2.28734500	3.24538100	2.36840600
F	-0.10282600	2.62293500	1.01423300
F	2.07097900	-1.48843300	-2.18115100
F	2.30651200	-5.48462300	0.25596200
F	0.72374800	-4.40001500	2.18852200
F	-0.18373100	-1.91243000	1.96221300
F	1.94602200	1.68692700	-2.35469900
F	1.77210100	0.24658700	2.15079900
F	4.23576200	2.95340400	-1.85090200
F	5.33598200	2.89693800	0.64620700
F	4.08147800	1.53670000	2.63969900
F	2.96952300	-4.00035000	-1.93386100
H	-1.75211600	-0.01366600	-1.96032000
H	0.14362600	0.05776400	-1.57089400
K	-0.55182100	2.60261800	-1.96415200

## Int2

C	-3.58070800	-1.72606200	-2.67152100
O	-4.95292300	-1.47320500	-2.58136500
O	-3.16930400	-2.32186500	-3.67438200
K	-0.63601900	-2.05806500	-2.73796300
O	-2.93757200	-1.29132400	-1.68364100
B	0.41522600	0.12456400	-0.12000600
C	1.94524500	0.35695200	-0.62464400
C	0.44719800	-0.97279300	1.09427100
C	-0.41295600	1.48260900	0.25525700
C	2.91970500	0.86340900	0.23183200
C	4.24771500	1.03594400	-0.12663600
C	4.65488700	0.68041200	-1.40789800
C	3.72671300	0.16187100	-2.29704500
C	2.40803700	0.01192700	-1.88401500
C	-0.01191500	2.80421100	0.08537000
C	-0.84460800	3.90211700	0.30307900
C	-2.15949000	3.70692500	0.69590800
C	-2.60248600	2.40581500	0.87741700
C	-1.73154300	1.35189900	0.67187200
C	0.33157400	-0.70324000	2.45479900
C	0.38612000	-1.68493400	3.43897800
C	0.56975100	-3.01158800	3.07687600
C	0.69332000	-3.33450800	1.73274000
C	0.63098000	-2.31665900	0.79316300
F	1.56239100	-0.51417500	-2.81359300
F	4.10452600	-0.19315400	-3.52921600
F	5.92614600	0.83454700	-1.77576200
F	5.13772300	1.53424400	0.73281200
F	2.56566100	1.22568600	1.47422200
F	-2.25514100	0.11620100	0.88879000
F	-2.98379700	4.73744900	0.88155500
F	-0.39525900	5.14233000	0.11247000
F	1.22740900	3.09998100	-0.32992500
F	0.76211200	-2.70260700	-0.50630500
F	0.13537900	0.55243300	2.88717700
F	0.86489000	-4.60689200	1.36159300

F	0.62387800	-3.96551100	4.00633600
F	0.25723500	-1.36535200	4.72837100
F	-3.89131000	2.15959000	1.21807700
H	-0.22885200	-0.35906100	-1.02025000
K	-4.65298800	-0.16894600	-0.19436200
H	-5.35959500	-1.83817600	-3.37869100

KHCO<sub>3</sub>-BCF(M062x/6-311++G\*\*)

Reactant

C	-2.98558600	-1.29871700	2.20295500
O	-3.74316300	-2.19022400	2.91520700
O	-3.52688700	-0.17881000	2.02070600
K	-4.29817700	1.96414900	1.33917200
O	-1.86840200	-1.68531600	1.80734700
B	0.54584600	-0.01304000	-0.10115200
C	-0.79313100	-0.56088400	-0.74611400
C	1.82672900	-0.94516600	0.02233800
C	0.82816100	1.55775100	-0.07660500
C	-0.90639800	-1.80504700	-1.36680600
C	-2.11709500	-2.33536300	-1.79595600
C	-3.28506500	-1.61040900	-1.61527900
C	-3.21434000	-0.36002300	-1.02136000
C	-1.99393200	0.12968100	-0.60555700
C	0.41559800	2.42770100	-1.08320400
C	0.73202300	3.77980700	-1.09094800
C	1.49340600	4.30908900	-0.05790000
C	1.93257500	3.47966700	0.96569300
C	1.60332500	2.13239500	0.92969600
C	3.06354800	-0.58158000	-0.50758000
C	4.19159200	-1.38672300	-0.41649300
C	4.10483300	-2.60634000	0.23872100
C	2.89296400	-3.01002500	0.78569200
C	1.78527700	-2.18590900	0.65995700
F	-2.02024400	1.34480100	-0.01155600
F	-4.33221000	0.37157700	-0.85199200
F	-4.45220000	-2.09383500	-2.02164900
F	-2.16279900	-3.52666800	-2.38574900
F	0.17223300	-2.55856900	-1.59451900
F	2.05718000	1.36896200	1.93282600
F	1.79467700	5.60300900	-0.04569400
F	0.30848700	4.57206700	-2.07589800
F	-0.31234900	1.97982100	-2.11510800
F	0.63632600	-2.61584900	1.17871700
F	3.21350900	0.57826700	-1.16604100
F	2.80647600	-4.18282100	1.40945600
F	5.17429100	-3.38759700	0.33761000

F	5.34816000	-1.00109300	-0.95381900
F	2.66333600	3.97954100	1.95970000
H	-3.21031200	-2.99326800	2.98316500
H	-0.40713600	-0.50918900	1.60975000
H	0.16046300	0.01969700	1.62842500

### TS1

C	-2.98558600	-1.29871700	2.20295500
O	-3.74316300	-2.19022400	2.91520700
O	-3.52688700	-0.17881000	2.02070600
K	-4.29817700	1.96414800	1.33917200
O	-1.86840200	-1.68531600	1.80734700
B	0.54584600	-0.01304000	-0.10115200
C	-0.79313100	-0.56088400	-0.74611400
C	1.82672900	-0.94516600	0.02233800
C	0.82816100	1.55775100	-0.07660500
C	-0.90639800	-1.80504700	-1.36680600
C	-2.11709500	-2.33536300	-1.79595600
C	-3.28506500	-1.61040900	-1.61527900
C	-3.21434000	-0.36002300	-1.02136000
C	-1.99393200	0.12968100	-0.60555700
C	0.41559800	2.42770100	-1.08320400
C	0.73202300	3.77980700	-1.09094800
C	1.49340500	4.30908900	-0.05790000
C	1.93257500	3.47966700	0.96569300
C	1.60332500	2.13239500	0.92969600
C	3.06354800	-0.58158000	-0.50758000
C	4.19159200	-1.38672200	-0.41649300
C	4.10483300	-2.60633900	0.23872100
C	2.89296400	-3.01002500	0.78569200
C	1.78527700	-2.18590900	0.65995700
F	-2.02024400	1.34480100	-0.01155600
F	-4.33221000	0.37157600	-0.85199200
F	-4.45220000	-2.09383600	-2.02164900
F	-2.16279900	-3.52666800	-2.38574900
F	0.17223300	-2.55856900	-1.59451900
F	2.05718000	1.36896200	1.93282600
F	1.79467600	5.60300900	-0.04569400
F	0.30848600	4.57206700	-2.07589800
F	-0.31234900	1.97982100	-2.11510800
F	0.63632600	-2.61584900	1.17871700
F	3.21350900	0.57826700	-1.16604100
F	2.80647700	-4.18282100	1.40945600
F	5.17429100	-3.38759600	0.33761000
F	5.34816000	-1.00109200	-0.95381900
F	2.66333600	3.97954100	1.95970000
H	-3.21031200	-2.99326800	2.98316500
H	-0.40713600	-0.50918900	1.60975000
H	0.16046300	0.01969700	1.62842500

### Int1

C	-2.45425800	-1.87240400	1.81947000
O	-3.38171900	-2.48885700	1.09360500
O	-2.72323500	-0.88227500	2.47261800
K	-3.86796100	1.36082800	2.39981200
O	-1.28165800	-2.46356500	1.74706900
B	0.30663100	0.03596100	0.41779200
C	-1.06022000	-0.20531000	-0.45624300
C	1.46727600	-1.08387200	0.19263600



C	0.95110500	1.51277300	0.14913600
C	-1.35160600	-1.22530800	-1.35905100
C	-2.59144900	-1.37896400	-1.98127100
C	-3.63015900	-0.50785800	-1.68897300
C	-3.38915000	0.51609600	-0.78655200
C	-2.13151900	0.64513500	-0.22525100
C	0.75689700	2.30051200	-0.98008600
C	1.35090000	3.54509500	-1.16125100
C	2.19238400	4.04803100	-0.18066700
C	2.42447200	3.29811300	0.96423700
C	1.80775700	2.06125200	1.10107200
C	2.16511100	-1.18417500	-1.00824600
C	3.20563600	-2.07546000	-1.22224200
C	3.59377700	-2.92372600	-0.19128900
C	2.93517000	-2.86166000	1.02679000
C	1.90005400	-1.94795800	1.18669900
F	-1.99177400	1.68327200	0.64920400
F	-4.38517200	1.35125700	-0.40495900
F	-4.83302000	-0.66192800	-2.23907600
F	-2.80229700	-2.38631100	-2.83032200
F	-0.43839200	-2.15484900	-1.66685100
F	2.07569800	1.37787200	2.22764500
F	2.77268200	5.23950800	-0.33420800
F	1.11935800	4.25827100	-2.26735200
F	-0.04644000	1.88403000	-1.97684900
F	1.29758000	-1.94917100	2.40489100
F	1.81517300	-0.39163000	-2.03375300
F	3.29746600	-3.67338600	2.02398600
F	4.58760900	-3.79295300	-0.37423100
F	3.83370900	-2.13416700	-2.39800100
F	3.23186400	3.77402100	1.91722700
H	-2.98358500	-3.22613700	0.60563200
H	-0.57675200	-1.91785400	2.15193000
H	-0.04813800	0.00964000	1.58104100

## Int2

C	-4.05431600	-1.41149800	-2.60589200
O	-4.97054700	-1.71621300	-3.51528300
O	-2.87598500	-1.63774800	-2.78154800
K	-0.35362800	-1.91460000	-3.04540400
O	-4.58049300	-0.85113200	-1.52902300
B	0.16892900	0.09358100	-0.21709400
C	1.70860700	0.48346800	-0.58846200
C	0.20063500	-1.09163500	0.91618400
C	-0.78802300	1.34165300	0.21599300
C	2.61068800	0.89403500	0.39156900
C	3.94384400	1.18431200	0.14146500
C	4.43620500	1.05953400	-1.15327500
C	3.58325800	0.64897400	-2.16519100

C	2.25668900	0.37401200	-1.85543500
C	-0.43684700	2.67727400	0.38218700
C	-1.34922400	3.67336500	0.72217700
C	-2.68649100	3.35469800	0.90567400
C	-3.08994400	2.03651200	0.74580900
C	-2.13921800	1.08848600	0.41119000
C	-0.00848400	-0.92206900	2.28330700
C	0.05791900	-1.96345100	3.20401000
C	0.34970600	-3.24918100	2.77099200
C	0.56945800	-3.47253300	1.41934000
C	0.49148800	-2.39807500	0.54716100
F	1.49006600	-0.03764000	-2.90901100
F	4.03719000	0.51064600	-3.41511600
F	5.71412500	1.32566800	-1.41694900
F	4.75779000	1.57897900	1.12020900
F	2.18193800	1.03509100	1.65320300
F	-2.60019400	-0.19204900	0.27244300
F	-3.57170800	4.29840000	1.22126300
F	-0.95084100	4.93758500	0.86447200
F	0.83022100	3.08340600	0.20977600
F	0.72202200	-2.69288400	-0.76771300
F	-0.29560300	0.28633800	2.78587900
F	0.84648500	-4.70259700	0.97609400
F	0.41593200	-4.25759600	3.63857400
F	-0.15258200	-1.73971700	4.50111800
F	-4.37439300	1.69549200	0.89933900
H	-5.84890500	-1.45889900	-3.19870200
H	-0.36819700	-0.36789000	-1.20079400
H	-3.88215400	-0.63233100	-0.88056800

$K_2H_2PO_4$ -BCF(M062x/6-311++G\*\*)

Reactant

C	-0.86187200	3.89693800	-0.27177800
C	-0.50150800	2.57690900	-0.06815700
F	-3.70637100	1.08424000	0.59582600
F	-4.43026700	3.61405100	0.22649800
F	-2.57168900	5.51200800	-0.35407400
F	0.05845200	4.82135400	-0.53989400
C	0.36240200	-0.23679200	1.28223600
F	-1.40021700	-2.28917400	2.14985200
F	-3.15737000	-4.22827900	1.65797300
F	-4.68842000	-4.16148400	-0.58797700
F	-4.43970400	-2.10082600	-2.34261400
C	0.88541500	0.62336800	2.24780600
C	2.07755000	0.37818400	2.91838200
C	2.80662600	-0.76797800	2.62099200
C	2.31591200	-1.65202400	1.67516400
H	-0.29094000	-0.02555900	-1.35535500
C	1.11745200	-1.38005000	1.04290100
F	0.24037700	1.74899800	2.58014600
F	2.52977200	1.23063700	3.83984100
F	3.95807700	-1.00796400	3.23744500
C	-3.03406200	-3.22132900	0.79541000

C	-3.68843900	-2.13465400	-1.24563700
F	3.01898700	-2.74229900	1.33631200
C	-2.77900100	-1.12534800	-0.97157900
C	-1.96044300	-1.11731700	0.16008900
C	-3.81754400	-3.18965300	-0.34981400
C	-2.12418300	-2.19835100	1.02570600
F	0.70840200	-2.28765200	0.14244200
B	-0.94146500	0.06083600	0.43567500
F	-2.69497700	-0.12392900	-1.85294100
F	0.81134700	2.29558500	-0.15165100
C	-1.40942900	1.55867200	0.21969600
C	-2.74198900	1.96396000	0.30476800
C	-3.14760100	3.28000500	0.11940500
C	-2.20206100	4.25166700	-0.17495300
H	0.45946100	-0.11953800	-1.23803500
P	2.99781600	-0.06046800	-2.54113800
O	2.48642200	-0.40133800	-1.08802100
O	4.03598300	1.05265400	-2.50059500
O	1.61406300	0.58763200	-3.20359100
O	3.33285400	-1.32465200	-3.31943600
K	3.47758900	1.88997000	-0.23689800
H	1.77056000	0.79094700	-4.13338700
K	2.84533100	-2.97849700	-1.54519900

## TS1

C	0.86187200	3.89693800	0.27177800
C	0.50150800	2.57690900	0.06815700
F	3.70637100	1.08424000	-0.59582600
F	4.43026700	3.61405100	-0.22649800
F	2.57168900	5.51200800	0.35407400
F	-0.05845200	4.82135400	0.53989400
C	-0.36240200	-0.23679200	-1.28223600
F	1.40021700	-2.28917400	-2.14985200
F	3.15737000	-4.22827900	-1.65797300
F	4.68842000	-4.16148400	0.58797700
F	4.43970400	-2.10082600	2.34261400
C	-0.88541500	0.62336800	-2.24780600
C	-2.07755000	0.37818400	-2.91838200
C	-2.80662600	-0.76797800	-2.62099200
C	-2.31591200	-1.65202400	-1.67516400
H	0.29094000	-0.02555900	1.35535500
C	-1.11745200	-1.38005000	-1.04290100
F	-0.24037700	1.74899800	-2.58014600
F	-2.52977200	1.23063700	-3.83984100
F	-3.95807700	-1.00796400	-3.23744500
C	3.03406200	-3.22132900	-0.79541000
C	3.68843900	-2.13465400	1.24563700
F	-3.01898700	-2.74229900	-1.33631200
C	2.77900100	-1.12534800	0.97157900
C	1.96044300	-1.11731700	-0.16008900
C	3.81754400	-3.18965300	0.34981400
C	2.12418300	-2.19835100	-1.02570600
F	-0.70840200	-2.28765200	-0.14244200
B	0.94146500	0.06083600	-0.43567500

F	2.69497700	-0.12392900	1.85294100
F	-0.81134700	2.29558500	0.15165100
C	1.40942900	1.55867200	-0.21969600
C	2.74198900	1.96396000	-0.30476800
C	3.14760100	3.28000500	-0.11940500
C	2.20206100	4.25166700	0.17495300
H	-0.45946100	-0.11953800	1.23803500
P	-2.99781600	-0.06046800	2.54113800
O	-2.48642200	-0.40133800	1.08802100
O	-4.03598300	1.05265400	2.50059500
O	-1.61406300	0.58763200	3.20359100
O	-3.33285400	-1.32465200	3.31943600
K	-3.47758900	1.88997000	0.23689800
H	-1.77056000	0.79094700	4.13338700
K	-2.84533100	-2.97849700	1.54519900

Int1

C	2.81969900	2.21624000	0.76991300
C	1.86705200	1.23054100	0.58342900
F	-0.86863200	3.19130000	-0.63954700
F	0.91621500	5.09430600	-0.25149000
F	3.42585800	4.49500100	0.66237900
F	4.06535900	1.88794500	1.18955100
C	-0.52432900	-0.86967400	1.06720600
F	-2.15031400	1.81019200	1.57966400
F	-4.74727000	2.41272400	1.19419500
F	-6.02360700	1.57099400	-1.05623400
F	-4.65881800	0.11358500	-2.91984400
C	-0.14083400	-0.67689100	2.39275000
C	-0.27177100	-1.64763300	3.38213200
C	-0.82551400	-2.88012800	3.06896100
C	-1.24345300	-3.11957600	1.76722100
H	-0.02800800	-0.35484900	-1.14272600
C	-1.08540900	-2.11879500	0.82113700
F	0.39453600	0.48819700	2.79008800
F	0.12855400	-1.40298100	4.63046500
F	-0.96051000	-3.81833800	4.00386400
C	-4.08262500	1.70319600	0.28162600
C	-4.04171700	0.54148200	-1.81435100
F	-1.78973900	-4.29351500	1.44178000
C	-2.70123100	0.24960500	-1.58965000
C	-1.99762800	0.65244900	-0.46605000
C	-4.73814200	1.27705500	-0.86863300
C	-2.74629100	1.37854400	0.45669800
F	-1.54152400	-2.41063400	-0.42537100
B	-0.45653500	0.22154400	-0.16022100
F	-2.09546600	-0.48579100	-2.56264000
F	2.28174900	-0.02970900	0.88448400
C	0.57537000	1.46303000	0.12058600
C	0.31872100	2.80549200	-0.15370000

C	1.24187500	3.83420800	0.03057300
C	2.51290700	3.53973100	0.49455300
H	1.70951700	-1.96967300	-0.06017600
P	2.72236100	-1.84015400	-2.03921100
O	1.60601300	-2.35175800	-0.94330300
O	4.10743000	-2.18819700	-1.58866100
O	2.69104200	-0.19520900	-1.83338200
O	2.10204600	-2.20697300	-3.34934600
K	4.95788300	-0.13557600	-0.38974100
H	1.83789500	0.20128000	-2.06144900
K	-0.38588200	-2.54483500	-2.78853900

## Int2

O	-3.44715900	-1.85207300	-1.91931900
K	-1.07737000	-2.50679200	-1.85705200
B	0.77314500	0.07941900	-0.21585200
C	2.23976800	-0.37044300	-0.75982600
C	0.60355100	-0.51741600	1.30232800
C	0.45500700	1.67937600	-0.31024000
C	3.40396700	0.02026900	-0.10271700
C	4.67643500	-0.37308400	-0.48827000
C	4.82183200	-1.21729400	-1.58354200
C	3.69402200	-1.64722600	-2.26482500
C	2.44319500	-1.21756000	-1.83673900
C	1.27350200	2.69952600	-0.78690600
C	0.87564100	4.03342100	-0.87512600
C	-0.40303900	4.40359800	-0.48732900
C	-1.25527600	3.41780100	-0.01565300
C	-0.81028000	2.11190300	0.06052200
C	0.64623300	0.20386200	2.49190300
C	0.52158100	-0.38006800	3.74892000
C	0.35339200	-1.75274700	3.85713700
C	0.31077800	-2.52090400	2.70151200
C	0.43729800	-1.88628000	1.47551200
F	1.38601100	-1.69508900	-2.55028400
F	3.81484700	-2.47005400	-3.31096200
F	6.03343300	-1.61329100	-1.97088900
F	5.75718000	0.04229700	0.17270700
F	3.30905400	0.83463300	0.95908500
F	-1.71470700	1.21363800	0.54143000
F	-0.80996600	5.66839100	-0.57879100
F	1.71087400	4.96003000	-1.34293400
F	2.51804400	2.44526900	-1.21136600
F	0.39172000	-2.69638100	0.38121800
F	0.80365900	1.53813600	2.48012700
F	0.14695900	-3.84368300	2.78014500
F	0.23170300	-2.32732600	5.05299200
F	0.55883400	0.36869900	4.85307500
F	-2.52275500	3.72450400	0.35503300
H	-0.07966000	-0.43903600	-0.90286800
K	-4.32077600	1.65956600	0.55688200
P	-4.81364800	-1.55050700	-1.36921100
O	-5.01723900	-0.51281000	-0.29665000
O	-5.80002000	-1.11693400	-2.59002000
O	-5.41985800	-2.97081700	-0.85982400
H	-6.20383200	-2.83578400	-0.31332300
H	-5.59819500	-1.61465500	-3.39188100

KH<sub>3</sub>PO<sub>4</sub>-BCF(M062x/6-311++G\*\*)

## Reactant

C	-0.42748200	3.69932900	0.08755600
C	-0.33258300	2.32450800	0.19824100
F	2.99874100	1.76681900	-1.02699900
F	2.85409700	4.40737800	-1.23939800
F	0.58745200	5.73457500	-0.52284400
F	-1.56018300	4.32943600	0.41773600
C	-0.37557600	-0.85588700	-0.62231000
F	1.96274200	-2.18011400	-1.68783100
F	4.39363700	-3.22776700	-1.37496900
F	6.03940800	-2.32782900	0.59084500
F	5.21376700	-0.33171300	2.24660400
C	-1.35150300	-0.37681300	-1.49181400
C	-2.38791400	-1.15122000	-1.98111300
C	-2.49772400	-2.47636000	-1.59737900
C	-1.55525200	-3.00589100	-0.72815400
H	0.59516300	0.06164900	1.72848500
C	-0.53419600	-2.19649200	-0.25688600
F	-1.37462300	0.92147700	-1.88412700
F	-3.34421200	-0.57879100	-2.73180400
F	-3.50868900	-3.21458000	-2.02611600
C	3.98625200	-2.25926100	-0.55764500
C	4.40649600	-0.78164700	1.28840800
F	-1.65927600	-4.27021000	-0.33078300
C	3.14285300	-0.24283400	1.10772500
C	2.25018800	-0.68297100	0.13149100
C	4.83025400	-1.80012000	0.44373800
C	2.72141000	-1.70175600	-0.69419900
F	0.32559900	-2.75166300	0.59728900
B	0.82408900	-0.00293300	-0.04277800
F	2.78009300	0.75645700	1.92774200
F	-1.42341400	1.68654200	0.66700000
C	0.79436200	1.58932800	-0.15723500
C	1.86068400	2.34900400	-0.63735500
C	1.81031400	3.73458300	-0.76468900
C	0.65839000	4.41553900	-0.40039900
H	-0.09639900	-0.27667600	1.73468400
P	-3.20482400	-0.79970100	1.94087300
O	-1.75007100	-1.04582400	2.21845500
O	-3.80420400	-0.96422600	0.57264900
O	-3.56725000	0.78451400	2.28436200
H	-3.10357800	1.09180700	3.07325700
K	-3.94059300	1.36366400	-0.35694500

O	-4.08290000	-1.60313300	3.04007400
H	-3.49667900	-2.11326900	3.61302500
<b>TS1</b>			
C	-0.42748200	3.69932900	0.08755600
C	-0.33258300	2.32450800	0.19824100
F	2.99874100	1.76681900	-1.02699900
F	2.85409700	4.40737800	-1.23939800
F	0.58745100	5.73457500	-0.52284400
F	-1.56018300	4.32943600	0.41773600
C	-0.37557600	-0.85588700	-0.62231000
F	1.96274200	-2.18011400	-1.68783100
F	4.39363700	-3.22776700	-1.37496900
F	6.03940800	-2.32782800	0.59084500
F	5.21376700	-0.33171300	2.24660400
C	-1.35150300	-0.37681300	-1.49181400
C	-2.38791400	-1.15122000	-1.98111300
C	-2.49772400	-2.47636000	-1.59737900
C	-1.55525200	-3.00589100	-0.72815400
H	0.59516300	0.06164900	1.72848500
C	-0.53419600	-2.19649200	-0.25688600
F	-1.37462300	0.92147700	-1.88412700
F	-3.34421200	-0.57879100	-2.73180400
F	-3.50868900	-3.21458000	-2.02611600
C	3.98625200	-2.25926100	-0.55764500
C	4.40649600	-0.78164700	1.28840800
F	-1.65927600	-4.27021000	-0.33078300
C	3.14285300	-0.24283400	1.10772500
C	2.25018800	-0.68297100	0.13149100
C	4.83025400	-1.80012000	0.44373800
C	2.72141000	-1.70175600	-0.69419900
F	0.32559900	-2.75166300	0.59728900
B	0.82408900	-0.00293300	-0.04277800
F	2.78009300	0.75645700	1.92774200
F	-1.42341400	1.68654200	0.66700000
C	0.79436200	1.58932800	-0.15723500
C	1.86068400	2.34900400	-0.63735500
C	1.81031400	3.73458300	-0.76468900
C	0.65839000	4.41553900	-0.40039900
H	-0.09639900	-0.27667600	1.73468400
P	-3.20482400	-0.79970100	1.94087300
O	-1.75007100	-1.04582400	2.21845500
O	-3.80420400	-0.96422600	0.57264900
O	-3.56725000	0.78451400	2.28436200
H	-3.10357800	1.09180700	3.07325700
K	-3.94059300	1.36366400	-0.35694500
O	-4.08290000	-1.60313300	3.04007400
H	-3.49667900	-2.11326900	3.61302500

**Int1**

C	-0.84211100	3.61059700	0.64440800
C	-0.55213900	2.26467700	0.76420400
F	2.93675500	2.20957300	-0.01373300
F	2.45227600	4.80514400	-0.18363700
F	-0.05896500	5.79433100	0.20062200
F	-2.10997700	4.04623100	0.78990700
C	-0.22185900	-0.70583400	-0.43197900
F	2.24224400	0.07717100	-1.87632000
F	4.66150400	-1.01463100	-2.34666600

F	6.02369900	-2.22691500	-0.32312100
F	4.93794900	-2.33360700	2.16842800
C	-0.95231700	-0.16212700	-1.47725000
C	-1.86852800	-0.86443200	-2.25010500
C	-2.08836100	-2.20829200	-2.00993600
C	-1.36654900	-2.81144200	-0.99013900
H	0.41525200	-0.25284400	1.74046800
C	-0.46169900	-2.06788100	-0.24285000
F	-0.88236300	1.16491300	-1.77131800
F	-2.61468900	-0.20600700	-3.15823000
F	-2.99131500	-2.89118100	-2.70682700
C	4.12798000	-1.07133400	-1.12343500
C	4.26896800	-1.74020600	1.17632300
F	-1.61102800	-4.09367600	-0.67125600
C	3.01518400	-1.17771400	1.39756400
C	2.28074700	-0.55073100	0.39901500
C	4.82654500	-1.68768100	-0.09216700
C	2.88326600	-0.52436800	-0.85445500
F	0.15911900	-2.71993400	0.74847800
B	0.79477300	0.05349300	0.62413900
F	2.53183100	-1.26917900	2.64550900
F	-1.61892700	1.46088400	1.05554300
C	0.68369300	1.68216600	0.52927400
C	1.68055400	2.60334300	0.22080100
C	1.45472700	3.97697400	0.12151500
C	0.18146000	4.48988600	0.32132900
H	-1.31595000	-0.67141100	1.95003200
P	-3.37951600	-1.40758300	1.58585000
O	-1.97449300	-1.30039700	2.30657700
O	-3.57168900	-0.53759700	0.40136900
O	-4.47993600	-1.10212200	2.69126100
H	-4.42237100	-1.66408300	3.47634400
K	-3.42601600	1.61200900	-0.88391200
O	-3.57940300	-2.97252300	1.36653600
H	-2.83996000	-3.45409500	0.96399600
<b>Int2</b>			
O	-1.88727300	-1.46724700	-3.34054100
K	0.52207600	-2.08417600	-3.29965200
B	0.18029500	0.10892800	-0.17315600
C	1.80425100	0.30498300	-0.20721900
C	-0.13273200	-1.10958100	0.88418200
C	-0.60901400	1.51489700	0.14794600
C	2.51372100	0.61659100	0.95108600
C	3.89045600	0.79010200	0.99255900
C	4.63052800	0.64521700	-0.17429000
C	3.97406200	0.33450400	-1.35520000
C	2.59478500	0.17527500	-1.33689200
C	-0.07623600	2.77579000	-0.12585400



C	-0.74445300	3.97098500	0.12123600
C	-2.02421200	3.94500400	0.65365600
C	-2.61690400	2.71879700	0.92004600
C	-1.90563000	1.55887500	0.65590900
C	-0.50449700	-0.97631500	2.22272100
C	-0.70770900	-2.05581700	3.07630000
C	-0.52535800	-3.34956500	2.60821600
C	-0.13831500	-3.53984400	1.28999000
C	0.04819100	-2.42825200	0.48336600
F	2.02905300	-0.11079100	-2.54617700
F	4.66450600	0.18311900	-2.48955100
F	5.95249800	0.79885200	-0.15887400
F	4.50966300	1.08876300	2.13366300
F	1.84848500	0.78506900	2.10292200
F	-2.57318700	0.40281300	0.90524800
F	-2.68010500	5.07745300	0.89100300
F	-0.16841200	5.13908800	-0.16105500
F	1.14428800	2.90082300	-0.67333400
F	0.45523800	-2.69852600	-0.78895100
F	-0.69535800	0.23361700	2.76127300
F	0.05590000	-4.77304400	0.81564400
F	-0.71147800	-4.39237300	3.41296800
F	-1.07174600	-1.86049500	4.34274700
F	-3.85572700	2.66567300	1.40907800
H	-0.18691000	-0.26888100	-1.28056700
P	-2.87377600	-0.95423800	-2.36311700
O	-2.78312400	0.60605000	-2.04937000
H	-1.88604300	0.92535100	-1.85020300
O	-4.35672800	-1.13530600	-2.89074100
H	-5.04375400	-0.92435700	-2.24386800
O	-2.84748100	-1.69439200	-0.95349100
H	-2.55889300	-1.14693500	-0.20229700

### K<sub>2</sub>CO<sub>3</sub>-BCF-Solvent (M062x/6-311++G\*\*)

#### Reactant

C	-2.55568900	-1.30591700	0.63169200
O	-3.25023100	-2.04921400	-0.17276300
O	-3.13338900	-0.38221900	1.32784900
K	-3.30764900	1.98213600	2.05747800
O	-1.28071000	-1.48620500	0.72054900
B	1.70557100	0.67983600	-0.60042900
C	0.28263800	0.44621400	-1.19519600
C	2.80658600	-0.44593800	-0.62785300
C	2.08901700	2.08458300	0.00244900
C	0.02792900	-0.47573600	-2.21508100
C	-1.23393800	-0.70168700	-2.73549500
C	-2.31750800	0.01916600	-2.25156600
C	-2.11699500	0.95474800	-1.24951700
C	-0.84564100	1.12908100	-0.73238200
C	1.65890800	3.28693300	-0.56210900
C	2.00253800	4.52923700	-0.05261500
C	2.80060500	4.60228900	1.08068100
C	3.25211500	3.43487300	1.68015000
C	2.90205200	2.21176300	1.13032600
C	4.16164400	-0.15691800	-0.80885700
C	5.15326000	-1.12577400	-0.80329100
C	4.80584000	-2.45240400	-0.59233400
C	3.47355600	-2.79066000	-0.40107600
C	2.50847300	-1.79689900	-0.43096000
F	-0.74498000	2.00772900	0.27741600
F	-3.13674600	1.69442200	-0.80382800
F	-3.51898500	-0.15939800	-2.77975800

F	-1.41889700	-1.59962600	-3.70893600
F	1.02818000	-1.18395100	-2.75910900
F	3.37701000	1.12139900	1.74629300
F	3.13055800	5.78370300	1.58844900
F	1.57160900	5.64805600	-0.63509800
F	0.88737400	3.28416600	-1.65650200
F	1.24551800	-2.18652300	-0.23986200
F	4.56468900	1.10313100	-1.01485700
F	3.13218100	-4.06396300	-0.19942200
F	5.74190400	-3.39309000	-0.57628800
F	6.43060300	-0.79435700	-0.99056600
F	4.01962000	3.49937900	2.76798200
H	0.46597600	-0.38996200	1.55770800
H	1.07795900	-0.06478500	1.84662700
C	-5.94429300	0.21984200	-0.48424000
C	-6.13991300	1.46050500	-1.37591500
C	-6.26047000	0.76253800	0.90154700
C	-5.98954500	2.64587500	-0.39731700
O	-5.71138900	2.08415000	0.88955300
H	-6.59707100	-0.60994100	-0.76818300
H	-4.90728900	-0.13172800	-0.48203000
H	-7.13510800	1.46866700	-1.82900000
H	-5.40254700	1.50319800	-2.17975300
H	-5.76923200	0.20534400	1.70244500
H	-7.34325700	0.81805600	1.09035600
H	-6.91251300	3.23662900	-0.33965700
H	-5.16148400	3.31360000	-0.64887100
K	-1.24599500	-3.66751500	-0.67951200
C	-1.21091500	-3.17841800	3.42074600
C	0.22512500	-3.35526700	2.90649000
C	-2.03162000	-4.12704500	2.52536700
C	0.19028000	-4.77887700	2.36775500
O	-1.08913100	-4.88406100	1.74259700
H	-1.28915700	-3.47610400	4.47101500
H	-1.55179000	-2.14735900	3.31055700
H	0.98221500	-3.21333800	3.68200700
H	0.39665100	-2.65491500	2.08477900
H	-2.67469400	-3.58491600	1.82506600
H	-2.64201800	-4.82149900	3.11468200
H	0.27303500	-5.51877500	3.17799300
H	0.94956200	-4.99508200	1.61115100
TS1			
C	-2.26305200	-1.24020400	0.90691100
O	-3.11144300	-2.07491800	0.40400800
O	-2.65817200	-0.18463100	1.53078500
K	-3.52719600	2.12658200	1.80194400
O	-0.99534300	-1.47892300	0.77290900
B	1.60899300	0.57700600	-0.56746100
C	0.21976100	0.38369100	-1.27914600
C	2.78018300	-0.48088900	-0.74202900
C	1.99372600	1.98586600	0.05192600
C	0.00234900	-0.52574300	-2.31426000
C	-1.25288000	-0.80098700	-2.83278500
C	-2.35974100	-0.13477900	-2.32895000
C	-2.19057600	0.80637600	-1.32703000
C	-0.92639300	1.03345700	-0.81514900
C	1.60888700	3.19636500	-0.52108300
C	1.97432700	4.43031200	-0.00284400
C	2.75258900	4.48422000	1.14423400
C	3.16297400	3.30493600	1.74992600
C	2.78964200	2.09262400	1.19201000
C	4.10495800	-0.10515600	-0.96610600
C	5.14327700	-1.01839900	-1.09472500

C	4.87679300	-2.37406600	-0.98562900
C	3.57401300	-2.79846700	-0.76276600
C	2.56359700	-1.85711000	-0.65740100
F	-0.84730300	1.91696600	0.19000000
F	-3.24783200	1.48650500	-0.87085300
F	-3.57026800	-0.38017700	-2.82023300
F	-1.40491400	-1.69363900	-3.81614800
F	1.02699400	-1.18808100	-2.87192300
F	3.22738400	0.98530800	1.80829500
F	3.10338100	5.65836900	1.65951800
F	1.58266100	5.56054400	-0.59347700
F	0.85857700	3.21490300	-1.63171200
F	1.32675200	-2.32426900	-0.45662300
F	4.44028000	1.18699700	-1.08903100
F	3.30599500	-4.10157800	-0.65953100
F	5.85961300	-3.26145900	-1.09982900
F	6.39064200	-0.60249500	-1.31822300
F	3.91443600	3.34839600	2.85114700
H	0.44359100	-0.47075500	1.08352600
H	1.12631200	-0.10500500	1.20753300
C	-6.49574500	-0.10724900	-1.05080600
C	-6.38612100	1.26929600	-1.71664000
C	-5.80399400	0.10845200	0.30060900
C	-6.51899900	2.19625700	-0.51467600
O	-5.83298000	1.53315100	0.54887600
H	-7.54880000	-0.37137200	-0.90982600
H	-6.01701100	-0.90111800	-1.62844200
H	-7.15764500	1.44553300	-2.46966700
H	-5.40409100	1.39475500	-2.18061100
H	-4.75868000	-0.21980000	0.30464700
H	-6.32928400	-0.39642700	1.11885500
H	-7.57457000	2.33873700	-0.24231200
H	-6.05559600	3.17654900	-0.65648900
K	-1.19728900	-3.86338400	-0.13895500
C	-1.20283500	-2.98019400	4.37491600
C	-0.05933900	-2.16694700	3.76200000
C	-1.63995800	-3.81756300	3.17972000
C	0.59244200	-3.17759800	2.81744600
O	-0.42769500	-4.13745200	2.47972400
H	-0.83621100	-3.62789100	5.17900500
H	-2.01226900	-2.35892100	4.76570700
H	0.64397400	-1.77998200	4.50351300
H	-0.46591700	-1.34112500	3.17108900
H	-2.30105700	-3.24071600	2.51774000
H	-2.12662900	-4.75827100	3.45228100
H	1.41620800	-3.71956200	3.29759500
H	0.94611400	-2.70386800	1.89752600
Int1			
C	2.61699900	-1.60699300	-0.96527600
O	3.29682700	-2.59237700	-0.61634500
O	2.97587400	-0.51321400	-1.45305900
K	3.65765200	1.82950800	-2.07535500
O	1.25537400	-1.78372800	-0.77434700
B	-1.34604500	0.48470300	-0.16755900
C	-0.10280900	0.57500300	0.90198600
C	-2.54699000	-0.54873000	0.25402100
C	-1.84766300	2.01356900	-0.43254500
C	-0.05723100	0.10071700	2.20842500
C	1.07281700	0.17230700	3.01515800
C	2.22907500	0.76383100	2.53005400
C	2.22609400	1.28384600	1.24527500
C	1.07580500	1.18303600	0.47899900
C	-2.30346700	2.81116800	0.61189600

C	-2.69785100	4.13126700	0.46330900
C	-2.63765600	4.71411300	-0.79537500
C	-2.18714800	3.96414800	-1.86939800
C	-1.80252500	2.64218100	-1.66932200
C	-3.91221400	-0.27895800	0.21046400
C	-4.90089900	-1.21392800	0.50604900
C	-4.54507500	-2.50151900	0.86650300
C	-3.19838800	-2.82922600	0.92043200
C	-2.25423400	-1.86492700	0.60877100
F	1.14272400	1.71744400	-0.76181700
F	3.32577500	1.88150800	0.75617300
F	3.31905900	0.84603100	3.29741900
F	1.05609200	-0.31951600	4.25966600
F	-1.13778300	-0.46951100	2.77343000
F	-1.37561100	1.98167100	-2.76232200
F	-3.00940800	5.98599100	-0.96693500
F	-3.13826700	4.84723800	1.50507100
F	-2.39949600	2.28348500	1.84852000
F	-0.96557900	-2.26683500	0.66926700
F	-4.37230300	0.93865700	-0.13610200
F	-2.82479300	-4.06930000	1.26598000
F	-5.47772500	-3.41257800	1.15296000
F	-6.19424700	-0.87889200	0.43500600
F	-2.12324600	4.52139500	-3.08570300
H	0.77884800	-0.97618600	-1.02098600
H	-0.87510200	0.05706400	-1.20635500
C	5.56676500	-0.38943400	0.98106700
C	6.18029000	0.90329900	1.55120200
C	6.00166100	-0.34131300	-0.47723600
C	6.40714400	1.78346000	0.30149400
O	5.90201900	1.04549400	-0.81597600
H	5.91167700	-1.28893900	1.49605600
H	4.47261100	-0.36524100	1.02146500
H	7.13220700	0.69671500	2.04718800
H	5.52084600	1.38567900	2.27406800
H	5.34372200	-0.90035000	-1.14301300
H	7.04525600	-0.67104700	-0.59447000
H	7.47392200	1.98792400	0.14567600
H	5.87135100	2.73571500	0.33862100
K	1.27486200	-4.07814300	0.52125600
C	-0.06218800	-2.82683500	-3.50892500
C	-1.34044400	-2.82571900	-2.64850600
C	0.77639500	-3.98599700	-2.92819000
C	-1.34263800	-4.23217500	-2.06100100
O	0.03375800	-4.51916700	-1.82477600
H	-0.29615700	-3.01375900	-4.55999200
H	0.46810000	-1.87371500	-3.44494400
H	-2.24295500	-2.60919700	-3.22489200
H	-1.25847000	-2.09043100	-1.84443400
H	1.74684800	-3.66475400	-2.54118700
H	0.92949400	-4.77809000	-3.67148200
H	-1.75774600	-4.96118300	-2.77226900
H	-1.87129100	-4.32393900	-1.10885700
<b>Int2</b>			
C	-3.24610500	1.69407200	1.37338700
O	-4.57728000	2.07003700	1.58067500
O	-2.45719200	1.93098500	2.31414700
K	0.02906700	1.46713100	2.92539800
O	-3.04337500	1.15896500	0.27028700
B	0.80426900	-0.39938700	-0.19589700
C	1.53958500	-1.67158500	0.51463200
C	1.98491200	0.60211000	-0.73380400
C	-0.30098200	-0.77549200	-1.33634200

C	2.43591900	-2.48276500	-0.17541900
C	3.12937400	-3.53477000	0.40171100
C	2.94083400	-3.81133200	1.74994000
C	2.06733100	-3.02860900	2.48651100
C	1.39775700	-1.98399300	1.85855400
C	-0.67582900	-2.03906900	-1.77825000
C	-1.70286600	-2.26590500	-2.68975800
C	-2.41787500	-1.19388400	-3.19495200
C	-2.08297500	0.09028000	-2.78902800
C	-1.04272700	0.26657000	-1.89114900
C	2.34230100	0.84685500	-2.05509400
C	3.36154400	1.71671400	-2.42731200
C	4.09195400	2.37759900	-1.45239700
C	3.78847500	2.15537200	-0.11713900
C	2.75335600	1.28897400	0.20031000
F	0.57265000	-1.25951100	2.65122100
F	1.88449900	-3.27862400	3.78863300
F	3.59650500	-4.82045400	2.32834700
F	3.97412100	-4.28455500	-0.31530000
F	2.64826500	-2.26207400	-1.48565600
F	-0.73410300	1.53504000	-1.57701100
F	-3.41813800	-1.39102800	-4.06069100
F	-2.02313200	-3.51286700	-3.06175800
F	-0.06526700	-3.14948000	-1.31550500
F	2.48871700	1.13773000	1.52199600
F	1.70086200	0.23679900	-3.06827600
F	4.48497300	2.78258000	0.83927600
F	5.07869700	3.20965800	-1.79303500
F	3.65492500	1.91154900	-3.71755700
F	-2.76509000	1.13724400	-3.27163400
H	0.19232600	0.20928900	0.65724300
C	-0.87735900	4.23805200	0.27567600
C	0.62309400	4.13690100	-0.10059400
C	-0.84388600	4.64298900	1.75204300
C	1.34429300	4.37042900	1.23849600
O	0.37504700	4.07974500	2.24593900
H	-1.41860800	4.96418700	-0.33534400
H	-1.36462200	3.26411700	0.17025000
H	0.92204900	4.88032100	-0.84333800
H	0.84963600	3.14633300	-0.50437200
H	-1.66692400	4.23245200	2.33859400
H	-0.80402400	5.73569100	1.86974300
H	1.66189500	5.41766600	1.33866900
H	2.20916700	3.72634900	1.41092500
K	-5.51209600	0.42463700	-0.42260800
C	-2.27386900	-2.49777700	1.28618300
C	-2.50072400	-1.48693300	2.41155400
C	-4.02018800	-1.33943000	2.40499400
C	-3.31633700	-2.04010400	0.27273700
H	-1.25825600	-2.46691000	0.88256500
H	-2.48669400	-3.51720400	1.62590400
H	-2.03585800	-0.53232100	2.14589700
H	-2.11756300	-1.81546600	3.38010500
H	-4.50076900	-2.07960900	3.05627800
H	-4.35590800	-0.33958900	2.69932000
H	-3.66456000	-2.83249600	-0.39672400
H	-2.93454800	-1.19200000	-0.31081000
O	-4.43912000	-1.58813000	1.05119600
H	-4.63554100	2.46002700	2.46319500

KHCO<sub>3</sub>-BCF-Solvent (M062x/6-311++G\*\*)

Reactant

C	2.08018900	-1.64457200	-1.59736200
O	1.51944400	-2.26770000	-2.70272000
O	2.31002500	-0.42193700	-1.76719200
K	3.13713400	1.94582400	-1.88728000
O	2.28646100	-2.35156100	-0.59506600
B	-1.42467600	0.05874700	0.48298600
C	-0.00807600	-0.29636000	1.04316100
C	-2.44711700	-1.07805200	0.12720500
C	-1.84310300	1.56271800	0.29183400
C	0.22310800	-1.40338100	1.86763700
C	1.46652100	-1.71290900	2.38755900
C	2.55774700	-0.92184500	2.05801500
C	2.38373000	0.17562300	1.23380100
C	1.12106500	0.47183700	0.75764800
C	-1.42422400	2.57339000	1.16117900
C	-1.79020600	3.90173700	1.01092700
C	-2.59688600	4.26809100	-0.05761900
C	-3.03293600	3.30239300	-0.95439000
C	-2.66232600	1.98140300	-0.76023500
C	-3.82469000	-0.93428100	0.31506900
C	-4.73945300	-1.92572100	-0.00052900
C	-4.28630100	-3.11714600	-0.55064500
C	-2.92814500	-3.30513000	-0.76587600
C	-2.03979100	-2.29945400	-0.41797600
F	1.02566000	1.55766100	-0.02847100
F	3.43199700	0.92969100	0.88276700
F	3.76425700	-1.22902200	2.51928700
F	1.63186600	-2.77385600	3.17903700
F	-0.78958100	-2.20785600	2.21704500
F	-3.11767200	1.09694500	-1.65613700
F	-2.94981400	5.53690900	-0.22044200
F	-1.37289600	4.82676300	1.87476300
F	-0.64383900	2.28533500	2.20934100
F	-0.74674900	-2.53787900	-0.64645100
F	-4.32319800	0.19352800	0.83678800
F	-2.49250900	-4.44631000	-1.29825500
F	-5.14962400	-4.07294500	-0.86938600
F	-6.04299700	-1.74694800	0.21217000
F	-3.80555000	3.65140200	-1.98242800
H	1.34896500	-3.18161800	-2.43813700
H	-0.09110900	-0.02248800	-2.04492300
H	-0.81731800	0.08965700	-2.16776700
C	5.51412300	-1.21038500	-0.44050700
C	6.31216600	-0.27143100	0.48348300
C	5.63137700	-0.51329700	-1.78962800
C	6.30830700	1.07737100	-0.26856800
O	5.54918500	0.87701900	-1.46634100
H	5.91300000	-2.22758900	-0.45692000
H	4.45767500	-1.25759400	-0.15943800
H	7.33674100	-0.62910200	0.61462000
H	5.85579500	-0.18723000	1.47129700
H	4.81549100	-0.74295000	-2.47848300
H	6.59786700	-0.72091100	-2.27264600
H	7.32549200	1.38923200	-0.53606200
H	5.82968500	1.88525000	0.29066600
TS1			
C	2.30716000	-1.17650700	-2.06772300
O	3.21168800	-2.09486700	-2.56825300
O	2.77957300	-0.03702900	-1.87306000
K	3.61270900	2.23915400	-1.22859100

O	1.14424100	-1.59144600	-1.86754800
B	-1.35634400	-0.02267600	0.05425000
C	-0.03120600	-0.54182900	0.75567800
C	-2.61823500	-0.98551300	-0.09511900
C	-1.68426300	1.54084700	0.05667800
C	0.07752500	-1.76245800	1.41987000
C	1.27048400	-2.23033900	1.95390600
C	2.42050700	-1.46549400	1.83574000
C	2.35875900	-0.23870000	1.19103900
C	1.15253500	0.19018900	0.66946900
C	-1.32510400	2.40078100	1.09138700
C	-1.68127800	3.74193800	1.11695200
C	-2.42799000	4.27128300	0.07474300
C	-2.81384800	3.45189400	-0.97664600
C	-2.44577000	2.11557900	-0.95864000
C	-3.86810200	-0.66699200	0.43152700
C	-4.97089300	-1.50417500	0.32022300
C	-4.84713100	-2.71075700	-0.35028700
C	-3.62078300	-3.07030600	-0.89268100
C	-2.54129800	-2.21456700	-0.74796000
F	1.16216600	1.38218600	0.05168400
F	3.45484000	0.52247600	1.08689800
F	3.56634700	-1.89604700	2.35564200
F	1.31725700	-3.40448900	2.58532600
F	-0.98769600	-2.55646500	1.58710100
F	-2.85002600	1.35783800	-1.99073800
F	-2.77056900	5.55597500	0.08297800
F	-1.31065800	4.52463100	2.13179700
F	-0.61787300	1.95213400	2.13793700
F	-1.37284100	-2.60835000	-1.26333800
F	-4.05995200	0.47689900	1.10620500
F	-3.49192500	-4.23348600	-1.53259700
F	-5.89407300	-3.52210400	-0.46833000
F	-6.14311100	-1.15827700	0.85491600
F	-3.53431300	3.95063800	-1.98128100
H	2.72942900	-2.92554900	-2.67674700
H	-0.39143600	-0.45847300	-1.56521200
H	-0.96231600	0.06176800	-1.61980800
C	5.62686600	-1.35827900	-0.33002800
C	6.35411400	-0.71263400	0.86359700
C	5.94725200	-0.39722000	-1.46555300
C	6.51179300	0.76565000	0.44217500
O	5.90000400	0.89186300	-0.84577900
H	5.95854100	-2.37920100	-0.53188900

H	4.54265100	-1.36731500	-0.18328700
H	7.33533000	-1.17040500	1.01379200
H	5.79101900	-0.81330000	1.79296800
H	5.20556400	-0.41411400	-2.26510300
H	6.95565700	-0.57194000	-1.86972700
H	7.56883600	1.05030200	0.36929100
H	6.00820500	1.46314300	1.11694500

Int1

C	1.64922500	-2.22372600	-1.64740500
O	2.40046900	-3.07659800	-0.96073700
O	2.07737700	-1.15981000	-2.03512700
K	1.73070900	1.46930700	-2.30993000
O	0.41751800	-2.68111700	-1.84751100
B	-0.73198200	-0.00739400	-0.21710100
C	0.25993500	-0.85946100	0.76366400
C	-2.22223700	-0.63869600	-0.42439500
C	-0.89780800	1.54990200	0.27093800
C	-0.02029700	-2.04505600	1.43474600
C	0.90194400	-2.71535900	2.23353500
C	2.17924100	-2.20245100	2.39000400
C	2.51430400	-1.02605600	1.73619700
C	1.56306100	-0.40393500	0.94512800
C	-0.77051400	2.02194300	1.57449400
C	-0.94285600	3.35448100	1.92921200
C	-1.26429200	4.28826700	0.95633800
C	-1.40624900	3.87148900	-0.35811300
C	-1.22322600	2.52942600	-0.66285300
C	-3.17508400	-0.63925100	0.58994000
C	-4.47124300	-1.10383900	0.43279200
C	-4.86763300	-1.60371800	-0.80118600
C	-3.95824400	-1.63001500	-1.84531200
C	-2.67120200	-1.14949900	-1.63316100
F	1.95938300	0.73458400	0.32841000
F	3.74227300	-0.51237700	1.87072900
F	3.07450300	-2.83196400	3.15339700
F	0.56610600	-3.85355500	2.85089400
F	-1.23093500	-2.62514000	1.34290600
F	-1.36374200	2.19032600	-1.96414600
F	-1.43073700	5.57216900	1.28049000
F	-0.80100300	3.74621900	3.19998900
F	-0.45935500	1.18696200	2.58192600
F	-1.83994000	-1.21266600	-2.70515700
F	-2.83794900	-0.18021600	1.80838000
F	-4.32450600	-2.11116800	-3.03801300
F	-6.11160300	-2.05396900	-0.97663900
F	-5.34145200	-1.08070300	1.44763800
F	-1.71156300	4.75917900	-1.31087700
H	1.89544200	-3.87267600	-0.73223000
H	-0.12267600	-1.99289200	-2.27704400
H	-0.19977700	0.01461000	-1.30582600
C	5.39192000	-0.68072400	-1.04898500
C	5.92099200	0.49005600	-0.21393900
C	4.98076700	0.03755800	-2.32380400
C	4.98833000	1.64116500	-0.61982600
O	4.37236300	1.25055100	-1.86253700
H	6.13721200	-1.46107200	-1.21836400
H	4.50512600	-1.12690600	-0.58430100
H	6.95319700	0.71548800	-0.49919300
H	5.89537400	0.30117700	0.86037600
H	4.24141200	-0.50296500	-2.91760900



H	5.85482700	0.27604100	-2.94599400
H	5.52534600	2.58341500	-0.76834100
H	4.19082300	1.79759200	0.11258500
Int2			
C	-3.43955500	1.71094200	-2.07467100
O	-4.28811200	1.99891300	-3.05286000
O	-2.72872900	0.73213200	-2.10381300
K	-1.54756300	-1.55447200	-2.65108600
O	-3.48199400	2.59614600	-1.08414800
B	0.66359900	0.15400200	-0.16592400
C	2.03691700	-0.60742800	-0.60979900
C	0.09725300	-0.63774500	1.15509600
C	0.81978500	1.76834300	0.04312300
C	3.12816000	-0.69805000	0.24922300
C	4.29540600	-1.38062500	-0.05337000
C	4.40216200	-2.02865000	-1.27759400
C	3.34171100	-1.97718700	-2.16678900
C	2.19339600	-1.27699000	-1.81318200
C	1.94783400	2.54387500	-0.20461600
C	1.98686800	3.92692200	-0.04781600
C	0.85597000	4.60678800	0.37033000
C	-0.30106900	3.88426800	0.62385200
C	-0.28275900	2.51111200	0.45116700
C	0.02576600	-0.17811200	2.46525900
C	-0.47161400	-0.93525400	3.52105700
C	-0.90961100	-2.22951600	3.29270600
C	-0.84182500	-2.74580500	2.00669100
C	-0.34975500	-1.94460600	0.98802200
F	1.19861400	-1.28168000	-2.73286600
F	3.42940300	-2.60187400	-3.34700800
F	5.51726700	-2.69226600	-1.59187600
F	5.31774400	-1.42259600	0.80812500
F	3.07819500	-0.07451800	1.44100900
F	-1.45169500	1.86818300	0.72595300
F	0.87466300	5.93238400	0.52175200
F	3.10994700	4.60560000	-0.30526700
F	3.09806700	1.98628000	-0.62750800
F	-0.32332600	-2.50134900	-0.24964700
F	0.44908000	1.05803700	2.78763900
F	-1.25220800	-3.99756200	1.76703000
F	-1.38268600	-2.97339200	4.29466800
F	-0.52069600	-0.42871300	4.75767200
F	-1.41355000	4.51258000	1.02188200
H	-4.77231000	2.81700100	-2.86058100
H	-0.16503000	0.01069100	-1.03872100
H	-2.84812800	2.32638400	-0.39399900
C	-4.97141600	-0.58684700	-0.10014900
C	-3.74130800	-1.19787000	0.59757800
C	-5.02587300	-1.32644200	-1.45848100
C	-3.63428700	-2.54449500	-0.10837600
O	-3.91074000	-2.22755500	-1.47236500
H	-5.87881300	-0.78535200	0.47553600
H	-4.88697800	0.49602700	-0.21572400
H	-3.86243200	-1.28888000	1.67977800
H	-2.84250300	-0.60288600	0.39445100
H	-4.92545200	-0.66900900	-2.32437000
H	-5.95197500	-1.90535400	-1.55637700
H	-4.38420400	-3.25341300	0.27186000
H	-2.65219400	-3.01914000	-0.06572100

K<sub>2</sub>H<sub>2</sub>PO<sub>4</sub>-BCF-Solvent (M062x/6-311++G\*\*)

Reactant

C	-1.29927100	3.93841500	-1.51960200
C	-1.01464200	2.79160000	-0.79718200
F	-4.24814200	2.05773100	0.60757800
F	-4.81397400	4.29172600	-0.74180100
F	-2.87947000	5.55428300	-2.17106500
F	-0.35226200	4.55672700	-2.22306700
C	-0.24520000	0.71192400	1.51045100
F	-1.95301300	-0.98079500	3.06230100
F	-3.66938800	-3.00701500	3.20385000
F	-5.33888700	-3.54037500	1.12818400
F	-5.26835000	-1.99789000	-1.10819100
C	0.33984700	1.82305500	2.12487200
C	1.52449700	1.75687100	2.84266600
C	2.18580300	0.53995600	2.95126700
C	1.65234600	-0.58282900	2.33869600
H	-0.96854800	-0.40141200	-1.38032300
C	0.46326400	-0.48208100	1.63986400
F	-0.25647300	3.02005900	2.06732700
F	2.02849200	2.84086300	3.43281500
F	3.31537200	0.45208000	3.64335300
C	-3.62936800	-2.25494300	2.10563900
C	-4.44935100	-1.73596900	-0.09079000
F	2.28586700	-1.75782300	2.42368800
C	-3.55175900	-0.68200900	-0.15469100
C	-2.65949000	-0.37067400	0.87731300
C	-4.48611100	-2.52869500	1.04871800
C	-2.74107300	-1.19547000	2.00379800
F	0.00097900	-1.61201000	1.09191300
B	-1.61953100	0.80027400	0.75716100
F	-3.54492500	0.02446900	-1.29060800
F	0.25091100	2.34988500	-0.84668900
C	-1.97249600	2.09535800	-0.05734100
C	-3.25770200	2.64078100	-0.07723300
C	-3.57700900	3.79902400	-0.76882700
C	-2.59068100	4.44802000	-1.49848800
H	-0.23264100	-0.32546100	-1.26282000
P	2.64954200	-0.95622000	-2.21091500
O	2.04709800	-0.59919100	-0.83116900
O	3.61595300	0.11172700	-2.73534100
O	1.31233300	-0.89542100	-3.21669400
O	3.16930800	-2.39733200	-2.27645500
K	3.06255000	1.93617100	-0.96008400
H	1.58900300	-1.05407800	-4.12814600
K	2.16905400	-3.19337000	0.00437300
C	-1.53672200	-3.56897800	-0.92760800
O	-0.15469100	-3.86118600	-1.18138200
C	0.07797600	-3.94605400	-2.60049100
C	-1.06887400	-3.17144600	-3.23137900
C	-2.22816900	-3.52177100	-2.29361000
H	-1.94870800	-4.33837200	-0.26554200
H	-1.58499000	-2.59998000	-0.41678800
H	1.06183800	-3.51133200	-2.80139300
H	0.06183900	-5.00259500	-2.90177200
H	-0.83788400	-2.10266600	-3.19429800
H	-1.25272400	-3.46321100	-4.26817800
H	-3.04074700	-2.79105800	-2.32530500
H	-2.64295500	-4.50274200	-2.54695700
C	5.42742300	0.98281300	1.31433100
O	5.58965400	1.50623100	-0.00135000
C	6.17356100	0.45897700	-0.79656100
C	5.74787200	-0.87511500	-0.14488900
C	4.92189500	-0.43668300	1.08043100

H	6.39350000	0.98042200	1.84120800
H	4.73693400	1.63809400	1.85323800
H	5.77895600	0.56517900	-1.80843800
H	7.26375200	0.58058100	-0.79483200
H	5.15011100	-1.47813100	-0.83398300
H	6.62441800	-1.45369500	0.15926100
H	3.85901900	-0.41607700	0.80846300
H	5.05661300	-1.08507400	1.94973100

TS1

C	-1.03487800	4.06310800	-1.36854500
C	-0.77320000	2.84905800	-0.75797300
F	-4.01513900	2.03635000	0.57574100
F	-4.54651600	4.37499900	-0.57043700
F	-2.59870100	5.74806700	-1.87942200
F	-0.07371000	4.73424500	-2.00250500
C	-0.05808800	0.60657200	1.48882600
F	-1.89073100	-0.92646100	3.01121300
F	-3.84941900	-2.69998500	3.26208000
F	-5.58018100	-3.14829500	1.21400100
F	-5.31388500	-1.76564000	-1.11543500
C	0.52840000	1.68913100	2.14067800
C	1.66984600	1.57410300	2.92631400
C	2.27910100	0.33561200	3.06871000
C	1.72852400	-0.76865500	2.43467700
H	-0.86353200	-0.02730000	-0.97331400
C	0.58570300	-0.61415000	1.67416200
F	-0.00691100	2.91419900	2.05267400
F	2.18201100	2.64135000	3.54087400
F	3.37266000	0.20474800	3.81319900
C	-3.71420700	-2.03327200	2.11624300
C	-4.46214000	-1.55457500	-0.11132800
F	2.30965400	-1.96938300	2.54124500
C	-3.42820400	-0.64131500	-0.23526600
C	-2.50633300	-0.37763700	0.77986100
C	-4.60071000	-2.26253700	1.07518300
C	-2.69425000	-1.10436500	1.95496300
F	0.09425600	-1.72414200	1.10126600
B	-1.35866300	0.70494100	0.58778500
F	-3.32458400	0.00057700	-1.40726000
F	0.48654700	2.39039900	-0.83317100
C	-1.73291100	2.09403500	-0.08736800
C	-3.00761800	2.65677900	-0.05219000
C	-3.31171300	3.87787600	-0.63978900
C	-2.32090600	4.58272300	-1.30598200
H	-0.10253200	-0.12228500	-0.86294200
P	2.25588600	-0.71812800	-2.34033200
O	1.81105900	-0.48233200	-0.87088300

O	3.20282400	0.37139500	-2.84793600
O	0.81262300	-0.53128600	-3.16059300
O	2.72132500	-2.15518000	-2.59159100
K	3.15830500	1.92727300	-0.77803000
H	0.93742800	-0.70466800	-4.10226800
K	2.11369300	-3.15292100	-0.24880900
C	-1.62058200	-3.75968400	-0.84065500
O	-0.25906500	-3.86601000	-1.28729700
C	-0.20670400	-3.76443300	-2.72461100
C	-1.50257700	-3.06891100	-3.10991400
C	-2.47705800	-3.69089600	-2.10674500
H	-1.85660400	-4.61930000	-0.20593400
H	-1.70959300	-2.84360200	-0.24236800
H	0.69757700	-3.20789000	-2.98424200
H	-0.16108100	-4.77621800	-3.15131500
H	-1.40017700	-1.99041100	-2.94410600
H	-1.78229000	-3.24377300	-4.15134200
H	-3.39188900	-3.11098500	-1.96748600
H	-2.76076100	-4.69780500	-2.43016200
C	5.50025900	0.37539700	1.21476400
O	5.62851400	1.06760200	-0.02444100
C	6.00205500	0.09361700	-1.01562300
C	5.49332800	-1.27199200	-0.50228000
C	4.80093700	-0.92339400	0.82924000
H	6.49384900	0.18091200	1.64460900
H	4.93920100	1.01593100	1.90089200
H	5.52514000	0.38677300	-1.95404700
H	7.09228100	0.10281600	-1.13031500
H	4.80307400	-1.72842300	-1.21743200
H	6.32883600	-1.95719700	-0.33548900
H	3.73643600	-0.72372600	0.64879400
H	4.89881900	-1.70423100	1.58771800

**Int1**

C	-2.76375200	-3.12449500	0.31119800
C	-1.91252300	-2.03257900	0.32148000
F	1.26411000	-3.65350400	-0.10268000
F	-0.33459200	-5.75586600	-0.11156800
F	-3.03563800	-5.46664200	0.14880000
F	-4.09049500	-2.95130300	0.42119300
C	0.02648400	0.29191800	1.36830600
F	2.07746700	-1.56532000	2.38973700
F	4.73827200	-1.87339600	2.34245700
F	6.11679500	-1.54371700	0.01090600
F	4.77462700	-0.88682400	-2.26698600
C	-0.45657400	-0.05963800	2.62589800
C	-0.71980300	0.85773000	3.63683100
C	-0.48639800	2.20698800	3.41604900
C	0.00946300	2.61085200	2.18606900
H	0.06135700	-0.15773200	-0.88520200

C	0.24329400	1.65638000	1.20491100
F	-0.70359300	-1.34633700	2.92942700
F	-1.19118800	0.45388000	4.82138800
F	-0.73322800	3.10419700	4.37290300
C	4.08737900	-1.53536400	1.22395400
C	4.10588500	-1.03620900	-1.11654100
F	0.24194800	3.90851500	1.95511200
C	2.73105700	-0.84688000	-1.06099500
C	1.97750800	-0.99328800	0.09514600
C	4.79283700	-1.37194500	0.03907600
C	2.71286800	-1.35074800	1.22241800
F	0.72409600	2.12771100	0.03525000
B	0.36634000	-0.73590300	0.13703000
F	2.13889800	-0.52303200	-2.23192700
F	-2.51464700	-0.82851000	0.46654000
C	-0.52753900	-2.10803600	0.19045400
C	-0.05127300	-3.40806600	0.04287900
C	-0.86548000	-4.53735100	0.03289900
C	-2.23655100	-4.39852700	0.16532000
H	-2.34336100	1.70837100	-1.06296200
P	-2.17304600	0.77380100	-3.02135200
O	-1.66038100	1.68785800	-1.77140000
O	-3.62473400	1.04776100	-3.30290800
O	-2.19243100	-0.74298800	-2.37933100
O	-1.08680900	0.88537900	-4.05283900
K	-4.77560900	-0.48412100	-1.39147400
H	-1.31711900	-1.00920700	-2.05553900
K	0.96084500	1.91741600	-2.62057500
C	3.68135700	2.30520800	0.07321900
O	3.34582800	2.15388300	-1.31760700
C	4.52397700	2.30199500	-2.12595500
C	5.70027700	2.11436100	-1.17525800
C	5.14920400	2.72897800	0.11399400
H	3.00953000	3.04362700	0.51804000
H	3.52186800	1.33963700	0.57172300
H	4.48068000	1.55867300	-2.92659100
H	4.53271800	3.30692400	-2.56817500
H	5.91400600	1.04990200	-1.03488100
H	6.60839600	2.60251400	-1.53485700
H	5.65501000	2.37384400	1.01437300
H	5.23267200	3.81984700	0.07707500
C	-3.41640900	1.98119700	1.26363800
O	-3.81389400	1.77425000	-0.10504500
C	-4.48943300	2.96534100	-0.58469500
C	-4.33010700	4.02232700	0.51745600
C	-3.16306700	3.47717300	1.34771200
H	-4.23118400	1.67256100	1.93086300
H	-2.54285200	1.35156200	1.44433300
H	-4.00609400	3.25003300	-1.52342100
H	-5.53624400	2.71995800	-0.78609400
H	-4.13811500	5.01417600	0.10483200
H	-5.23375500	4.07395400	1.13143400
H	-2.20677000	3.71955400	0.86990900
H	-3.14843100	3.84994600	2.37448800
<b>Int2</b>			
O	-0.41416000	2.64649400	-1.23502800
K	-1.68975300	0.94889200	-2.66300600
B	-0.05794400	-1.34262100	-0.30813200
C	-1.21996700	-2.48745700	-0.25530500
C	-0.37100100	-0.33376500	0.95143500
C	1.46620900	-1.93435600	-0.35399300
C	-1.31597600	-3.36251000	0.82177900
C	-2.31698500	-4.30983400	0.96332900

C	-3.30215200	-4.40094600	-0.01149000
C	-3.26198600	-3.54339700	-1.09909400
C	-2.23272400	-2.61265800	-1.19400900
C	1.85188400	-3.26093000	-0.51883800
C	3.17818700	-3.67752100	-0.60339000
C	4.19966700	-2.74684100	-0.52682900
C	3.87147600	-1.40768900	-0.37386700
C	2.53670600	-1.04621500	-0.30709300
C	0.38436200	-0.10652400	2.09338000
C	0.00666100	0.75347000	3.11697000
C	-1.19765900	1.42875700	3.03946400
C	-2.00262100	1.23108000	1.92914500
C	-1.56655900	0.37969500	0.92676000
F	-2.27155100	-1.80078900	-2.27664700
F	-4.21244700	-3.61658700	-2.03875500
F	-4.28026900	-5.30330500	0.10152300
F	-2.34888200	-5.13364600	2.01747400
F	-0.38237900	-3.31388100	1.79113600
F	2.29115900	0.27651300	-0.16594800
F	5.47682700	-3.12812700	-0.60508600
F	3.47376200	-4.97288500	-0.76143900
F	0.93952300	-4.24673200	-0.62008700
F	-2.39971100	0.24438100	-0.13164500
F	1.58553400	-0.70866500	2.27058500
F	-3.18122900	1.85431400	1.83899800
F	-1.57134200	2.26998400	4.00832900
F	0.82213700	0.95704700	4.16341800
F	4.83820900	-0.48457700	-0.28149200
H	-0.18777300	-0.69396600	-1.32350000
C	-4.55168100	3.98169700	-0.54919100
C	-5.74827300	3.04484200	-0.73349600
C	-3.71537500	3.65667100	-1.78047400
C	-5.07782700	1.79355100	-1.29616800
O	-3.93845800	2.25816300	-2.03917700
H	-4.82972700	5.03721400	-0.50291700
H	-3.98913400	3.72242900	0.35208200
H	-6.45218900	3.46252600	-1.46101600
H	-6.28788500	2.84084100	0.19401400
H	-2.64316800	3.80373100	-1.62335400
H	-4.04643200	4.23310800	-2.65431500
H	-5.72064500	1.22060400	-1.97034700
H	-4.72564500	1.13663900	-0.49259600
K	3.08461400	1.92137600	1.84047900
C	5.46556000	1.75332700	-2.33499800
C	3.94668800	1.70056400	-2.59320400
C	3.40871600	2.73474600	-1.61027200
C	5.58160600	2.40156700	-0.93745400
H	5.91608200	0.75933400	-2.35966100
H	5.96864900	2.37059500	-3.08336400
H	3.54393700	0.71386600	-2.34641200
H	3.68468000	1.93046800	-3.62833200
H	3.50763400	3.75364600	-2.01383000
H	2.37631800	2.57035500	-1.29456900
H	6.08500600	3.37508500	-0.99333100
H	6.10207600	1.77546800	-0.20935300
O	4.24579100	2.59214000	-0.46293800
P	-0.02500300	3.48274600	-0.04680700
O	0.93249000	2.99332300	1.00235800
O	0.59042500	4.90285200	-0.57831700
O	-1.43017300	3.92763900	0.65909400
H	-1.28083200	4.34294600	1.51982100
H	0.13845600	5.20371100	-1.37806900

KH<sub>3</sub>PO<sub>4</sub>-BCF-Solvent (M062x/6-311++G\*\*)

## Reactant

C	0.31253400	3.62287800	0.10785100
C	0.44358400	2.24583600	0.05969200
F	3.81635500	1.93547700	-1.15604400
F	3.57883100	4.59020800	-1.09953100
F	1.26586100	5.74360400	-0.25511900
F	-0.82997700	4.17950500	0.51862200
C	0.47204200	-0.82453900	-0.78874400
F	2.71787300	-2.40699300	-1.65116400
F	5.03503200	-3.59372900	-1.09638200
F	6.69631300	-2.54966400	0.78362300
F	6.00386800	-0.27558500	2.10180500
C	-0.46670300	-0.39449500	-1.73226200
C	-1.56263700	-1.14797800	-2.10601800
C	-1.78112000	-2.37414400	-1.49589500
C	-0.88886900	-2.84099000	-0.54535000
H	1.42516500	0.13331100	2.27740200
C	0.21549200	-2.07333200	-0.21595300
F	-0.32058300	0.79313600	-2.34145500
F	-2.43048300	-0.69005500	-3.01343900
F	-2.85908300	-3.08608900	-1.80465600
C	4.69425200	-2.47944900	-0.45004900
C	5.18995800	-0.78600900	1.17832100
F	-1.11522000	-4.00765600	0.06096000
C	3.98911900	-0.16720300	0.86976100
C	3.09025900	-0.66830400	-0.07640900
C	5.54551500	-1.94894600	0.50885000
C	3.49221000	-1.84327000	-0.71771200
F	1.05133100	-2.58082600	0.69324000
B	1.71912000	0.03016300	-0.39519900
F	3.70428200	0.95332800	1.54507500
F	-0.62414200	1.53610100	0.45241700
C	1.60880000	1.59934500	-0.35608800
C	2.65421800	2.44512000	-0.73346000
C	2.55630500	3.82864300	-0.71374000
C	1.37661700	4.42195500	-0.28602600
H	0.76742300	-0.21300000	2.20840100
P	-2.47461700	-0.83900900	1.96285200
O	-1.14776400	-1.43801100	2.32238400
O	-2.92526700	-0.58917500	0.55240400
O	-2.62018700	0.64259500	2.68018700
H	-2.12151200	0.70165300	3.50567800
K	-3.39900600	2.00790000	0.40375300
C	-6.08189100	-0.06169900	0.95807600
O	-5.88619100	1.00579800	0.01482700
C	-6.16721700	0.48313600	-1.28402300
C	-5.58581000	-0.92356100	-1.24861300
C	-5.95152300	-1.38207000	0.17295500
H	-5.31798500	0.03777500	1.73341900
H	-7.07270700	0.04641400	1.41546200
H	-7.25469300	0.46375100	-1.44968400
H	-5.70804300	1.14836700	-2.01977500
H	-5.99324000	-1.57171500	-2.02830100
H	-4.49839300	-0.87328800	-1.34804400
H	-6.90137500	-1.92459600	0.17554600
H	-5.17683200	-2.01608400	0.60665400
O	-3.65627200	-1.70710100	2.69021100
H	-3.30070200	-2.21359800	3.43250700

## TS1

C	0.33851400	3.70468600	-0.00141000
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C	0.41974300	2.33014700	0.12791000
F	3.75666500	1.72638600	-1.07544200
F	3.62770600	4.36725700	-1.34203600
F	1.37365900	5.72214700	-0.64028800
F	-0.77861700	4.35454800	0.33732000
C	0.34178700	-0.84954800	-0.61108700
F	2.60117000	-2.29594200	-1.61539700
F	4.99972800	-3.40367200	-1.29917800
F	6.71104700	-2.47652100	0.59936700
F	5.97950900	-0.38429800	2.18082100
C	-0.52966400	-0.41145700	-1.60373700
C	-1.56369800	-1.18995700	-2.10148000
C	-1.77749500	-2.45326800	-1.57972500
C	-0.94247900	-2.93161400	-0.58005700
H	1.37592300	0.12381200	1.66729000
C	0.09295500	-2.13479100	-0.12727600
F	-0.40119900	0.81213000	-2.14426100
F	-2.37212800	-0.71372800	-3.05460300
F	-2.78432100	-3.20214800	-2.02391500
C	4.63979600	-2.38474800	-0.51731900
C	5.14149300	-0.84526800	1.25162900
F	-1.14903500	-4.14705200	-0.06510200
C	3.89469400	-0.27153300	1.06716800
C	2.97072100	-0.71864100	0.12404400
C	5.51686200	-1.91244700	0.44683600
C	3.39204800	-1.79082600	-0.65907800
F	0.88812300	-2.64851300	0.82061600
B	1.55689500	-0.00174300	-0.04816900
F	3.57757300	0.76808500	1.85638800
F	-0.66609900	1.70287700	0.61053800
C	1.54626700	1.58474900	-0.21216500
C	2.61759300	2.32612300	-0.70481000
C	2.57583300	3.70748800	-0.85707300
C	1.42978400	4.40175600	-0.50188000
H	0.68331600	-0.21365000	1.68240800
P	-2.34606700	-0.60635800	1.98534900
O	-0.93229000	-0.91853300	2.39639300
O	-2.78251600	-0.44889100	0.56037900
O	-2.80554700	0.81032500	2.69627600
H	-2.34612500	0.96875100	3.53157900
K	-3.47450300	2.08723600	0.32035600
C	-5.96665200	-0.22185900	1.02492500
O	-5.86831800	0.85914500	0.08239100
C	-6.13200400	0.31920700	-1.21262700



C	-5.44138800	-1.03835700	-1.19393700
C	-5.73368600	-1.52574800	0.23484300
H	-5.20918500	-0.05706200	1.79537300
H	-6.96061400	-0.19829500	1.48829500
H	-7.21744200	0.21516300	-1.35874600
H	-5.74003400	1.01966300	-1.95452000
H	-5.81567200	-1.71566000	-1.96527600
H	-4.36397800	-0.90246700	-1.32136800
H	-6.62996300	-2.15214500	0.25728700
H	-4.89559100	-2.08778200	0.64981300
O	-3.33636000	-1.70592300	2.67401900
H	-2.91848400	-2.12127800	3.44039800

### Int1

C	0.57931600	3.91007700	0.41637700
C	0.53896500	2.53190900	0.53629700
F	3.98754500	1.68916100	-0.00545200
F	4.10404800	4.31827600	-0.24105000
F	1.86766800	5.85309000	0.02754000
F	-0.53185000	4.64658600	0.54871400
C	0.24344500	-0.56747600	-0.33192800
F	2.82506400	-0.17126900	-1.91773100
F	4.92214400	-1.77281700	-2.45475800
F	5.99891200	-3.31580500	-0.48286300
F	4.94821600	-3.22870600	2.02846900
C	-0.31817400	-0.02447000	-1.48296500
C	-1.27399900	-0.67559400	-2.25278600
C	-1.70691100	-1.94082100	-1.88690200
C	-1.18057200	-2.52971600	-0.74885300
H	1.12242600	-0.06636300	1.77504300
C	-0.23100700	-1.83695700	-0.01178400
F	0.05080200	1.19507200	-1.92431000
F	-1.77572200	-0.09875000	-3.35358200
F	-2.61235300	-2.58417600	-2.62827300
C	4.40556700	-1.73514500	-1.22069800
C	4.42341500	-2.46993000	1.05856300
F	-1.59271400	-3.74425900	-0.37569800
C	3.34010900	-1.63483700	1.31472900
C	2.75346700	-0.83081100	0.34721900
C	4.95950000	-2.52000200	-0.21764800
C	3.32532900	-0.92258100	-0.91758700
F	0.23862600	-2.45880700	1.09081200
B	1.42876700	0.08093300	0.60451000
F	2.87304900	-1.64392100	2.57674900
F	-0.67760600	1.99047900	0.78913600
C	1.63642300	1.68771600	0.39446100
C	2.82800100	2.35691700	0.13749600
C	2.92444200	3.74031900	0.01093100
C	1.79344400	4.52593800	0.14842100
H	-0.38827400	-0.17700200	2.23957400
P	-2.56444200	-0.56729800	2.14781000
O	-1.16780200	-0.26243700	2.83247300
O	-2.90928900	0.15441800	0.90740400
O	-3.59881200	-0.23212400	3.31249700
H	-3.39293000	-0.60526900	4.18267900
K	-3.19859300	2.24871500	-0.54916300
C	-5.93415400	0.25252200	0.22455300
O	-5.24539100	0.55806600	-0.99593100
C	-5.11529600	-0.64627300	-1.75186900

C	-4.91468000	-1.74179100	-0.71113300
C	-5.81960700	-1.27024000	0.43836700
H	-5.45265000	0.82193800	1.02472600
H	-6.97901900	0.57219100	0.13646000
H	-6.03043400	-0.81705700	-2.33739200
H	-4.27457200	-0.51926300	-2.43915300
H	-5.18586200	-2.73001100	-1.08941600
H	-3.87309900	-1.75750300	-0.38271800
H	-6.80527000	-1.73920600	0.37582000
H	-5.39433200	-1.51040600	1.41612100
O	-2.61743000	-2.14625800	1.90599200
H	-2.11474700	-2.68608300	2.53427400

## Int2

O	-2.43389900	1.26646700	-1.32281100
K	-1.77515200	-0.86102200	-2.65584900
B	1.06050300	-0.14704100	-0.35519100
C	1.54297000	-1.69817200	-0.20948800
C	0.10737100	0.16174000	0.94515000
C	2.26235500	0.94166200	-0.55113500
C	2.26899000	-2.13219000	0.89579100
C	2.64261600	-3.44950000	1.10769900
C	2.27454300	-4.41414900	0.17863100
C	1.54326700	-4.03764700	-0.93611000
C	1.19544500	-2.70149600	-1.10048000
C	3.62311300	0.68409300	-0.67612600
C	4.57949100	1.67190400	-0.89389000
C	4.18995000	2.99556400	-1.00220900
C	2.84264200	3.30996500	-0.89202900
C	1.93363800	2.28789300	-0.67711800
C	0.41364300	0.93397100	2.06172300
C	-0.45427200	1.11378200	3.13582600
C	-1.69218700	0.49311600	3.12702400
C	-2.03853400	-0.30647900	2.04721200
C	-1.14196600	-0.44930200	1.00100200
F	0.47317800	-2.41667000	-2.21078500
F	1.17641500	-4.95906000	-1.83445900
F	2.62091800	-5.69101500	0.35818900
F	3.34870700	-3.80417400	2.18713800
F	2.65526400	-1.23309800	1.81982000
F	0.63236100	2.66591700	-0.58063000
F	5.09341100	3.95501700	-1.21605700
F	5.87277900	1.35115100	-1.01018100
F	4.10474000	-0.57144400	-0.59934700
F	-1.52537000	-1.27339300	0.00008300
F	1.60067600	1.56224800	2.16100700
F	-3.22155600	-0.93121600	2.03314000
F	-2.53909400	0.65379800	4.14585700
F	-0.10246100	1.87787000	4.17555400
F	2.44234300	4.58134200	-1.00158800
H	0.35931600	-0.04477100	-1.33776700
C	-5.50692000	-0.30639400	-0.32410100
C	-5.62401500	-1.78211700	0.06668200
C	-5.15112800	-0.42245400	-1.79761800
C	-4.51097000	-2.43110200	-0.76372800
O	-4.25286600	-1.53880500	-1.86594000
H	-6.42273600	0.26349300	-0.15139400
H	-4.68302900	0.17562700	0.21160600
H	-6.60234800	-2.17237000	-0.23136800
H	-5.49336900	-1.95910200	1.13599100
H	-4.62947500	0.45263100	-2.19223000
H	-6.04100200	-0.62989900	-2.40795900

H	-4.79450100	-3.41078500	-1.16029100
H	-3.58509100	-2.53117700	-0.18887400
P	-2.61156400	2.57689700	-0.66096000
O	-2.13752700	3.83084400	-1.53132800
H	-2.19002300	3.68452700	-2.48733400
O	-4.13227600	2.81720700	-0.26760700
H	-4.32524200	3.67367600	0.14297700
O	-1.86615500	2.82026900	0.71852400
H	-0.90290600	2.68986700	0.66553000
S			