

## Supporting Information

### **Efficient glycolysis of PET catalyzed by a metal-free phosphazene base: the important role of EG<sup>-</sup>**

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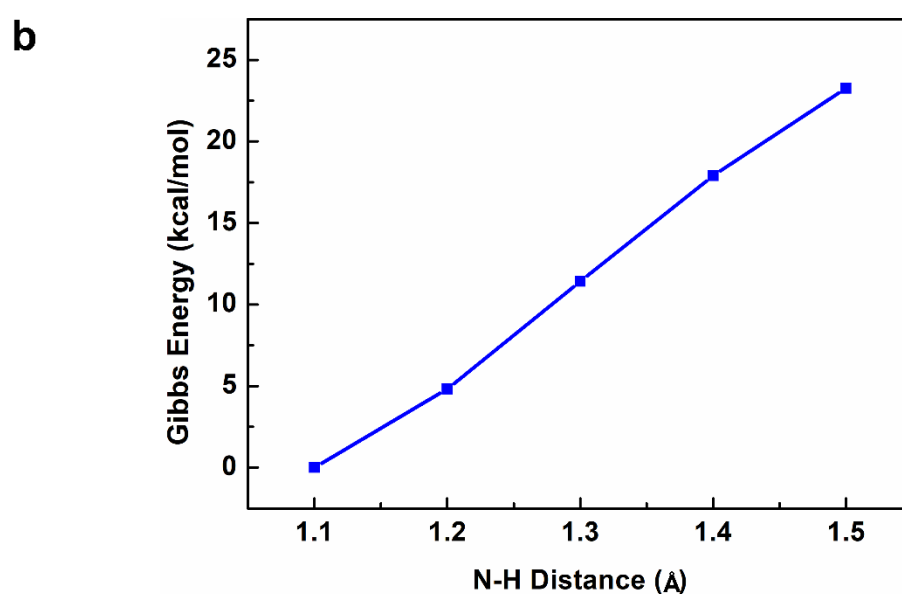
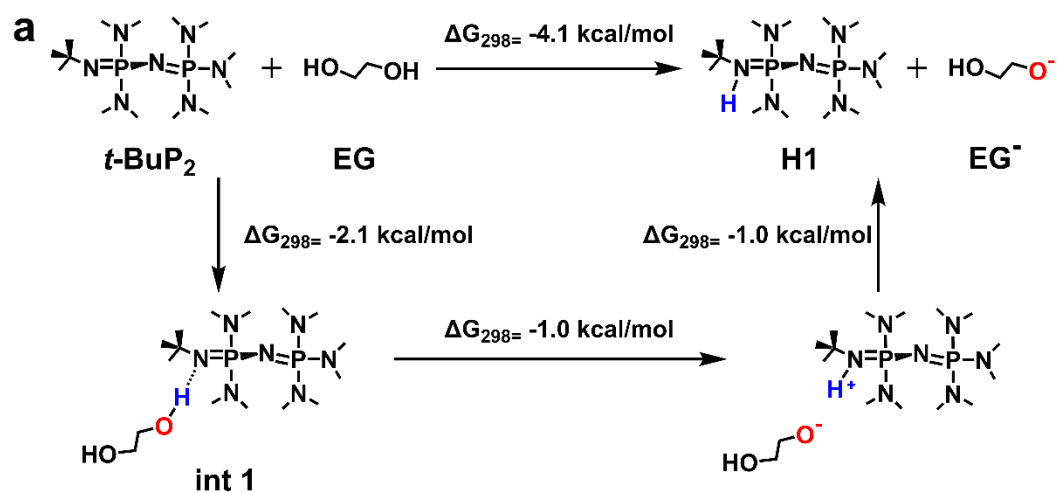
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### Complete Representation of Reference 36

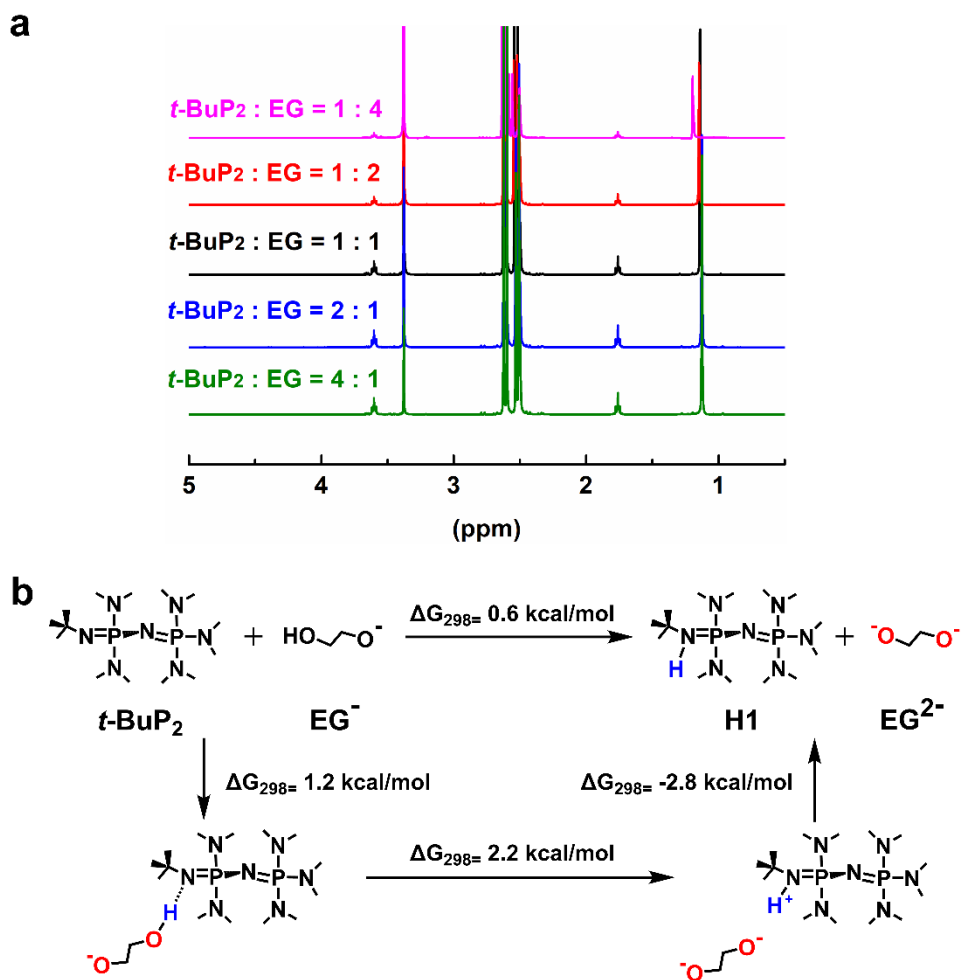
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**Table S1.** Reaction energies of EG<sup>-</sup> generation through the proton abstraction of organic bases.

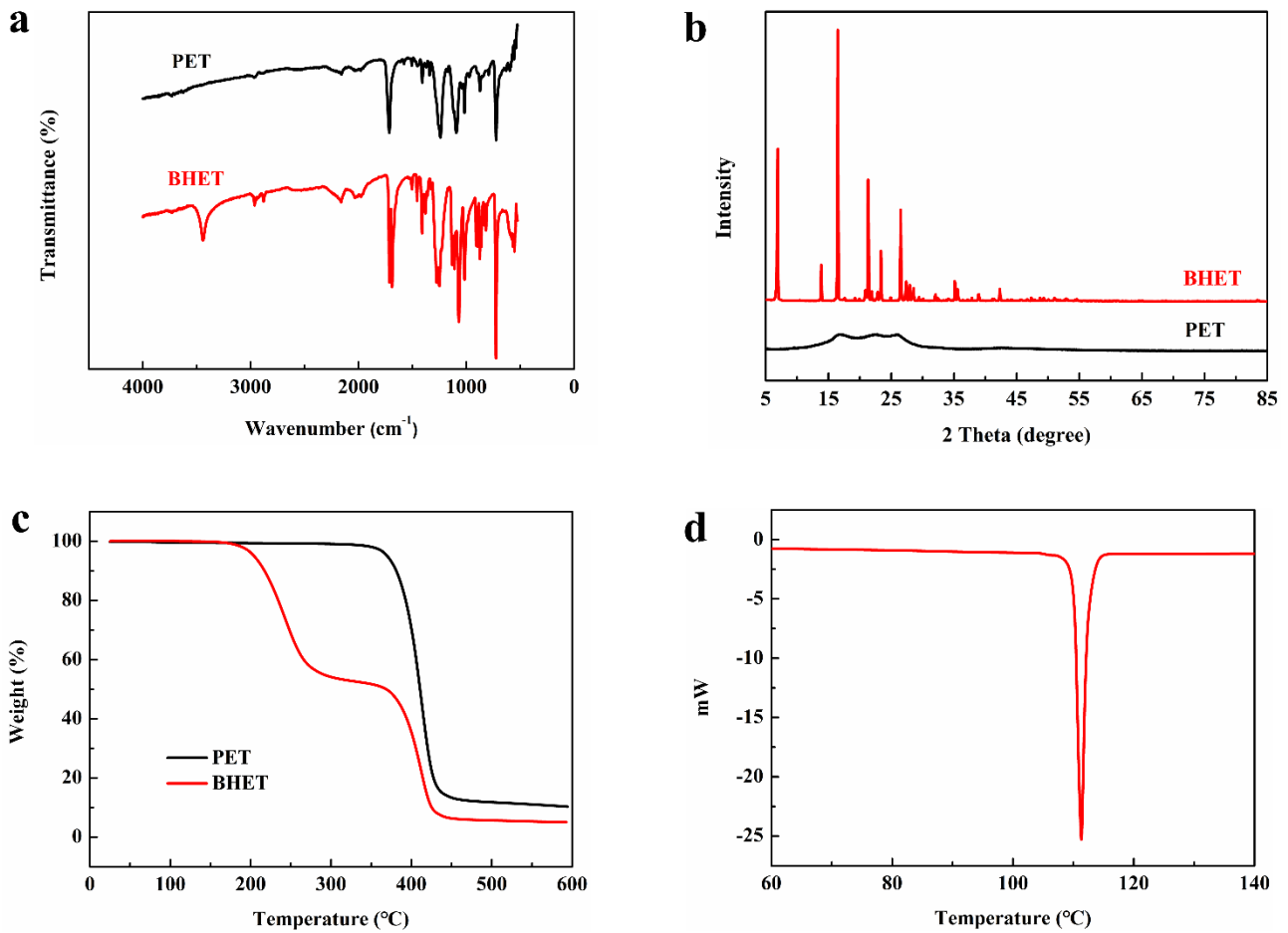
Organic Base + EG → Organic Base H <sup>+</sup> + EG <sup>-</sup>	
Organic Base	$\Delta G_{298.15}$ (kcal/mol)
Py	25.4
DMAP	17.5
DBU	8.4
TBD	6.4
<i>t</i> -BuP <sub>1</sub>	2.4
<i>t</i> -BuP <sub>2</sub>	-4.1



**Fig S1.** (a) The total and sub-step reaction formulas and Gibbs reaction energies of the proton migration from EG to *t*-BuP<sub>2</sub>; (b) The relative Gibbs energies of the **int 1** for the proton migration from EG to *t*-BuP<sub>2</sub> through fixed optimizations (with respect to the N-H distance 1.1).



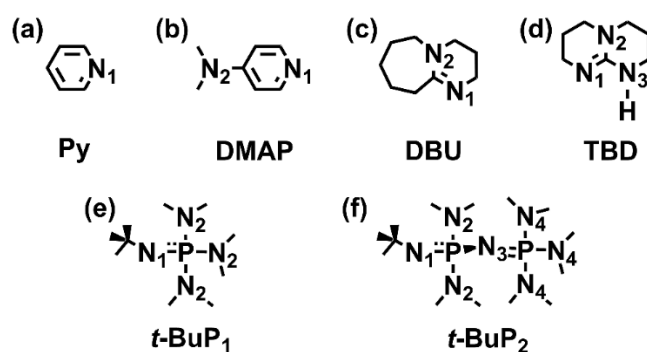
**Fig S2.** a)  $^1\text{H}$  NMR spectrum of  $t\text{-BuP}_2$  and EG mixed in different molar ratios. b) The total and sub-step reaction formulas and reaction energies of abstracting the second proton from ethylene glycol.



**Fig S3.** (a) FT-IR spectra of PET particles and main product; (b) XRD spectra of PET particles and main product; (c) TGA curves of PET particles and main product; (d) DSC curve of main product.

**Table S2.** Linear regression results for the data in Figure 5(a).

Temp.(K)	Rate constant	$R^2$
443	0.00828	0.99016
453	0.01493	0.99067
463	0.03291	0.99036
473	0.06591	0.98792



**Fig S4.** Structural formulas of organic bases with different nitrogen sites.

**Table S3.** Reaction energies of EG with different organic bases (kcal/mol).

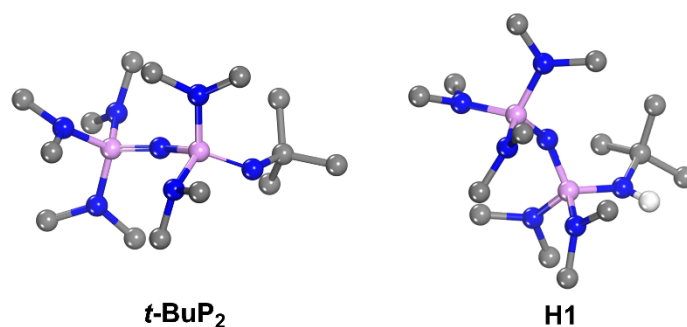
Organic Base + EG $\rightarrow$ Organic Base H <sup>+</sup> + EG <sup>-</sup>	
Organic Base	$\Delta G_{298.15}$
Py <sup>1</sup>	25.4
DMAP <sup>1</sup>	17.5
DMAP <sup>2</sup>	31.8
DBU <sup>1</sup>	8.4
DBU <sup>2</sup>	35.3
TBD <sup>1</sup>	6.4
TBD <sup>2</sup>	36.1
TBD <sup>3</sup>	32.3
<i>t</i> -BuP <sub>1</sub> <sup>1</sup>	2.4
<i>t</i> -BuP <sub>1</sub> <sup>2</sup>	24.2

1: N1 of the organic base abstract hydrogen of hydroxyl in EG.

2: N2 of the organic base abstract hydrogen of hydroxyl in EG.

3: N3 of the organic base abstract hydrogen of hydroxyl in EG.

Figure S3 showed that the organic bases had different nitrogen sites, and the reaction energies of these nitrogen sites in organic bases abstracting the hydrogen of hydroxyl in EG were listed in Table 1. As shown in Table 1, the reaction energies of N1 in organic bases abstracting H from EG were 25.4, 17.5, 8.4 and 6.4 kcal/mol, respectively, which was much lower than the N2 and N3, indicating that the N2 and N3 in organic bases hardly possessed the ability for abstracting proton in EG.



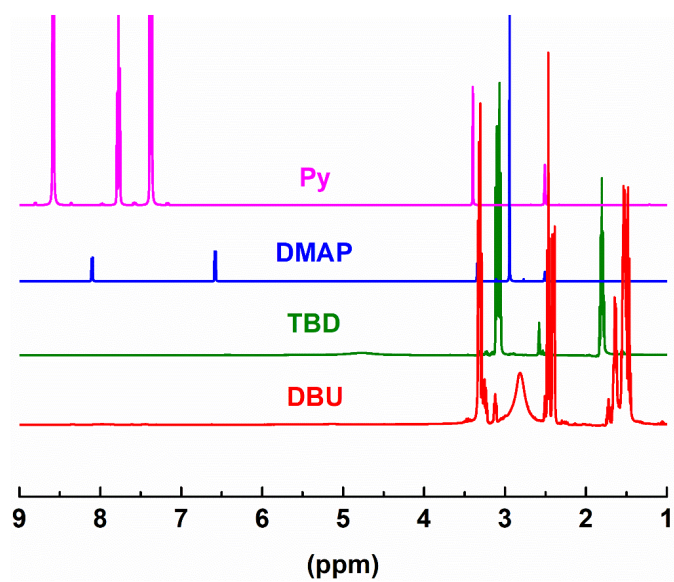
**Fig S5.** Optimized geometries of  $t\text{-BuP}_2$  and H1.

**Table S4.** Reaction energies of four different nitrogen sites in  $t\text{-BuP}_2$  to abstract hydrogen from EG and the relative energies E of the four products after abstracting H from EG (with respect to the H1) (kcal/mol).

$t\text{-BuP}_2 + \text{EG} \rightarrow \text{H } t\text{-BuP}_2^+ + \text{EG}^-$		
Organic Base <sup>a</sup>	$\Delta G_{298.15}$	E
H1	-4.1	0
H2	16.7	20.8
H3	23.9	28.0
H4	31.4	35.4

a: H1 is the product after N1 in  $t\text{-BuP}_2$  abstracting hydrogen from EG. H2 is the product after N2 in  $t\text{-BuP}_2$  abstracting hydrogen from EG. H3 is the product after N3 in  $t\text{-BuP}_2$  abstracting hydrogen from EG. H4 is the product after N4 in  $t\text{-BuP}_2$  abstracting hydrogen from EG.

The optimized geometries of  $t\text{-BuP}_2$  and H1 (the product after N1 in  $t\text{-BuP}_2$  abstracting hydrogen from EG) were showed in Figure S4, and Table S4 showed the reaction energies of four different nitrogen sites in  $t\text{-BuP}_2$  to abstract hydrogen from EG. As shown in Table S4, the reaction energies of N1, N2 and N3 in organic bases abstracting H from EG were 16.7, 23.9 and 31.4 kcal/mol, respectively, suggesting that they were thermodynamically unfavorable.



**Fig S6.** <sup>1</sup>H NMR spectrum of organic bases.



**t-BuP<sub>2</sub>**

P	-1.64626700	-0.19797600	-0.04632000
N	-2.23802800	-0.52185200	1.47509400
N	-2.07822100	-1.44299300	-1.06420100
N	-0.10461800	-0.07410000	-0.02968200
N	-2.41804500	1.18148100	-0.57857500
P	1.36524300	0.53726500	0.10791800
N	1.70106000	1.25734500	-1.38662800
N	1.24102200	1.84735100	1.19671800
N	2.51951500	-0.41554100	0.58940400
C	0.74587200	2.17618500	-1.97809700
H	0.89039500	3.21163600	-1.62642200
H	0.86157800	2.17321200	-3.06988100
H	-0.27755000	1.86984800	-1.74942300
C	3.06102600	1.47809800	-1.84446000
H	3.15965800	1.17991700	-2.89756800
H	3.35095800	2.53883500	-1.77224500
H	3.76214200	0.88822800	-1.25127800
C	2.41842800	2.69680900	1.31574500
H	2.14395900	3.61962000	1.84093100
H	3.23628500	2.21542000	1.87773900
H	2.79518000	2.97723500	0.32917600
C	0.66841500	1.54359800	2.50127700
H	1.35599200	0.96641400	3.14268300
H	0.43264100	2.48257100	3.01685000
H	-0.26084600	0.97938100	2.39084000
C	-3.23927400	-2.28901300	-0.84323700
H	-3.02020700	-3.29477800	-1.22093600
H	-3.45835800	-2.37643600	0.22223900
H	-4.13825800	-1.92039400	-1.35957100
C	-1.59269600	-1.43477100	-2.43662400

H	-1.29391400	-2.44850000	-2.73027000
H	-2.36553800	-1.08615100	-3.13788900
H	-0.72193500	-0.78070600	-2.53002000
C	-3.63370900	1.18965000	-1.37460700
H	-4.51895100	1.43224400	-0.76773600
H	-3.54680500	1.94776400	-2.16333400
H	-3.79936100	0.22391800	-1.85331000
C	-2.16924200	2.42831100	0.13036000
H	-2.92206300	2.60645600	0.91355700
H	-1.17669600	2.41906600	0.58921200
H	-2.20563500	3.26452300	-0.57870800
C	-1.55058900	-1.45859500	2.34956900
H	-1.67675200	-1.13832000	3.39101400
H	-1.95113100	-2.47898100	2.25167600
H	-0.48224000	-1.47528000	2.12552000
C	-3.61425300	-0.25327600	1.86291400
H	-3.63144600	0.28401500	2.81963100
H	-4.12182800	0.36006500	1.11666300
H	-4.18652500	-1.18410700	1.98466900
C	2.77555400	-1.78381600	0.13475600
C	1.88231100	-2.78219300	0.89367300
C	2.55655400	-2.00123200	-1.37497300
C	4.24244700	-2.10146300	0.45597700
H	1.99794700	-2.65298000	1.97713200
H	0.82737800	-2.62550600	0.64187700
H	2.14014600	-3.82015600	0.64427000
H	3.18584700	-1.32860900	-1.96895400
H	2.80815800	-3.03200100	-1.65613900
H	1.51037100	-1.82740400	-1.65484000
H	4.50330500	-3.13016800	0.17607100
H	4.91091200	-1.41991700	-0.08509400

H	4.43470800	-1.98090900	1.52936100
EG			
C	-0.57533700	0.49309500	0.00017000
H	-0.51795200	1.13149100	-0.89075300
H	-0.51790100	1.13117800	0.89137600
C	0.57533700	-0.49309500	-0.00019500
H	0.51793000	-1.13119300	-0.89139100
H	0.51792400	-1.13147500	0.89073900
O	1.78082800	0.26318100	-0.00021600
H	2.52671600	-0.34644800	0.00168000
O	-1.78082800	-0.26318100	0.00021200
H	-2.52671600	0.34644900	-0.00147300
H1			
P	-1.63958100	-0.31235800	0.13976000
N	-2.30425000	0.00674300	1.62260700
N	-2.10968600	-1.81896300	-0.36831000
N	-0.06315600	-0.34801300	0.26727700
N	-2.26497300	0.83531000	-0.87004500
P	1.18787300	0.53426000	-0.12452100
N	0.87338300	1.53233900	-1.41391100
N	1.67431800	1.43635200	1.17075700
N	2.49158400	-0.37247800	-0.57477400
C	0.48627200	0.95606800	-2.69385500
H	-0.27242200	1.59071700	-3.16673000
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C	1.44738200	2.86631000	-1.50566400
H	2.47545800	2.85755700	-1.89761800
H	0.82774700	3.46441300	-2.18300700

H	1.44040800	3.35922000	-0.53126900
C	3.01536100	1.99327200	1.28284800
H	3.00723800	3.08068500	1.12586200
H	3.41045900	1.79517600	2.28685300
H	3.68446300	1.53839200	0.55099100
C	0.71278100	2.05025600	2.07373300
H	1.08904500	1.98045000	3.10147200
H	0.55800900	3.11215000	1.83425000
H	-0.24805300	1.53551600	2.02935700
C	-3.46860900	-2.29400600	-0.14395200
H	-3.44355900	-3.38033000	-0.00374800
H	-3.89242600	-1.85094900	0.75927200
H	-4.13198900	-2.07031200	-0.99171300
C	-1.41137400	-2.51444900	-1.44167400
H	-1.29431300	-3.57148000	-1.17492500
H	-1.96823800	-2.45941100	-2.38799300
H	-0.41968900	-2.08662000	-1.59249900
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H	-4.12389300	0.82136600	-1.87368300
H	-2.69900000	1.12850000	-2.89604700
H	-3.02587500	-0.50623100	-2.31237500
C	-2.12471100	2.25388100	-0.57873500
H	-3.11017500	2.70880600	-0.40559500
H	-1.51218100	2.41751100	0.31024400
H	-1.64484700	2.76640100	-1.42143400
C	-1.76000800	-0.61819700	2.81974600
H	-1.81651500	0.08848100	3.65620800
H	-2.32452000	-1.52233200	3.08968700
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C	-3.64459000	0.55015600	1.79548400
H	-3.60533000	1.44473100	2.42973600

H	-4.08418800	0.82305600	0.83403600
H	-4.30360200	-0.18461600	2.27752500
C	3.02071000	-1.61385600	0.03602100
C	2.97605000	-1.52898000	1.56321000
C	2.21717200	-2.83002600	-0.44110600
C	4.47492400	-1.73486800	-0.42701500
H	3.56032400	-0.68065000	1.93397800
H	1.94984500	-1.43750300	1.93501600
H	3.40199400	-2.44631500	1.98383100
H	2.19098000	-2.86973300	-1.53682400
H	2.67355100	-3.75756200	-0.07616500
H	1.18851900	-2.78424800	-0.07057300
H	4.93031900	-2.64453100	-0.02116900
H	4.53354300	-1.78773500	-1.52159300
H	5.06263000	-0.87294800	-0.09136900
H	2.72636400	-0.28049200	-1.55488000

1 EG<sup>-</sup>

C	0.67629600	0.47502700	-0.00009100
H	0.55404400	1.13897900	0.88414000
H	0.55429800	1.13863900	-0.88464800
C	-0.50821000	-0.48946200	0.00003400
H	-0.45712500	-1.13130800	0.89095300
H	-0.45726000	-1.13131700	-0.89085800
O	-1.73064400	0.25641700	0.00019200
H	-2.46992800	-0.36092500	-0.00115500
O	1.88907600	-0.20234900	0.00004700

2 [BHET]<sub>3</sub>

C	-0.98339000	0.99302700	-0.03162500
C	0.35799700	1.34780500	-0.03145900

C	1.34307000	0.35778700	-0.03139200
C	0.98338600	-0.99285600	-0.03152600
C	-0.35800300	-1.34763400	-0.03096300
C	-1.34307300	-0.35761800	-0.03099100
H	-1.74466600	1.76504800	-0.03151800
H	0.64286600	2.39456700	-0.03132700
H	1.74466200	-1.76487700	-0.03133600
H	-0.64286800	-2.39439600	-0.03044700
C	2.76936400	0.78397600	-0.02961400
O	3.13601700	1.94766100	-0.01965000
O	3.61844700	-0.24157500	-0.03954900
C	5.01690800	0.07433100	-0.03472300
H	5.26094300	0.64150000	0.86756400
H	5.26193200	0.66688700	-0.92022200
C	5.72735900	-1.26314700	-0.05354500
H	5.48587800	-1.82840800	-0.95765900
H	5.47898900	-1.85733900	0.82997400
O	7.12600700	-0.94833600	-0.04254400
C	-2.76936500	-0.78381600	-0.02876700
O	-3.13599300	-1.94750800	-0.01846300
O	-3.61845500	0.24171000	-0.03876000
C	-5.01691000	-0.07420500	-0.03365500
H	-5.26079300	-0.64129900	0.86872000
H	-5.26206200	-0.66684900	-0.91906000
C	-5.72738300	1.26326300	-0.05250500
H	-5.47896800	1.85750700	0.83096600
H	-5.48596100	1.82846700	-0.95667000
O	-7.12602400	0.94843100	-0.04140800
H	16.47334000	4.14147200	0.24031200
C	9.76341000	-0.20341700	0.00589400
C	11.10550900	0.15133300	0.02264100

C	12.08856100	-0.84137400	-0.01052500
C	11.72466900	-2.18907700	-0.06000000
C	10.38404100	-2.54370100	-0.07570100
C	9.40075500	-1.55209400	-0.04296400
H	9.00335600	0.56939500	0.03187700
H	11.38352000	1.19852600	0.06121200
H	12.49088400	-2.95666500	-0.08511400
H	10.09759200	-3.58935300	-0.11363000
C	13.53894500	-0.50244000	0.00685100
O	14.43336500	-1.33242600	-0.03505200
O	13.76690100	0.80548800	0.07484800
C	15.13873200	1.23129200	0.10002900
H	15.64051700	0.89222200	-0.81068800
H	15.63589400	0.80006400	0.97355400
C	15.10436700	2.74400500	0.17756700
H	14.58237400	3.15225800	-0.69633900
H	14.57659900	3.06109700	1.08526500
O	16.45849800	3.17523800	0.20373000
C	7.97379400	-1.97508400	-0.06047100
O	7.60511600	-3.13785500	-0.08824900
C	-9.76338900	0.20344600	0.00705200
C	-11.10547600	-0.15136200	0.02349600
C	-12.08856400	0.84127500	-0.01065600
C	-11.72472100	2.18896900	-0.06076500
C	-10.38410500	2.54365300	-0.07617500
C	-9.40078500	1.55211100	-0.04249400
H	-9.00330400	-0.56930700	0.03382800
H	-11.38344700	-1.19854400	0.06261700
H	-12.49096200	2.95650600	-0.08663500
H	-10.09768900	3.58929400	-0.11463400
C	-13.53893700	0.50228100	0.00637000

O	-14.43338200	1.33221900	-0.03592200
O	-13.76685700	-0.80564800	0.07450100
C	-15.13867800	-1.23148900	0.09958500
H	-15.64041000	-0.89248400	-0.81118300
H	-15.63591000	-0.80022600	0.97305500
C	-15.10429600	-2.74419900	0.17720300
H	-14.58223200	-3.15248600	-0.69664400
H	-14.57660400	-3.06124900	1.08495900
O	-16.45843200	-3.17542600	0.20327600
H	-16.47329700	-4.14166300	0.23975300
C	-7.97383800	1.97515000	-0.05981800
O	-7.60519500	3.13792600	-0.08784500
3			
C	0.84503100	0.35568300	-0.86126600
C	-0.54009600	0.45476600	-0.85295400
C	-1.28557900	-0.12409900	-1.88308700
C	-0.64182000	-0.80464700	-2.91913900
C	0.74189700	-0.90429900	-2.92796500
C	1.48843900	-0.32406700	-1.89964500
H	1.41995000	0.80436100	-0.05901500
H	-1.03685400	0.97461700	-0.04179300
H	-1.22482400	-1.25485300	-3.71550800
H	1.24450000	-1.43199500	-3.73160600
C	-2.77338000	-0.06166600	-1.90167500
O	-3.46622100	-0.62822300	-2.73005900
O	-3.27162900	0.69953600	-0.92530200
C	-4.69641800	0.82877600	-0.83172000
H	-4.85858800	1.75678800	-0.28247800
H	-5.13258300	0.90909600	-1.82986600
C	-5.26853100	-0.35257000	-0.06657500



H	-4.80580800	-0.44341600	0.91951400
H	-5.15420300	-1.29098800	-0.61415200
O	-6.66544500	-0.05269100	0.08175300
C	2.97007600	-0.45754000	-1.94370300
O	3.57784300	-1.05230100	-2.81895800
O	3.57805700	0.14339200	-0.92255100
C	5.00884300	0.05480800	-0.87554000
H	5.43481500	0.51661300	-1.77025600
H	5.30643100	-0.99581900	-0.82626200
C	5.41676100	0.81413000	0.37450900
H	5.11813500	1.86068100	0.30893600
H	4.99354800	0.36338100	1.27455600
O	6.84885600	0.83963000	0.45951800
H	17.07076800	3.62297800	-0.72123300
C	-9.31651300	0.63041300	0.25199100
C	-10.66008600	0.96226900	0.36189200
C	-11.53024200	0.12114400	1.06056700
C	-11.05190500	-1.05250800	1.64786200
C	-9.71000800	-1.38464800	1.53711900
C	-8.83912500	-0.54422000	0.83961700
H	-8.64511500	1.28572600	-0.29129100
H	-11.02700600	1.87394300	-0.09596700
H	-11.73092300	-1.70239500	2.18958500
H	-9.33509900	-2.29553800	1.99163000
C	-12.97753500	0.44150700	1.20287500
O	-13.77511400	-0.26009800	1.80480700
O	-13.32132100	1.57848700	0.60492700
C	-14.70025100	1.97114100	0.69266100
H	-14.97416900	2.09917000	1.74378800
H	-15.32743600	1.19586900	0.24348000
C	-14.81416900	3.27739500	-0.06646800

H	-14.15638000	4.03136600	0.38270300
H	-14.52196700	3.13055600	-1.11329300
O	-16.17600200	3.67481700	0.02710400
H	-16.28952600	4.50592000	-0.45405800
C	-7.40608000	-0.93862700	0.74377100
O	-6.94708700	-1.96414200	1.21896100
C	-1.92497600	-3.38314100	-0.70757000
H	-2.27213200	-4.44170400	-0.70182200
H	-2.07240500	-3.03907700	-1.75569500
C	-0.41486300	-3.42734600	-0.50651500
H	-0.02118900	-2.40378900	-0.44749200
H	0.06417500	-3.94140800	-1.35384400
O	-2.60267600	-2.60036500	0.21197400
O	-0.12083400	-4.12467700	0.71127900
H	0.81948600	-4.03631600	0.89892400
C	10.96619000	1.12938400	0.48084600
C	9.58103300	1.03826500	0.45465500
C	8.94494300	-0.06329100	1.03334000
C	9.69851900	-1.07178700	1.63883500
C	11.08184100	-0.97896700	1.66767900
C	11.71895600	0.12067200	1.08785600
H	11.45601400	1.98460500	0.02927100
H	9.00047500	1.82256100	-0.01759200
H	9.20048700	-1.92540700	2.08611000
H	11.67003700	-1.75982000	2.13786500
C	7.46294400	-0.20499800	1.02046600
O	6.86725700	-1.16692400	1.47491300
C	13.20649700	0.17981700	1.13741500
O	13.90378700	-0.66206600	1.68108600
O	13.70669200	1.24847800	0.52415700
C	15.13627900	1.39124100	0.52136800

H	15.58598100	0.52679000	0.02478000
H	15.49625900	1.44834000	1.55256300
C	15.42929800	2.67161800	-0.23371000
H	15.04551200	2.59951900	-1.25853100
H	14.94804800	3.52108900	0.26599500
O	16.84330800	2.81976200	-0.23294900

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C	1.26247000	-0.81791900	-0.13592800
C	-0.08310800	-1.16476400	-0.12987700
C	-1.06305900	-0.18815700	0.05498700
C	-0.68511300	1.14785500	0.22242600
C	0.65635900	1.49703000	0.21816000
C	1.63825300	0.51638600	0.04117700
H	2.01497100	-1.58603000	-0.27817800
H	-0.37521800	-2.19996500	-0.27276700
H	-1.43937600	1.91338500	0.36739700
H	0.94764700	2.53395500	0.35152300
C	-2.50162600	-0.61434300	0.07067400
O	-2.85533800	-1.76019400	-0.23216900
O	-3.34178900	0.44514500	-0.06600000
C	-4.72880200	0.13420600	-0.13802200
H	-5.01837500	-0.49708000	0.70824200
H	-4.95332400	-0.38927800	-1.07291600
C	-5.44337300	1.46847900	-0.08187500
H	-5.15335300	2.11115100	-0.91778100
H	-5.24797800	1.98382700	0.86241600
O	-6.84308400	1.16366200	-0.17872100
C	3.06152200	0.93238600	0.05278900
O	3.44642400	2.06658100	0.29401300
O	3.90259600	-0.06476100	-0.22913200

C	5.30155400	0.24467100	-0.21423000
H	5.59623900	0.55573600	0.79191600
H	5.50986200	1.04982600	-0.92366900
C	5.99817500	-1.03726600	-0.62073500
H	5.77497600	-1.85042500	0.07524800
H	5.72134600	-1.33466800	-1.63559500
O	7.40001700	-0.73803400	-0.57168700
H	16.83866600	3.72740100	1.56367700
C	-9.47827600	0.42701100	-0.33909200
C	-10.81860700	0.07761900	-0.43323800
C	-11.79893300	1.07358100	-0.44152900
C	-11.43393000	2.41909400	-0.35434500
C	-10.09505600	2.76813800	-0.25982600
C	-9.11441700	1.77342100	-0.25246300
H	-8.72043300	-0.34838600	-0.33245700
H	-11.09734200	-0.96796700	-0.49988400
H	-12.19781700	3.18940500	-0.36127700
H	-9.80789400	3.81208300	-0.19214200
C	-13.24694400	0.74032400	-0.54268500
O	-14.13998100	1.57303100	-0.54394400
O	-13.47523700	-0.56633200	-0.63290300
C	-14.84500600	-0.98706500	-0.73549700
H	-15.29487800	-0.54296700	-1.62802000
H	-15.39265300	-0.65824300	0.15230300
C	-14.81017400	-2.49866900	-0.83200500
H	-14.23267900	-2.80441300	-1.71290000
H	-14.33953500	-2.92112900	0.06398000
O	-16.16175800	-2.92557400	-0.94150200
H	-16.17649500	-3.89105200	-0.99665900
C	-7.68847800	2.19008100	-0.15036400
O	-7.32214000	3.35036000	-0.05202200

C	-1.98771600	-1.70409600	2.70100800
H	-1.88427900	-2.50338200	1.93802900
H	-0.97238100	-1.51325100	3.10194800
C	-2.84804700	-2.26056100	3.83209900
H	-2.84347900	-1.56581000	4.68526700
H	-2.48537300	-3.23594300	4.17377100
O	-2.58062200	-0.57592300	2.15632500
O	-4.18692400	-2.43395400	3.36561200
H	-4.32163200	-1.68639800	2.75909300
C	10.04873300	-0.08143200	-0.29001200
C	11.39483500	0.24560100	-0.19761400
C	12.36333600	-0.65969300	-0.63947100
C	11.98099700	-1.89303000	-1.17227100
C	10.63671300	-2.22265100	-1.25842300
C	9.66773900	-1.31757400	-0.81881100
H	9.30045700	0.62357200	0.05409200
H	11.68725700	1.20433900	0.21559800
H	12.73568400	-2.59292000	-1.51488500
H	10.33645200	-3.18108600	-1.66844900
C	13.81708900	-0.34578900	-0.55977900
O	14.69601000	-1.06989800	-0.99988500
O	14.06738000	0.81116400	0.04593000
C	15.44471000	1.20091600	0.16984100
H	15.87949900	1.31453500	-0.82737600
H	15.99134800	0.43089100	0.72145900
C	15.44085400	2.51550200	0.92304400
H	14.86971500	3.26745700	0.36498200
H	14.97954300	2.38006600	1.90871000
O	16.80124900	2.90765400	1.05197900
C	8.23633400	-1.71237300	-0.92392600
O	7.85529400	-2.81152300	-1.29212000

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C	1.21881800	-1.05338000	-0.19829200
C	-0.12267600	-1.40645200	-0.30772600
C	-1.07314400	-0.86899400	0.55678500
C	-0.66238000	0.03537800	1.54266200
C	0.67109600	0.39914300	1.65515500
C	1.62201100	-0.14649200	0.78505700
H	1.94588800	-1.48199700	-0.87998400
H	-0.43673300	-2.10851100	-1.07351500
H	-1.39138500	0.45503400	2.22932200
H	0.98196700	1.10316700	2.42073200
C	-2.54957800	-1.30204200	0.45125100
O	-2.83984200	-2.11989300	-0.51752900
O	-3.27585500	-0.04947700	0.42159800
C	-4.66280200	-0.17811500	0.17139800
H	-5.11135500	-0.94958200	0.80891900
H	-4.85292200	-0.43533600	-0.87768800
C	-5.26692500	1.17405600	0.49291700
H	-4.83273600	1.96228500	-0.12885600
H	-5.13666600	1.42823300	1.54854800
O	-6.67194100	1.06413400	0.20387600
C	3.03813700	0.25998400	0.94204000
O	3.43421200	1.08804500	1.74925200
O	3.86470000	-0.37554100	0.10741700
C	5.25522600	-0.04456000	0.19907100
H	5.61677500	-0.24937700	1.21040600
H	5.39737200	1.01429500	-0.03407600
C	5.94717500	-0.92869300	-0.81746700
H	5.80565200	-1.98743800	-0.58442600
H	5.59408900	-0.72419000	-1.83178200

O	7.33893200	-0.59677600	-0.71819100
H	16.63011300	3.84218300	2.00167100
C	-9.33334100	0.67575200	-0.32561000
C	-10.68239600	0.50761700	-0.60720700
C	-11.56187200	1.58498900	-0.47042100
C	-11.08730900	2.82989000	-0.05052400
C	-9.74016000	2.99702600	0.23348500
C	-8.86013800	1.92100200	0.09635400
H	-8.65354000	-0.16199400	-0.43298900
H	-11.04598500	-0.46032300	-0.93313500
H	-11.77357400	3.66363100	0.05373200
H	-9.36807700	3.96193300	0.56113300
C	-13.01546100	1.44653200	-0.76309400
O	-13.81748900	2.36373200	-0.68357300
O	-13.35947400	0.21340400	-1.12262500
C	-14.74474800	-0.01794400	-1.42438100
H	-15.04692400	0.62545900	-2.25558600
H	-15.35081700	0.21368500	-0.54387900
C	-14.85279200	-1.48265400	-1.79630400
H	-14.22216300	-1.69594600	-2.66784700
H	-14.52191900	-2.10805800	-0.95824200
O	-16.22230900	-1.72014000	-2.09379500
H	-16.32581100	-2.64631200	-2.35201700
C	-7.42122400	2.14090500	0.41335300
O	-6.96903100	3.19859600	0.82399400
C	-2.34624500	-3.06248000	2.12635500
H	-2.46754400	-3.78521100	1.30924600
H	-1.27173600	-2.95190800	2.33979500
C	-3.04830700	-3.56812600	3.36707800
H	-2.94266100	-2.83831500	4.18127700
H	-2.59365400	-4.50975900	3.68646400

O	-2.92522300	-1.81884400	1.78094900
O	-4.42667100	-3.84062900	3.12827400
H	-4.82555900	-3.03841200	2.76857200
C	9.95840800	0.14590200	-0.41911500
C	11.29232800	0.50453300	-0.28033900
C	12.26871900	-0.13460900	-1.04906300
C	11.90613300	-1.13219400	-1.95715700
C	10.57347700	-1.49006500	-2.09652700
C	9.59692400	-0.85247000	-1.32773100
H	9.20370400	0.64355900	0.17932100
H	11.56873600	1.27968200	0.42533900
H	12.66757200	-1.62532300	-2.55202900
H	10.28825200	-2.26431100	-2.80080500
C	13.71034600	0.21941300	-0.92865600
O	14.59969700	-0.31601000	-1.57130700
O	13.93719400	1.18556700	-0.04382200
C	15.30116900	1.59643500	0.14166300
H	15.70296300	1.95937600	-0.80853500
H	15.89264400	0.74358400	0.48678600
C	15.26809100	2.69917300	1.18013400
H	14.65439600	3.53395800	0.82071600
H	14.83900100	2.32130800	2.11614400
O	16.61596000	3.10882000	1.37133500
C	8.17799000	-1.26629200	-1.50560900
O	7.80905500	-2.12774600	-2.28709400

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C	0.06190500	-3.34363500	0.00269900
C	1.15078700	-4.19240700	0.12116500
C	2.39113900	-3.83484400	-0.41520200
C	2.52773700	-2.61228800	-1.07738000



C	1.43792100	-1.75754400	-1.19718400
C	0.20155100	-2.11739500	-0.65982500
H	-0.89530000	-3.63343500	0.42242200
H	1.04447000	-5.14127100	0.63706000
H	3.48074400	-2.32744600	-1.50924500
H	1.54847900	-0.80956400	-1.71385900
C	3.53867000	-4.79444000	-0.26927900
O	3.35681100	-6.00687000	-0.06384500
O	4.01121600	-4.17453700	1.59462200
C	4.41959200	-2.85665900	1.73529300
H	4.03931100	-2.41013500	2.67201000
H	4.03511200	-2.21652600	0.91852800
C	5.94443000	-2.74258300	1.74251700
H	6.38839800	-3.25822800	0.89039900
H	6.37268900	-3.13665500	2.66581700
O	6.35212100	-1.35048600	1.72583600
C	-0.93845400	-1.18295400	-0.81976400
O	-0.87023100	-0.09735800	-1.37678300
O	-2.07364500	-1.64653800	-0.29250300
C	-3.23360800	-0.81572600	-0.41978700
H	-3.44204200	-0.63565600	-1.47799700
H	-3.06224200	0.13703400	0.08843600
C	-4.35690300	-1.59476600	0.23234200
H	-4.50938800	-2.55806200	-0.26180100
H	-4.16814800	-1.75274800	1.29753200
O	-5.52609900	-0.78117000	0.06633800
C	6.80643000	1.49848600	-0.46577200
C	7.10678700	2.85078100	-0.38536700
C	7.28482000	3.44860700	0.86540700
C	7.16350800	2.68806300	2.03055900
C	6.86571500	1.33518200	1.94982000

C	6.68606800	0.73742800	0.69926500
H	6.66411900	1.03035600	-1.43402400
H	7.19933300	3.43676800	-1.29277100
H	7.30169300	3.15623300	2.99936000
H	6.77052000	0.74914600	2.85686500
C	7.60113800	4.89781500	0.99758000
O	7.73700200	5.47231800	2.06635900
O	7.72123300	5.51283700	-0.17521700
C	8.01575600	6.91862300	-0.15108200
H	8.96377100	7.08231700	0.36908300
H	7.21481500	7.44709700	0.37377400
C	8.10235800	7.35101200	-1.60053200
H	8.89917900	6.79582200	-2.11008600
H	7.15115200	7.15142800	-2.10879900
O	8.38576000	8.74393400	-1.58862300
H	8.45962400	9.05057000	-2.50288800
C	6.35527300	-0.70961100	0.56722600
O	6.11536900	-1.24121700	-0.51028800
C	5.71256800	-5.27642400	-1.09380400
H	6.14591100	-5.49107900	-0.10979800
H	5.34691000	-6.21042500	-1.53292400
C	6.73753500	-4.65886700	-2.01780500
H	6.24790600	-4.34721900	-2.95040600
H	7.47850800	-5.42503500	-2.26308300
O	4.63168000	-4.35366400	-0.95253500
O	7.45566800	-3.57669800	-1.44430600
H	6.84658100	-2.85055700	-1.23194200
C	-10.19213000	0.05160100	0.54670600
C	-9.08670200	-0.75978200	0.75870500
C	-7.82854200	-0.36046300	0.30251400
C	-7.67709100	0.85767300	-0.36599200

C	-8.78264500	1.66905500	-0.57757600
C	-10.04138700	1.26857400	-0.12407600
H	-11.16718000	-0.26321500	0.90103900
H	-9.19982900	-1.70575500	1.27744900
H	-6.70227900	1.17198900	-0.72145500
H	-8.66956400	2.61462200	-1.09704100
C	-6.67108000	-1.26535900	0.54272400
O	-6.74975900	-2.34206000	1.11166500
C	-11.20319100	2.16514400	-0.37988500
O	-11.12365100	3.23530200	-0.96267200
O	-12.34761200	1.67954900	0.09069900
C	-13.53315000	2.46597900	-0.11928800
H	-13.68501800	2.60622500	-1.19390100
H	-13.41326700	3.44000200	0.36305700
C	-14.67723500	1.68126600	0.50082300
H	-14.73682000	0.68141300	0.05489100
H	-14.52135600	1.57406200	1.57706800
O	-15.90092300	2.38286100	0.33706600
H	-16.16373000	2.34105100	-0.59373400
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C	-0.50694900	-3.41375600	0.53213300
C	-1.81208500	-3.78896300	0.82054500
C	-2.50668100	-4.62616600	-0.05684700
C	-1.89206900	-5.08296100	-1.22512200
C	-0.58804900	-4.70884700	-1.51335500
C	0.10775700	-3.87472400	-0.63508700
H	0.02870700	-2.76503100	1.21599100
H	-2.28617900	-3.43034200	1.72715200
H	-2.43532200	-5.73098600	-1.90467100
H	-0.10693100	-5.06355700	-2.41867000

C	-3.90758300	-5.05509400	0.21934600
O	-4.55418300	-5.77366800	-0.52635000
O	-9.59081800	-2.78980800	0.33304600
C	-9.10298400	-1.48638500	0.40327800
H	-9.91798000	-0.74227300	0.46108500
H	-8.47349700	-1.32640300	1.30145500
C	-8.25456900	-1.16491100	-0.82185000
H	-8.85160000	-1.19711000	-1.73865600
H	-7.41373100	-1.85956200	-0.91352300
O	-7.73311500	0.17305400	-0.65113100
C	1.50753300	-3.50228900	-0.97716000
O	2.09129800	-3.88142700	-1.97933300
O	2.07107600	-2.70647600	-0.07023100
C	3.42785100	-2.30717100	-0.30912300
H	3.48830400	-1.75739200	-1.25208700
H	4.06440800	-3.19428100	-0.35822100
C	3.79259600	-1.41605100	0.86511400
H	3.15926000	-0.52890800	0.89096000
H	3.71812800	-1.95197600	1.81366500
O	5.12531600	-0.91696400	0.68259500
H	13.44752700	5.24967100	-1.85306000
C	-6.75975700	2.67693700	-0.10567800
C	-6.26774900	3.95112100	0.14279900
C	-5.44151800	4.57423300	-0.79636300
C	-5.11029400	3.91776300	-1.98411100
C	-5.60148500	2.64435900	-2.23153800
C	-6.42725500	2.02035100	-1.29357400
H	-7.39931100	2.19688500	0.62635400
H	-6.52773700	4.45540200	1.06659600
H	-4.46890300	4.40475100	-2.71109200
H	-5.34546000	2.13159600	-3.15266800

C	-4.89143400	5.93867300	-0.56618200
O	-4.16182600	6.52223000	-1.35240300
O	-5.27521500	6.46583000	0.59270300
C	-4.79147100	7.78119100	0.90734200
H	-5.13042500	8.48501200	0.14188000
H	-3.69813300	7.76875800	0.93450800
C	-5.37123400	8.12298100	2.26482800
H	-6.46694200	8.10920100	2.21877700
H	-5.03892900	7.38912200	3.00905300
O	-4.89595500	9.42254400	2.59094100
H	-5.24566600	9.66968600	3.45823700
C	-6.93099100	0.64859700	-1.59222500
O	-6.63306900	0.02377700	-2.60014800
C	-5.72955200	-4.89533100	1.74431600
H	-5.95784800	-5.92725300	1.46710600
H	-5.74624500	-4.79528700	2.83092800
C	-6.69938200	-3.91621200	1.10251300
H	-6.67411300	-4.03457000	0.00929900
H	-6.37150100	-2.89091300	1.33576900
O	-4.37435500	-4.57725000	1.36969500
O	-7.98332000	-4.17949600	1.61665600
H	-8.68081700	-3.61274000	1.06570300
C	8.84230600	0.76793400	0.06323100
C	7.58569100	0.21509400	0.27057600
C	7.46952600	-1.05529200	0.84113100
C	8.61391600	-1.77025100	1.20282500
C	9.86887900	-1.21803000	0.99530400
C	9.98626800	0.05182000	0.42516000
H	8.92791100	1.75374400	-0.37959300
H	6.70045600	0.77362000	-0.01154300
H	8.51920500	-2.75656500	1.64437200

H	10.75986400	-1.77069000	1.27377700
C	6.14225100	-1.68583500	1.07965200
O	5.99201200	-2.78441800	1.58700000
C	11.35299600	0.60625000	0.21728200
O	12.37937000	0.01603200	0.51496900
O	11.34736700	1.81743400	-0.33141200
C	12.62426900	2.42729800	-0.57961800
H	13.20080300	1.79453200	-1.26045600
H	13.16463000	2.53482600	0.36511900
C	12.33163800	3.77740500	-1.20168900
H	11.76044500	3.64750200	-2.12893700
H	11.74602700	4.39241500	-0.50775700
O	13.59407900	4.37569200	-1.46584300
6			
C	0.04377200	-3.35081300	-0.20962200
C	1.40040700	-3.59768000	-0.37185000
C	2.08503900	-4.37195900	0.56886800
C	1.40781800	-4.89709600	1.67205000
C	0.05276800	-4.65075700	1.83439600
C	-0.63214200	-3.87704100	0.89445300
H	-0.48346600	-2.74930600	-0.94148700
H	1.92167300	-3.18617000	-1.22870500
H	1.94352200	-5.49600800	2.40082600
H	-0.47575400	-5.05679800	2.69035200
C	3.54250500	-4.65530100	0.43636000
O	4.17917400	-5.31230200	1.24441400
O	8.88562200	-1.54063200	0.82604400
C	8.17311200	-0.35922900	0.61072900
H	8.84240600	0.51871300	0.56750400
H	7.61890300	-0.37960700	-0.34744500

C	7.16934100	-0.14340800	1.73402800
H	7.67303900	-0.01725600	2.69745300
H	6.46527500	-0.97845100	1.80061200
O	6.43441900	1.06222300	1.42958900
C	-2.08473500	-3.63285800	1.10799500
O	-2.71910900	-4.06545900	2.05633300
O	-2.63383800	-2.88485900	0.15274100
C	-4.03180300	-2.59156300	0.28269900
H	-4.20680400	-2.04933100	1.21585100
H	-4.60120600	-3.52437800	0.28662200
C	-4.37252800	-1.72658300	-0.91800400
H	-3.77790700	-0.81267100	-0.91789700
H	-4.22560300	-2.26411000	-1.85723700
O	-5.73297200	-1.28449700	-0.80807800
H	-14.35085300	4.53841400	1.40367700
C	5.15491200	3.37184700	0.69593100
C	4.48417600	4.53281400	0.33583600
C	3.42658000	4.99853600	1.12167000
C	3.04364000	4.29876800	2.26842400
C	3.71491200	3.13963100	2.62862800
C	4.77190100	2.67283000	1.84378400
H	5.97517000	3.01457800	0.08361000
H	4.78609100	5.07187000	-0.55497100
H	2.22177800	4.66317500	2.87567800
H	3.41991800	2.59437900	3.51892100
C	2.68144000	6.23870600	0.76957900
O	1.75233600	6.68549600	1.42378600
O	3.13095400	6.81929700	-0.33898100
C	2.47375200	8.02498900	-0.76039300
H	2.56211600	8.78025200	0.02574000
H	1.41699900	7.81514000	-0.94879100

C	3.18192300	8.46334100	-2.02602100
H	4.24305000	8.64587400	-1.81734600
H	3.10104000	7.68116700	-2.79061600
O	2.53927600	9.65667900	-2.45505600
H	2.97133100	9.96673900	-3.26306000
C	5.46935800	1.42342400	2.26338700
O	5.18200400	0.79357300	3.27097500
C	5.49017500	-4.27919300	-0.87663100
H	5.80420800	-5.27696300	-0.56128400
H	5.62016200	-4.17659800	-1.95518300
C	6.25437700	-3.19389500	-0.13676800
H	6.09156200	-3.29885600	0.94526300
H	5.86410200	-2.21230100	-0.44451700
O	4.07516000	-4.11877700	-0.65896800
O	7.61903500	-3.33197800	-0.46426500
H	8.14596400	-2.63944200	0.07398500
C	-9.53871000	0.23003800	-0.32807400
C	-8.25267900	-0.26925000	-0.48316100
C	-8.05909900	-1.52664700	-1.06154100
C	-9.15577000	-2.28200000	-1.48396200
C	-10.44045100	-1.78298900	-1.32888600
C	-10.63498900	-0.52656500	-0.75029300
H	-9.68501400	1.20518600	0.12250100
H	-7.40468100	0.31976500	-0.15289700
H	-9.00142600	-3.25795000	-1.93176300
H	-11.29450900	-2.36705600	-1.65499200
C	-6.69707400	-2.10062200	-1.24042000
O	-6.47766500	-3.19517900	-1.73100100
C	-12.03023800	-0.02849800	-0.59571100
O	-13.02052800	-0.65865600	-0.93138700
O	-12.09240700	1.18143500	-0.04829900



C	-13.39879300	1.74325700	0.15533000
H	-13.97495600	1.08928700	0.81617500
H	-13.90982300	1.83250100	-0.80747000
C	-13.17262900	3.10153900	0.78724600
H	-12.62660800	2.98832400	1.73172200
H	-12.58521300	3.73606000	0.11263800
O	-14.46021000	3.66038200	1.01288100
C	10.20488900	-1.12142100	-2.07763000
H	9.30402600	-1.73607400	-2.22110900
H	9.90174300	-0.06391700	-2.12378400
C	11.18951300	-1.40652700	-3.19567400
H	11.46251000	-2.46973000	-3.18683500
H	12.10063000	-0.81157500	-3.04817800
O	10.56115400	-1.06088200	-4.42771800
H	11.17026800	-1.25039700	-5.14936900
O	10.82675800	-1.41981300	-0.84344600
H	10.09501700	-1.48183000	-0.14122100

TS<sub>6/7</sub>

C	-0.36159600	-3.11564000	0.44403200
C	-1.72477400	-3.26940900	0.65835300
C	-2.45262400	-4.17937400	-0.11318700
C	-1.81272600	-4.93338200	-1.09976900
C	-0.45208900	-4.77670800	-1.31707000
C	0.27630400	-3.86795300	-0.54584800
H	0.20003100	-2.40875300	1.04427900
H	-2.21748100	-2.68162800	1.42464400
H	-2.38194400	-5.63831200	-1.69631000
H	0.04750400	-5.35911400	-2.08394800
C	-3.91821700	-4.36896300	0.07857300
O	-4.58890000	-5.15635800	-0.56919300

O	-8.90670600	-0.95718000	-1.06052800
C	-8.13541200	0.19467500	-0.82300700
H	-8.75018900	1.10285400	-0.90938600
H	-7.70183100	0.18258200	0.19090400
C	-7.00759300	0.24410500	-1.83864100
H	-7.38736100	0.40016100	-2.85275800
H	-6.41400400	-0.67448000	-1.81114200
O	-6.16724900	1.35631400	-1.47340700
C	1.73289900	-3.72455900	-0.81623100
O	2.32118200	-4.30023500	-1.71702400
O	2.34127500	-2.89602100	0.03050700
C	3.74693500	-2.68705400	-0.16469400
H	3.91773400	-2.25068000	-1.15260900
H	4.27124800	-3.64286300	-0.08852800
C	4.16544900	-1.72519100	0.93344900
H	3.61087400	-0.78920000	0.86111600
H	4.02827000	-2.16166600	1.92505800
O	5.53942500	-1.35917300	0.74117700
H	14.32103700	4.10730800	-1.70690600
C	-4.64096600	3.44882700	-0.58209000
C	-3.85798000	4.51230100	-0.15380500
C	-2.67694400	4.82512300	-0.83221100
C	-2.28268200	4.07037400	-1.93963200
C	-3.06613600	3.00923800	-2.36863300
C	-4.24685500	2.69568900	-1.69135300
H	-5.55569200	3.20849200	-0.05194600
H	-4.16755700	5.09312600	0.70768100
H	-1.36547400	4.31670300	-2.46414600
H	-2.76390100	2.42265600	-3.22977700
C	-1.80842000	5.95620100	-0.40313500
O	-0.73401600	6.22461300	-0.91741300

O	-2.32336300	6.65389100	0.60470200
C	-1.55591200	7.76560000	1.09324300
H	-1.41549400	8.49126400	0.28702200
H	-0.58134400	7.40971600	1.43911700
C	-2.36192700	8.35714800	2.23164100
H	-3.34678700	8.67430600	1.86783700
H	-2.50061500	7.60820700	3.02076000
O	-1.62059400	9.46899100	2.71649600
H	-2.10964200	9.86958300	3.44862600
C	-5.05934000	1.54522300	-2.17884000
O	-4.74207200	0.84339300	-3.12730100
C	-5.83678400	-3.63646400	1.27732200
H	-6.19274500	-4.66651300	1.20125900
H	-5.95797400	-3.28050700	2.30154500
C	-6.55625600	-2.72232500	0.30077000
H	-6.41663700	-3.08687100	-0.72567100
H	-6.12463600	-1.71359000	0.36847000
O	-4.41877900	-3.58756100	1.03370500
O	-7.92608500	-2.71668800	0.65375000
H	-8.38552200	-2.10618000	0.01623500
C	9.38991500	-0.01548500	0.12634700
C	8.08874600	-0.44634000	0.34675200
C	7.85908800	-1.67826600	0.96515000
C	8.93431600	-2.47820300	1.35944300
C	10.23404200	-2.04963100	1.13501200
C	10.46492500	-0.81729600	0.51914400
H	9.56453000	0.94123400	-0.35277000
H	7.25671300	0.17679500	0.03890700
H	8.75112700	-3.43420300	1.83844200
H	11.07135100	-2.66908600	1.43839900
C	6.47978200	-2.17569300	1.22226600

O	6.22850300	-3.21430700	1.80962200
C	11.87494000	-0.39225000	0.29516900
O	12.84646400	-1.07833200	0.57078100
O	11.97263500	0.82140900	-0.23844300
C	13.29458100	1.32119700	-0.49664300
H	13.80052200	0.65878300	-1.20481800
H	13.85898300	1.35525500	0.43949100
C	13.10645400	2.70838500	-1.07600100
H	12.51867900	2.65234600	-2.00025500
H	12.57568100	3.34441700	-0.35717700
O	14.40772100	3.21840900	-1.33540400
C	-11.06789400	-0.43606800	1.10590100
H	-10.05465600	-0.12257200	1.42210500
H	-11.76356700	0.33370400	1.48282600
C	-11.38645700	-1.75274600	1.80472800
H	-10.66232800	-2.51837300	1.49420900
H	-12.39174600	-2.08865500	1.51524000
O	-11.31761100	-1.54980300	3.21789500
H	-11.52164800	-2.38040600	3.66092600
O	-11.15582100	-0.56232900	-0.28630500
H	-9.98433100	-0.77861500	-0.71490400
7			
C	2.35272100	0.64136600	-1.33587700
C	3.73649600	0.74906800	-1.30651200
C	4.51936700	-0.16742400	-2.01420900
C	3.91600000	-1.19673100	-2.74023400
C	2.53234500	-1.28880000	-2.78781300
C	1.74834700	-0.36897200	-2.08946000
H	1.74759300	1.34892400	-0.78056700
H	4.20442000	1.54043400	-0.73099800

H	4.52899100	-1.91163400	-3.27879400
H	2.05849400	-2.07778900	-3.36183700
C	6.00582300	-0.06859200	-2.03931600
O	6.74192800	-0.98892400	-2.35316900
O	7.92693500	-0.17746300	2.55603100
C	6.57267700	-0.19077500	2.17985600
H	5.91337400	-0.16970300	3.06183500
H	6.31510600	0.67817800	1.55250500
C	6.30354800	-1.46019000	1.39442200
H	6.60983400	-2.34597400	1.96012300
H	6.81205800	-1.45659500	0.42668500
O	4.87938500	-1.51465900	1.19216500
C	0.26875100	-0.50389100	-2.16686100
O	-0.31046500	-1.29256300	-2.89560700
O	-0.37172300	0.33654000	-1.35574400
C	-1.80410800	0.33107100	-1.40269200
H	-2.18292900	-0.68986000	-1.31481800
H	-2.13200500	0.75604800	-2.35541400
C	-2.24363000	1.17629400	-0.22135500
H	-1.89077400	0.74167000	0.71486200
H	-1.88905000	2.20568300	-0.30698600
O	-3.67360400	1.15124700	-0.13083700
H	-13.59999300	-1.68029300	2.42349400
C	2.15038500	-1.64171200	1.19049100
C	0.76376800	-1.70413700	1.15545400
C	0.13148600	-2.66304100	0.35976200
C	0.88914500	-3.55380100	-0.40484300
C	2.27403600	-3.49731100	-0.36024600
C	2.90766600	-2.54259700	0.43797200
H	2.63854300	-0.89354400	1.80438400
H	0.17859900	-1.00391500	1.74088500

H	0.39279800	-4.28933300	-1.02882100
H	2.86626200	-4.18835700	-0.95048600
C	-1.35235900	-2.75683000	0.28800900
O	-1.95392100	-3.46481900	-0.50399100
O	-1.96501800	-1.98712500	1.18329900
C	-3.40091500	-2.01734300	1.20195200
H	-3.74019800	-3.05044000	1.32041200
H	-3.78380600	-1.61447000	0.25943700
C	-3.82718600	-1.17413700	2.38662800
H	-3.33897400	-1.54145100	3.29787200
H	-3.54514100	-0.12574700	2.23412700
O	-5.23918500	-1.30731400	2.48343000
H	-5.56185400	-0.69522300	3.15895000
C	4.39681800	-2.50976500	0.45868500
O	5.10480400	-3.31853600	-0.12170000
C	7.85043600	1.41859800	-1.81541200
H	8.27826600	0.86144500	-2.65193500
H	7.91909300	2.48957100	-2.01317600
C	8.53477100	1.07486000	-0.50641200
H	8.46728000	-0.00017500	-0.30633500
H	8.04645800	1.61654600	0.31039200
O	6.43999500	1.15067900	-1.72123600
O	9.89084800	1.47789500	-0.64291100
H	10.34268400	1.31572500	0.19333700
C	-7.75203000	0.75876500	0.26519300
C	-6.37569000	0.86775600	0.12091700
C	-5.83861800	1.87099000	-0.68974600
C	-6.68140000	2.76300300	-1.35687200
C	-8.05641200	2.65518500	-1.21055900
C	-8.59511300	1.65319300	-0.39963400
H	-8.16388500	-0.02198100	0.89510700

H	-5.72930300	0.16962400	0.64138800
H	-6.25992000	3.53935300	-1.98661700
H	-8.71428700	3.34716700	-1.72552700
C	-4.36863700	2.01717700	-0.87037100
O	-3.84897300	2.83812900	-1.60736800
C	-10.07647200	1.57188100	-0.26780800
O	-10.85293500	2.34436800	-0.80725300
O	-10.47534000	0.56530300	0.50398400
C	-11.89006500	0.41012400	0.69855500
H	-12.37214900	0.23832400	-0.26804800
H	-12.29536200	1.31887800	1.15261700
C	-12.05785100	-0.78279100	1.61741400
H	-11.63540100	-1.68033200	1.14964900
H	-11.53873100	-0.60014800	2.56612200
O	-13.45574500	-0.93252900	1.82749200
C	8.80345800	2.87816800	2.85826100
H	9.47876100	3.62001100	3.32482000
H	9.38347400	2.41662700	2.03378100
C	7.63766300	3.63666200	2.23113100
H	7.10213700	4.20065500	3.00754600
H	6.93371200	2.92228300	1.78126700
O	8.14679200	4.52449300	1.23309600
H	7.41144600	5.00987700	0.84406600
O	8.36380100	1.92863400	3.78109500
H	8.11239800	0.72117000	3.08767600

[BHET]<sub>2</sub>

C	-5.77785600	0.05422800	-0.00919600
C	-4.40326400	-0.13910500	-0.02500000
C	-3.88309300	-1.43605900	-0.03982400
C	-4.74179100	-2.53781300	-0.04030000

C	-6.11504400	-2.34439900	-0.02468100
C	-6.63607900	-1.04849900	-0.00834200
H	-6.17804200	1.06168000	0.00347100
H	-3.74058800	0.71893200	-0.02472000
H	-4.33351200	-3.54280000	-0.05225700
H	-6.78529800	-3.19744600	-0.02435600
C	-2.41567600	-1.68590600	-0.05270000
O	-1.91021700	-2.79652900	-0.05929700
O	-1.69741800	-0.56458100	-0.05505400
C	-0.27089300	-0.70707700	-0.06056000
H	0.03949000	-1.25224700	-0.95596100
H	0.04556200	-1.25362900	0.83192600
C	0.27092600	0.70717100	-0.06073700
H	-0.04554300	1.25394600	0.83160800
H	-0.03945400	1.25210700	-0.95628300
O	1.69744800	0.56468200	-0.05520400
C	-8.11624000	-0.88319700	0.01365700
O	-8.90621300	-1.81400100	0.02178300
O	-8.49709600	0.39049000	0.02601300
C	-9.90921900	0.65189000	0.05945100
H	-10.33958400	0.20205100	0.95872800
H	-10.37960900	0.21766900	-0.82731500
C	-10.05340600	2.15996100	0.07739000
H	-9.54655400	2.57382300	0.95753700
H	-9.60410300	2.59126800	-0.82537400
O	-11.44870200	2.42953200	0.12562600
H	-11.57876400	3.38780700	0.14969000
C	4.40326000	0.13917200	-0.02470800
C	5.77784300	-0.05419800	-0.00869400
C	6.63609600	1.04850200	-0.00809700
C	6.11510200	2.34441600	-0.02492200



C	4.74185500	2.53786900	-0.04073600
C	3.88312700	1.43613600	-0.03998600
H	3.74054700	-0.71883600	-0.02422900
H	6.17799800	-1.06165900	0.00432100
H	6.78538800	3.19743700	-0.02484800
H	4.33361000	3.54286400	-0.05308100
C	8.11624800	0.88315800	0.01417200
O	8.90625500	1.81392500	0.02270300
O	8.49704700	-0.39054600	0.02627400
C	9.90917300	-0.65199600	0.05953000
H	10.33955100	-0.20265400	0.95906100
H	10.37956500	-0.21730100	-0.82699200
C	10.05332100	-2.16007600	0.07674600
H	9.54626900	-2.57432600	0.95659900
H	9.60420900	-2.59096700	-0.82630800
O	11.44859700	-2.42969800	0.12513600
H	11.57858400	-3.38798900	0.14895900
C	2.41571300	1.68600300	-0.05307400
O	1.91025700	2.79662400	-0.06004200

[BHET]-

C	0.73910500	-0.37874000	0.00019400
C	-0.64941100	-0.36816300	0.00008200
C	-1.33646900	0.84888800	-0.00013700
C	-0.62951700	2.05371400	-0.00023500
C	0.75726900	2.04239500	-0.00008700
C	1.44553500	0.82692800	0.00012000
H	1.26926600	-1.32448300	0.00036100
H	-1.19365600	-1.30588500	0.00015800
H	-1.16625700	2.99645500	-0.00041300
H	1.30909500	2.97635600	-0.00015400

C	-2.82420900	0.90548500	-0.00027000
O	-3.46709800	1.94363000	-0.00057500
O	-3.39284300	-0.29686200	-0.00005400
C	-4.82887200	-0.34004600	-0.00005800
H	-5.20666700	0.16533700	-0.89344800
H	-5.20668900	0.16573700	0.89309400
C	-5.20435300	-1.80779800	0.00026600
H	-4.79778100	-2.29972600	-0.89163100
H	-4.79782200	-2.29932800	0.89240000
O	-6.62551300	-1.85625000	0.00024300
H	-6.90214200	-2.78283200	0.00050300
C	2.93699000	0.85805000	0.00032100
O	3.58820000	1.89361100	0.00084900
O	3.48563900	-0.34680800	-0.00009600
C	4.93291500	-0.42765700	0.00009800
H	5.31023100	0.08025700	0.89345000
H	5.31054600	0.08111000	-0.89262900
C	5.32669100	-1.90220700	-0.00055600
H	4.84831100	-2.37247800	0.88409600
H	4.84890000	-2.37154700	-0.88602200
O	6.70919400	-2.03408000	-0.00014100

[BHET]

C	0.69422100	-0.35753300	0.00051200
C	-0.69422700	-0.35753200	0.00051300
C	-1.39035600	0.85424000	0.00009200
C	-0.69337400	2.06480300	-0.00030500
C	0.69337500	2.06480300	-0.00030500
C	1.39035300	0.85423800	0.00009300
H	1.23141100	-1.29927300	0.00085100
H	-1.23141800	-1.29927200	0.00086100

H	-1.23789400	3.00301900	-0.00062700
H	1.23789700	3.00301800	-0.00062800
C	-2.87897600	0.89915900	0.00006500
O	-3.52918500	1.93245700	0.00014800
O	-3.43781900	-0.30753700	-0.00010500
C	-4.87365700	-0.36183600	-0.00004500
H	-5.25517700	0.14107000	-0.89322600
H	-5.25507800	0.14084800	0.89330000
C	-5.23845000	-1.83230000	-0.00021600
H	-4.82853700	-2.32104200	-0.89235500
H	-4.82841000	-2.32128400	0.89173000
O	-6.65918300	-1.89039200	-0.00010600
H	-6.92989400	-2.81871300	-0.00005500
C	2.87897300	0.89915000	0.00005800
O	3.52919000	1.93244100	0.00001500
O	3.43781500	-0.30754800	0.00007700
C	4.87365300	-0.36183500	0.00005900
H	5.25512800	0.14084100	0.89338800
H	5.25510700	0.14108200	-0.89314000
C	5.23845600	-1.83229500	-0.00013700
H	4.82855700	-2.32125700	0.89188400
H	4.82841100	-2.32106300	-0.89220000
O	6.65918900	-1.89037800	-0.00026900
H	6.92990300	-2.81869800	-0.00015700