

Supplementary Information

Novel uncharged triazole salicylaldoxime derivatives as potential acetylcholinesterase reactivators: comprehensive computational study, synthesis and in vitro evaluation

Mohammad Hadi Baghersad*,¹, Azizollah Habibi² and Arash dehdashti nejad¹

¹ Applied Biotechnology Research Center, Baqiyatallah University of Medical Sciences, Tehran, Iran.

² Faculty of Chemistry, Kharazmi University, No. 43, P. Code 15719-14911, Mofatteh Street, Enghelab Ave., Tehran, Iran.

Corresponding author: Hadibaghersad@bmsu.ac.ir

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Computational results

S1. The energy of optimized structures

The energy of optimized structures at the theoretical M062X/6-31G* level in the aqueous phase for species involved in reactivating the serine-POX (SON) molecule through studied oximes.

AE	-643759.3811	AZ	-643754.0200	BE	-2257202.653	BZ	-2257196.561
C1_{AE}	-1443810.037	C1_{AZ}	-1443805.742	C1_{BE}	-3057256.034	C1_{BZ}	-3057248.093
TS1_{AE}	-1443806.077	TS1_{AZ}	-1443801.349	TS1_{BE}	-3057252.829	TS1_{BZ}	-3057243.803
IN_{AE}	-1443816.003	IN_{AZ}	-1443814.083	IN_{BE}	-3057260.494	IN_{BZ}	-3057256.495
TS2_{AE}	-1443813.897	TS2_{AZ}	-1443813.223	TS2_{BE}	-3057259.996	TS2_{BZ}	-3057255.784
C2_{AE}	-1443827.563	C2_{AZ}	-1443827.052	C2_{BE}	-3057274.219	C2_{BZ}	-3057269.650
CE							
CE	-772044.2415	CZ	-772041.4792	DE	-2385487.366	DZ	-2385483.919
C1_{CE}	-1572094.643	C1_{CZ}	-1572093.530	C1_{DE}	-3185541.799	C1_{DZ}	-3185535.760
TS1_{CE}	-1572090.140	TS1_{CZ}	-1572088.274	TS1_{DE}	-3185536.851	TS1_{DZ}	-3185530.508
IN_{CE}	-1572098.230	IN_{CZ}	-1572098.705	IN_{DE}	-3185542.723	IN_{DZ}	-3185540.989
TS2_{CE}	-1572096.186	TS2_{CZ}	-1572097.513	TS2_{DE}	-3185541.611	TS2_{DZ}	-3185539.730
C2_{CE}	-1572108.009	C2_{CZ}	-1572109.482	C2_{DE}	-3185554.430	C2_{DZ}	-3185551.797
EE							
EE	-715595.9676	EZ	-715590.5874	FE	-2329039.422	FZ	-2329033.122
C1_{EE}	-1515646.708	C1_{EZ}	-1515642.618	C1_{FE}	-3129093.845	C1_{FZ}	-3129085.130
TS1_{EE}	-1515642.617	TS1_{EZ}	-1515638.143	TS1_{FE}	-3129089.042	TS1_{FZ}	-3129080.523
IN_{EE}	-1515652.479	IN_{EZ}	-1515650.293	IN_{FE}	-3129096.894	IN_{FZ}	-3129092.755
TS2_{EE}	-1515650.441	TS2_{EZ}	-1515649.408	TS2_{FE}	-3129096.452	TS2_{FZ}	-3129091.881
C2_{EE}	-1515663.604	C2_{EZ}	-1515662.609	C2_{FE}	-3129110.287	C2_{FZ}	-3129105.037
2-PAM							
2-PAM	-286146.9395						
C1_(2-PAM)	-1086193.381						
TS1_(2-PAM)	-1086186.711						
IN_(2-PAM)	-1086188.872						
TS2_(2-PAM)	-1086185.549						
C2_(2-PAM)	-1086196.157						
C1_(2-PAM)	-1086193.381						
AChE-POX							
AChE-POX	-800041.2208						

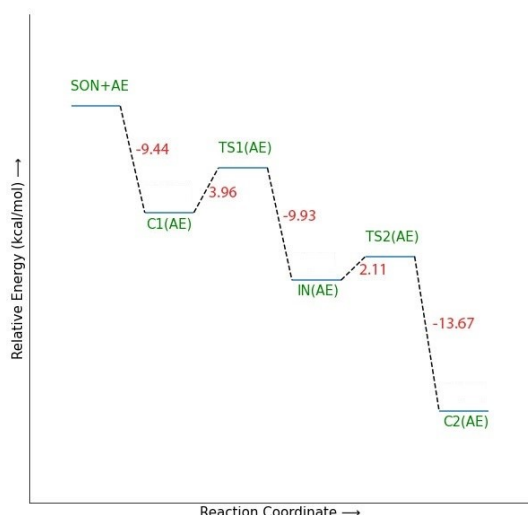
S2. The binding energy, O(Oxime)-P(POX) distance

The binding energy, O(Oxime)-P(POX) distance, and amino acids interacting with oximes in the AChE-POX complex based on docking calculations.

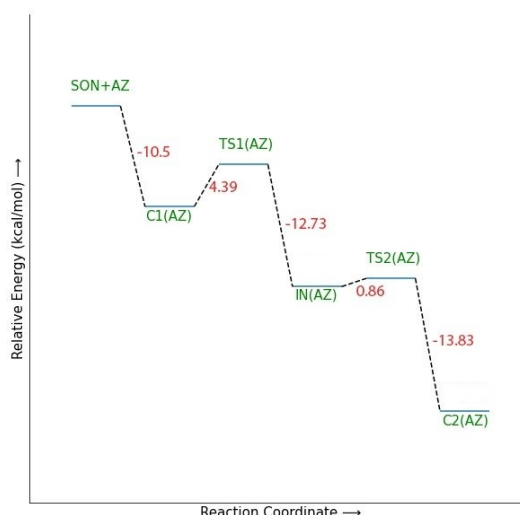
	Energy (kcal/mol)	Distance O-P (nm)	Interaction Residues
2-PAM	-4.96	0.73	TRP86, TRP117, TYR119, GLY120, GLY121, TYR133, GLU202, SON203, TYR337, HIS447, GLU448, ILE451
AE	-6.72	0.37	ASP74, TRP86, GLY120, GLY121, TYR124, SER125, GLY126, LEU130, TYR133, GLU202, SON203, ALA204, TYR337, TYR341, HIS447, GLY448, TYR449
BE	-8.16	0.38	ASP74, TRP86, GLY120, GLY121, TYR124, SER125, GLY126, LEU130, TYR133, GLU202, SON203, VAL294, PHE295, PHE297, TYR337, PHE338, TYR341
CE	-7.35	0.37	GLN71, TYR72, VAL73, ASP74, TRP86, ASN87, PRO88, TYR119, GLY120, GLY121, TYR124, SER125, GLY126, ALA127, LEU130, TYR133, GLU202, SON203, TYR337, TYR341, HIS447
DE	-6.04	0.36	GLN71, TYR72, VAL73, ASP74, TRP86, ASN87, PRO88, TYR119, GLY120, GLY121, SER125, GLY126, ALA127, LEU130, TYR133, GLU202, SON203, TYR337, PHE338, TYR341
EE	-7.59	0.49	TYR72, VAL73, ASP74, TRP86, ASN87, TYR119, GLY120, GLY121, TYR124, SER125, GLY126, ALA127, LEU130, TYR133, GLU202, SON203, TYR337, TYR341, HIS447, GLU202, SON203, TYR337, TYR341, HIS447, GLY448
FE	-7.14	0.35	GLN71, TYR72, VAL73, ASP74, THR83, TRP86, ASN87, PRO88, TYR119, GLY120, GLY121, TYR124, SER125, GLY126, ALA127, LEU130, TYR133, GLU202, SON203, TYR337, TYR341
AZ	-6.94	0.33	ASP74, TRP86, GLY120, GLY121, GLY122, TYR124, SER125, GLY126, LEU130, TYR133, GLU202, SON203, TYR341, HIS447, GLY448
BZ	-7.16	0.45	TYR72, VAL73, ASP74, THR75, LEU76, TRP86, ASN87, PRO88, GLY120, GLY121, TYR124, SER125, GLY126, ALA127, LEU130, TYR133, SON203, TYR341
CZ	-6.78	0.36	TYR72, VAL73, ASP74, TRP86, ASN87, PRO88, TYR119, GLY120, GLY121, GLY122, TYR124, SER125, GLY126, ALA127, LEU130, TYR133, SON203, TYR337, TYR341, HIS447
DZ	-6.83	0.47	ASP74, TRP86, TYR119, GLY120, GLY121, TYR124, SER125, GLY126, ALA127, LEU130, TYR133, SON203, PHE295, PHE297, TYR337, PHE338, TYR341
EZ	-6.05	0.52	ASP74, TRP86, TRP117, GLY120, GLY121, TYR124, SER125, TYR133, GLU202, SON203, TYR337, TYR341, HIS447, GLY448, TYR449, ILE451
FZ	-6.87	0.55	TYR72, VAL73, ASP74, TRP86, ASN87, TYR119, GLY120, GLY121, TYR124, SER125, GLY126, ALA127, LEU130, TYR133, GLU202, SON203, TYR337, HIS447, GLY448, TYR449

S3. The energy diagram of the optimized structures

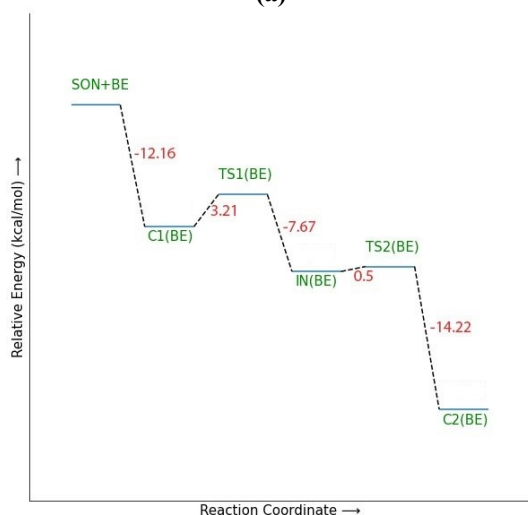
The energy diagram of the optimized structures at the theoretical M062X/6-31G* level for reactivating AChE-POX by (a) AE, (b) AZ, (c) BE, (d) BZ, (e) CE, (f) CZ, (g) DE, (h) DZ, (i) EE, (j) EZ, (k) FE, and (l) FZ in the aqueous phase.



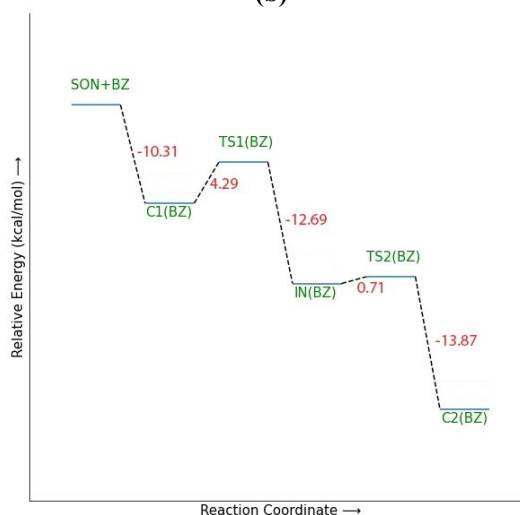
(a)



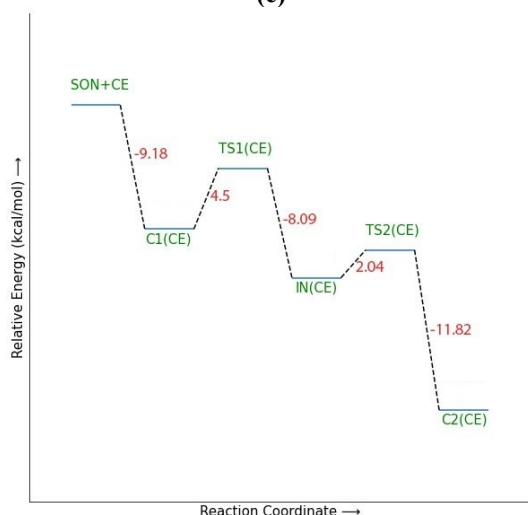
(b)



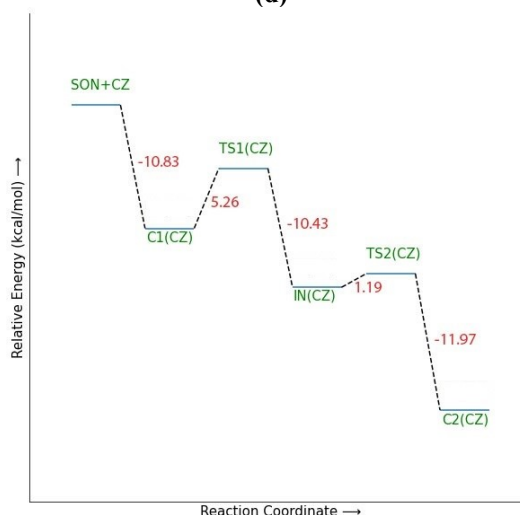
(c)



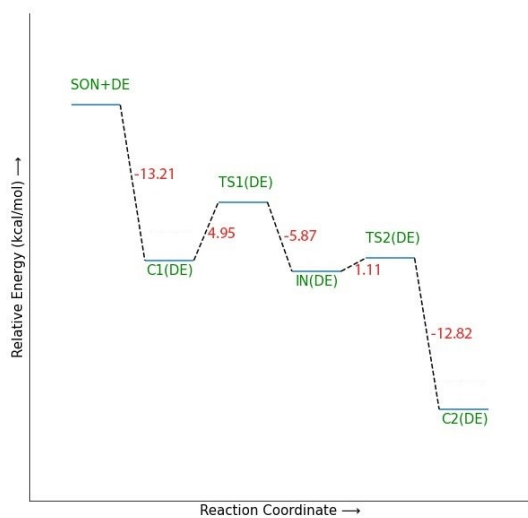
(d)



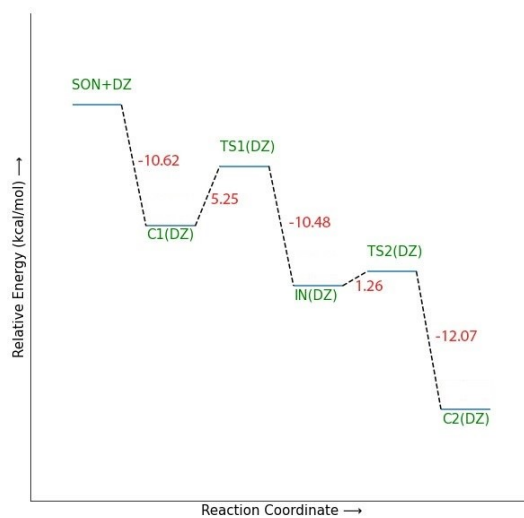
(e)



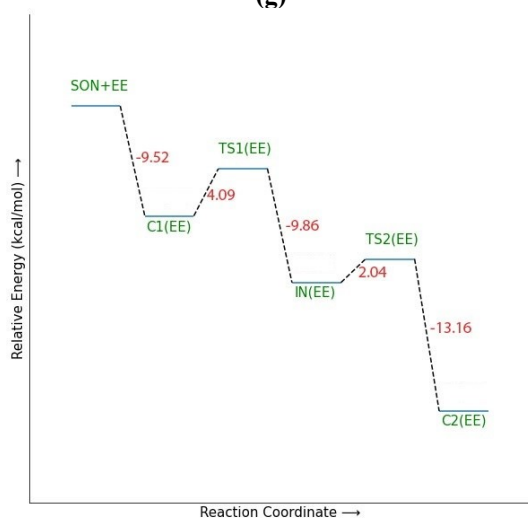
(f)



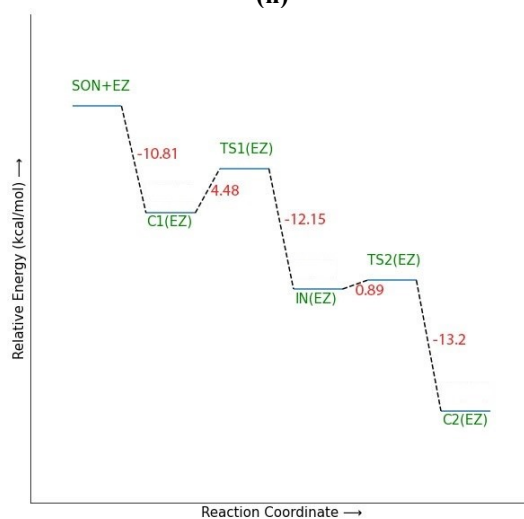
(g)



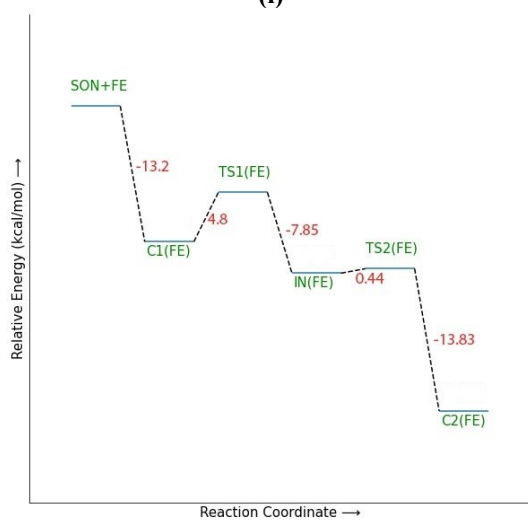
(h)



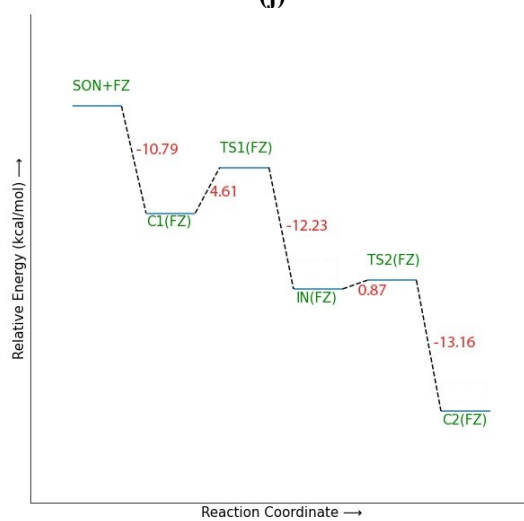
(i)



(j)



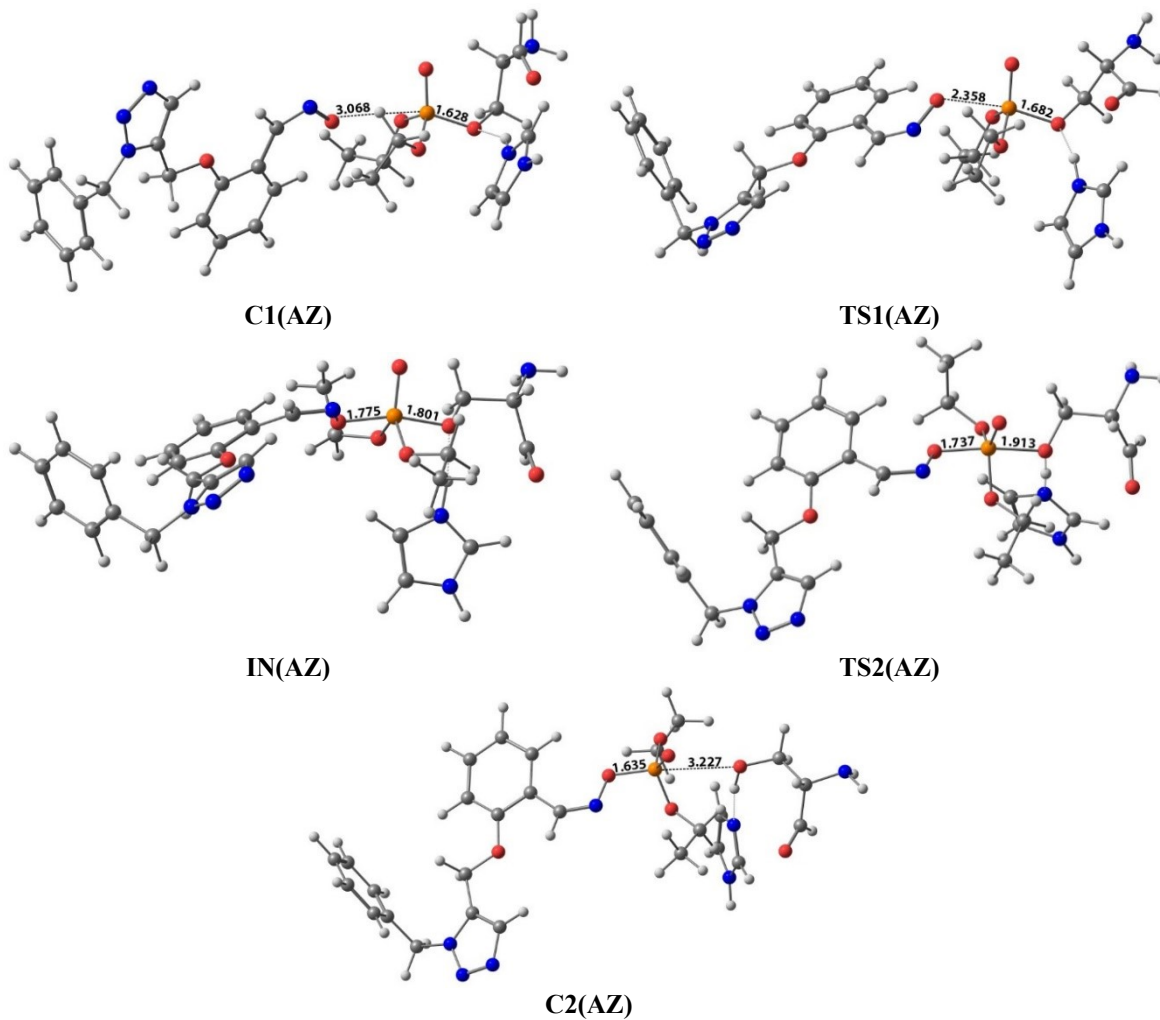
(k)



(l)

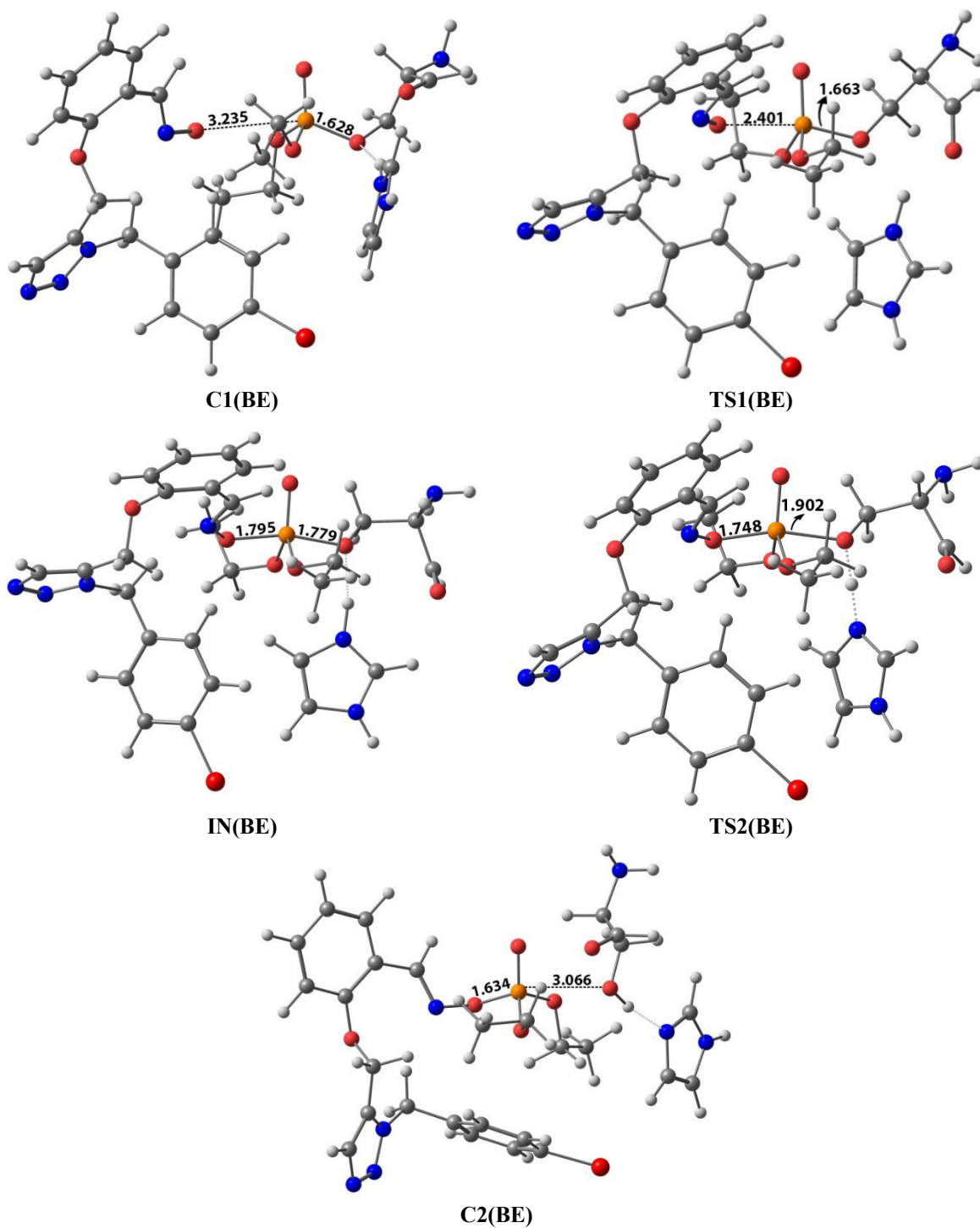
S4. The optimized structures of species involved in reactivating SON by AZ

The optimized structures at the theoretical M062X/6-31G* level and the selected bond lengths (Å) of species involved in reactivating SON by AZ in the aqueous phase.



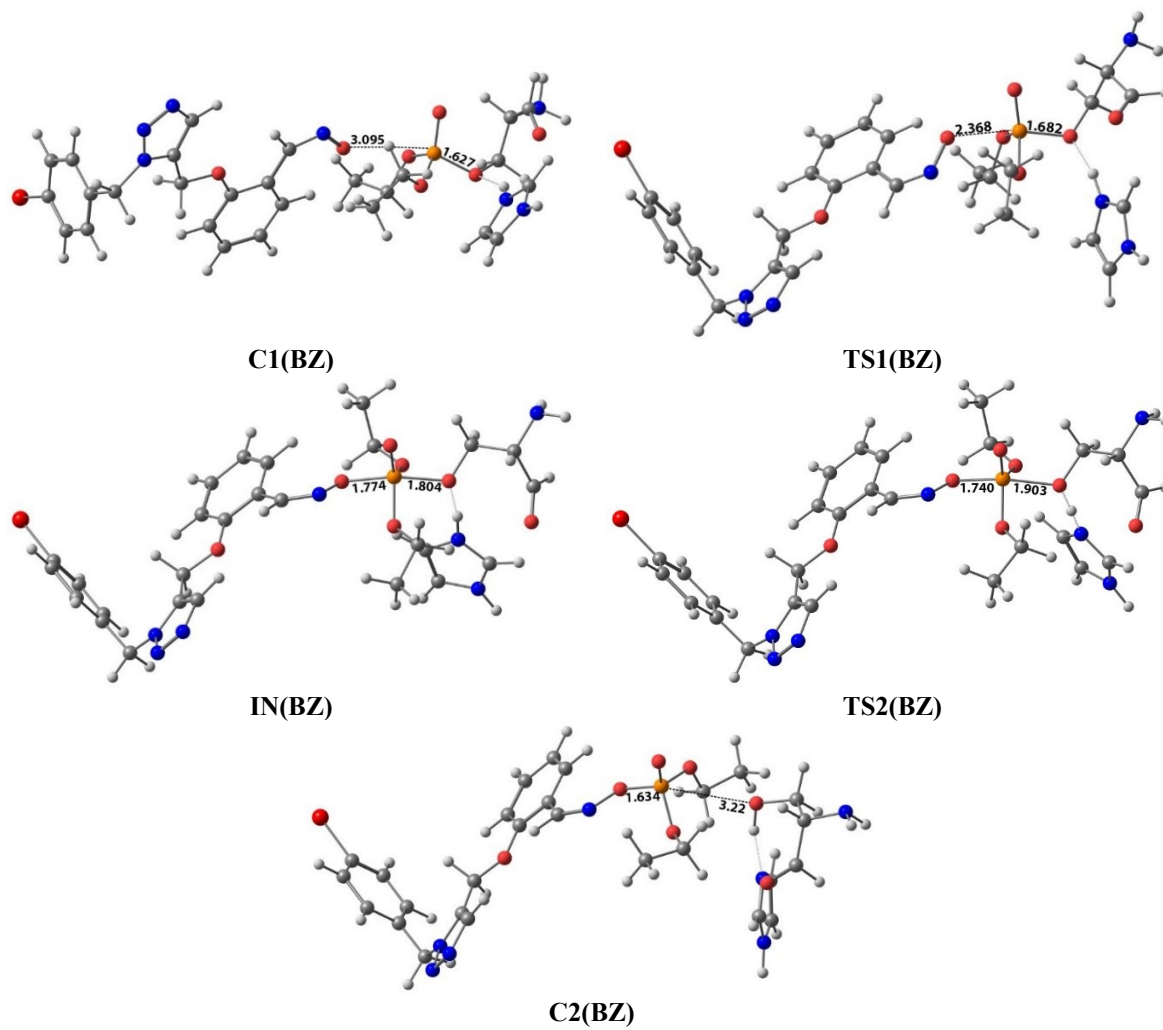
S5. The optimized structures of species involved in reactivating SON by BE

The optimized structures at the theoretical M062X/6-31G* level and the selected bond lengths (Å) of species involved in reactivating SON by BE in the aqueous phase.



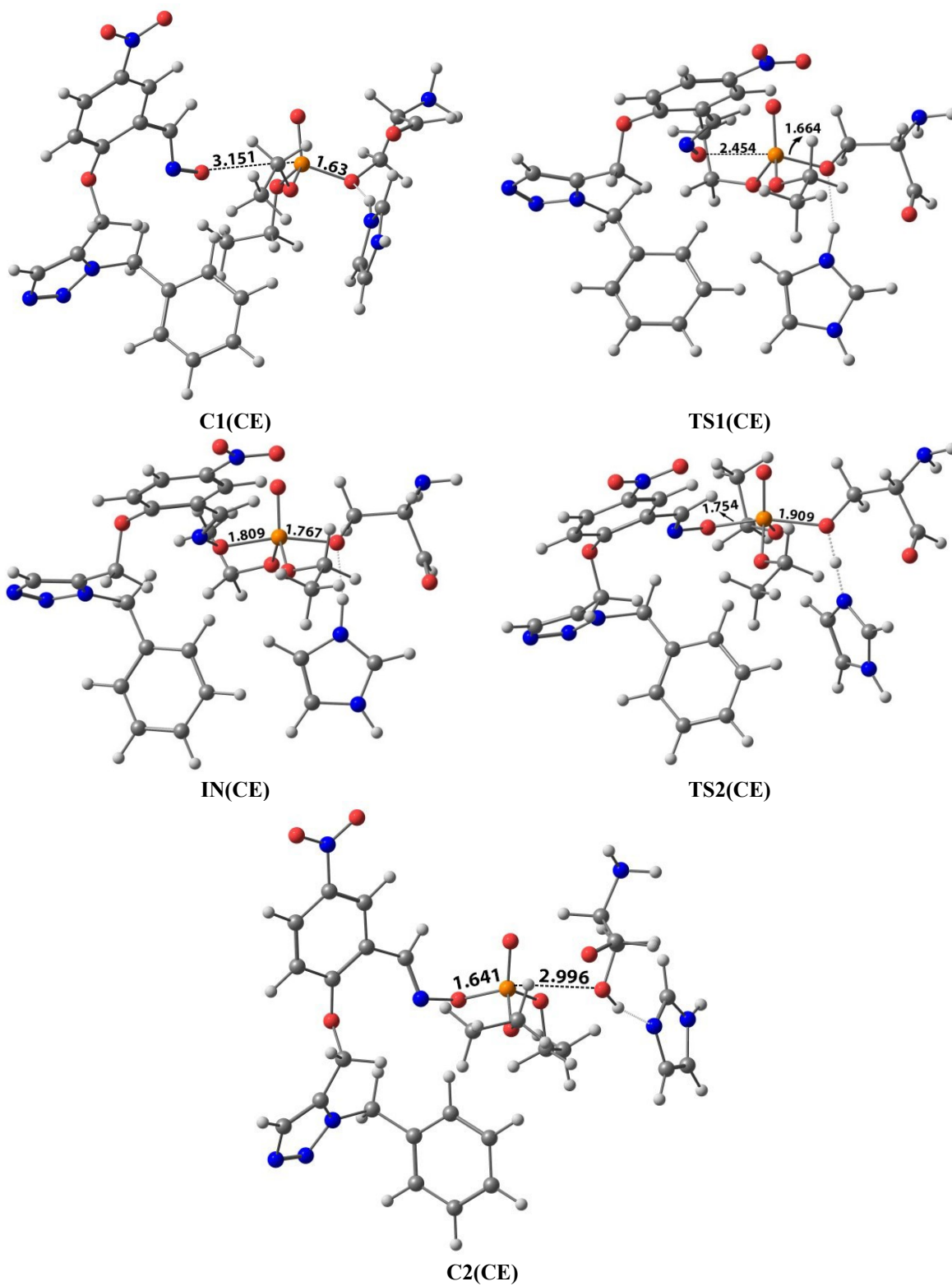
S6. The optimized structures of species involved in reactivating SON by BZ

The optimized structures at the theoretical M062X/6-31G* level and the selected bond lengths (Å) of species involved in reactivating SON by BZ in the aqueous phase.



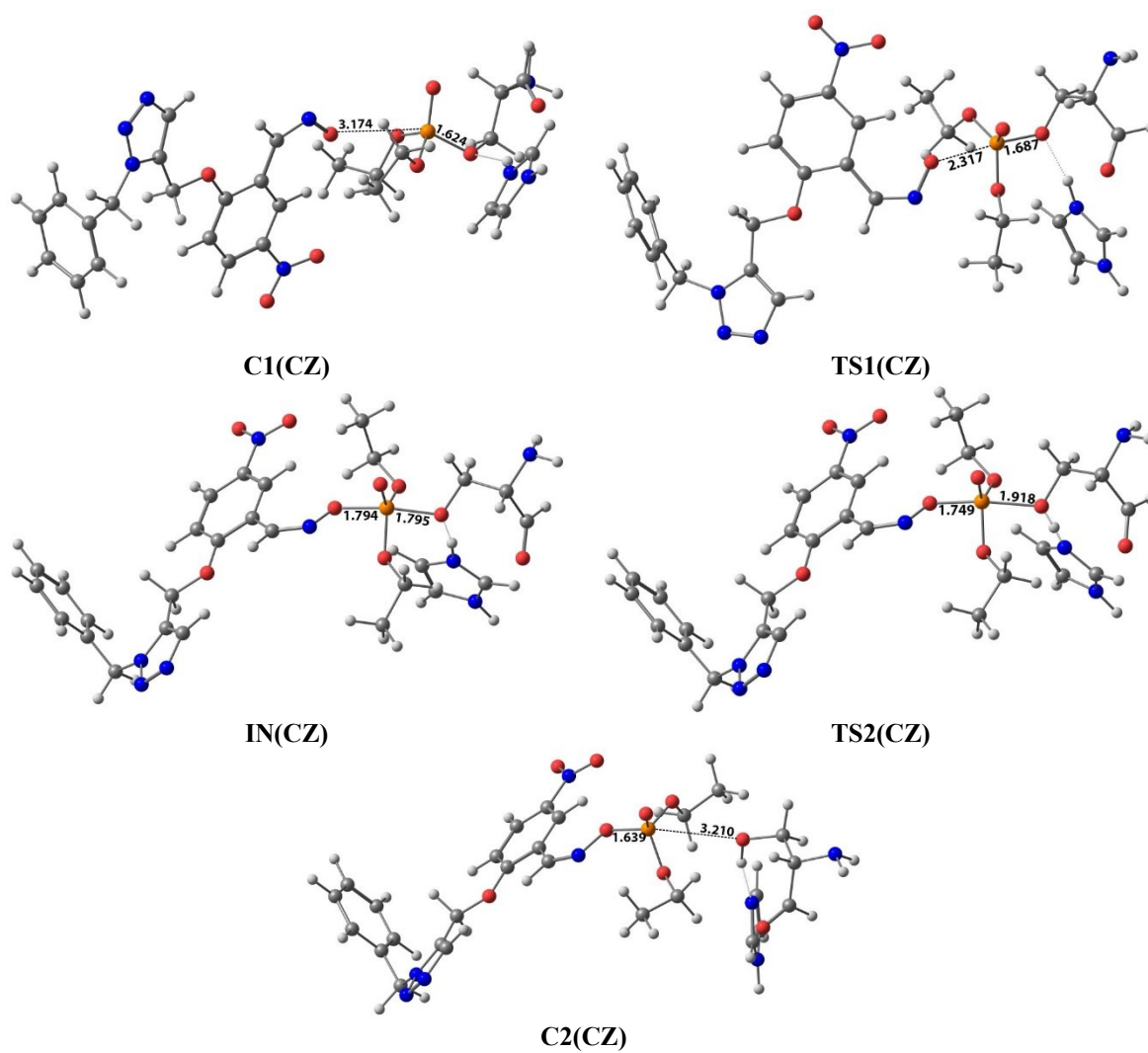
S7. The optimized structures of species involved in reactivating SON by CE

The optimized structures at the theoretical M062X/6-31G* level and the selected bond lengths (Å) of species involved in reactivating SON by CE in the aqueous phase.



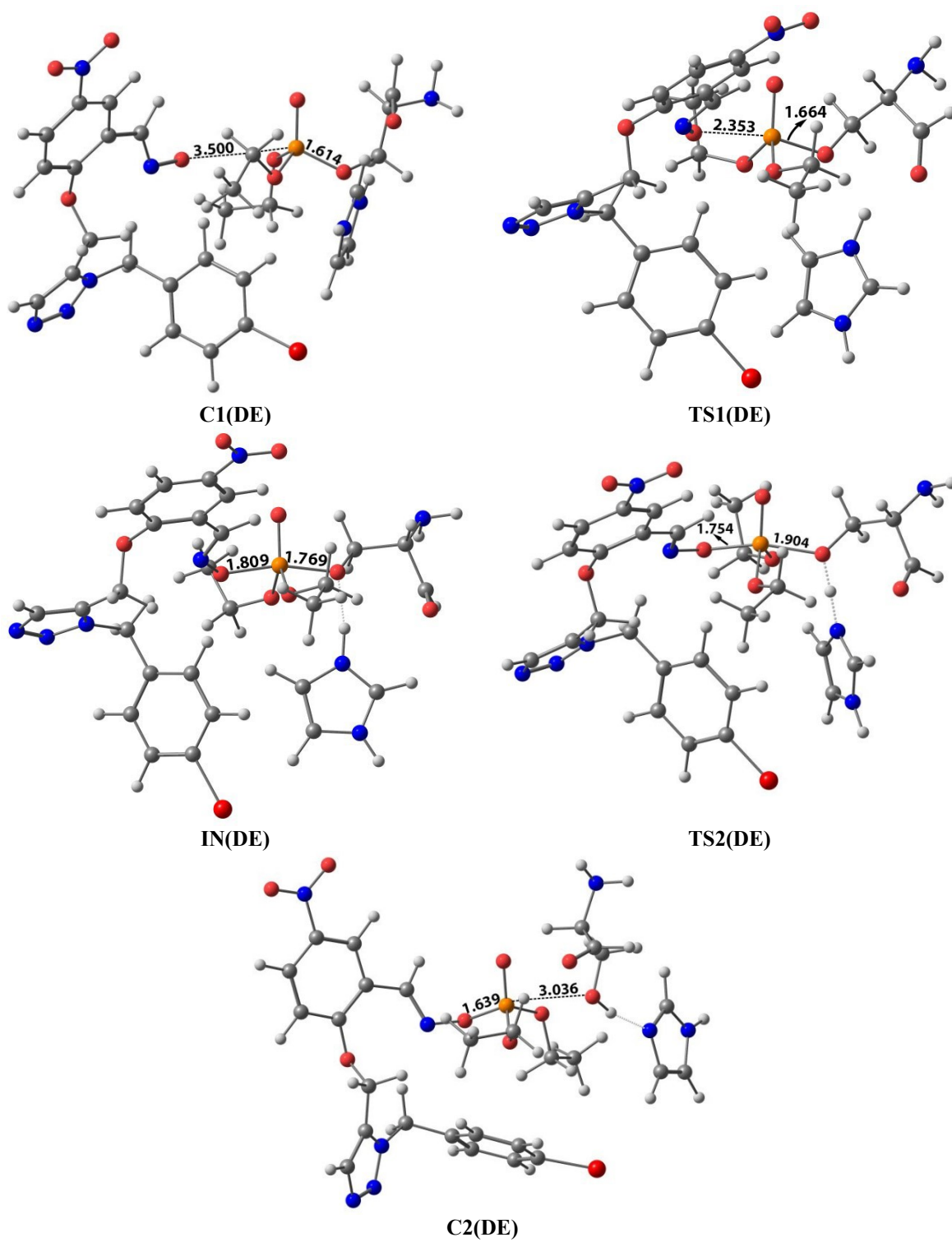
S8. The optimized structures of species involved in reactivating SON by CZ

The optimized structures at the theoretical M062X/6-31G* level and the selected bond lengths (Å) of species involved in reactivating SON by CZ in the aqueous phase.

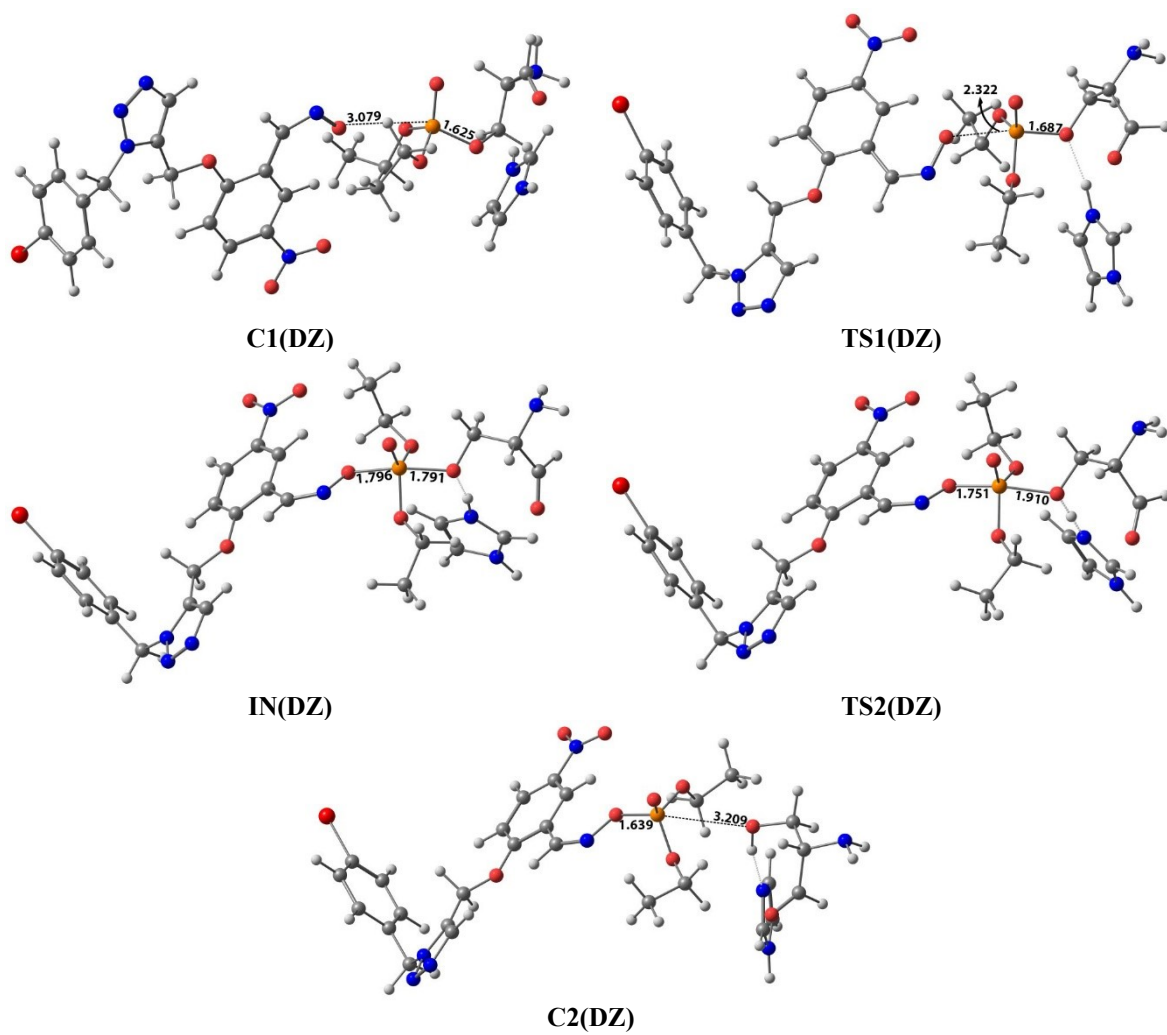


S9. The optimized structures species involved in reactivating SON by DE

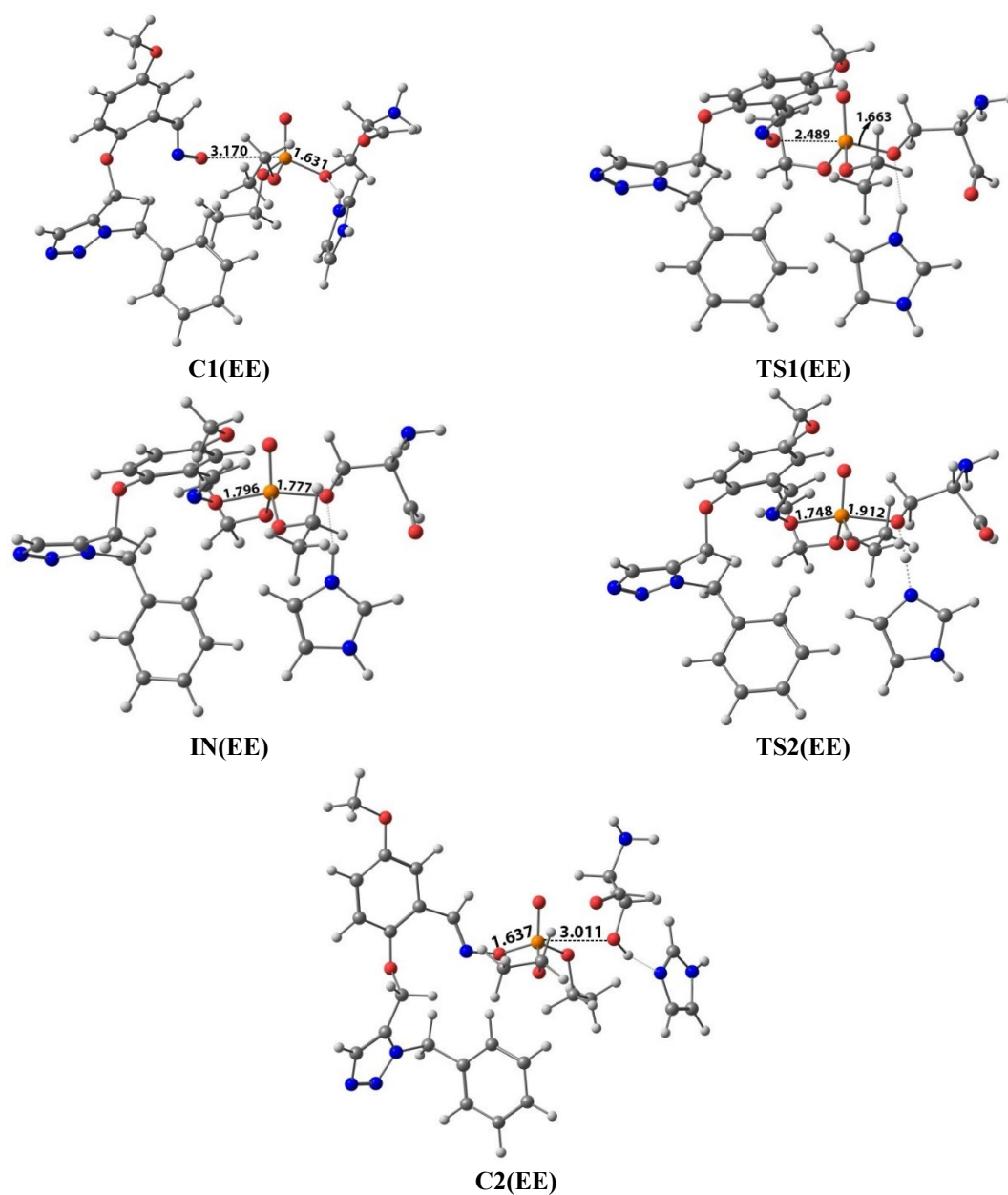
The optimized structures at the theoretical M062X/6-31G* level and the selected bond lengths (Å) of species involved in reactivating SON by DE in the aqueous phase.



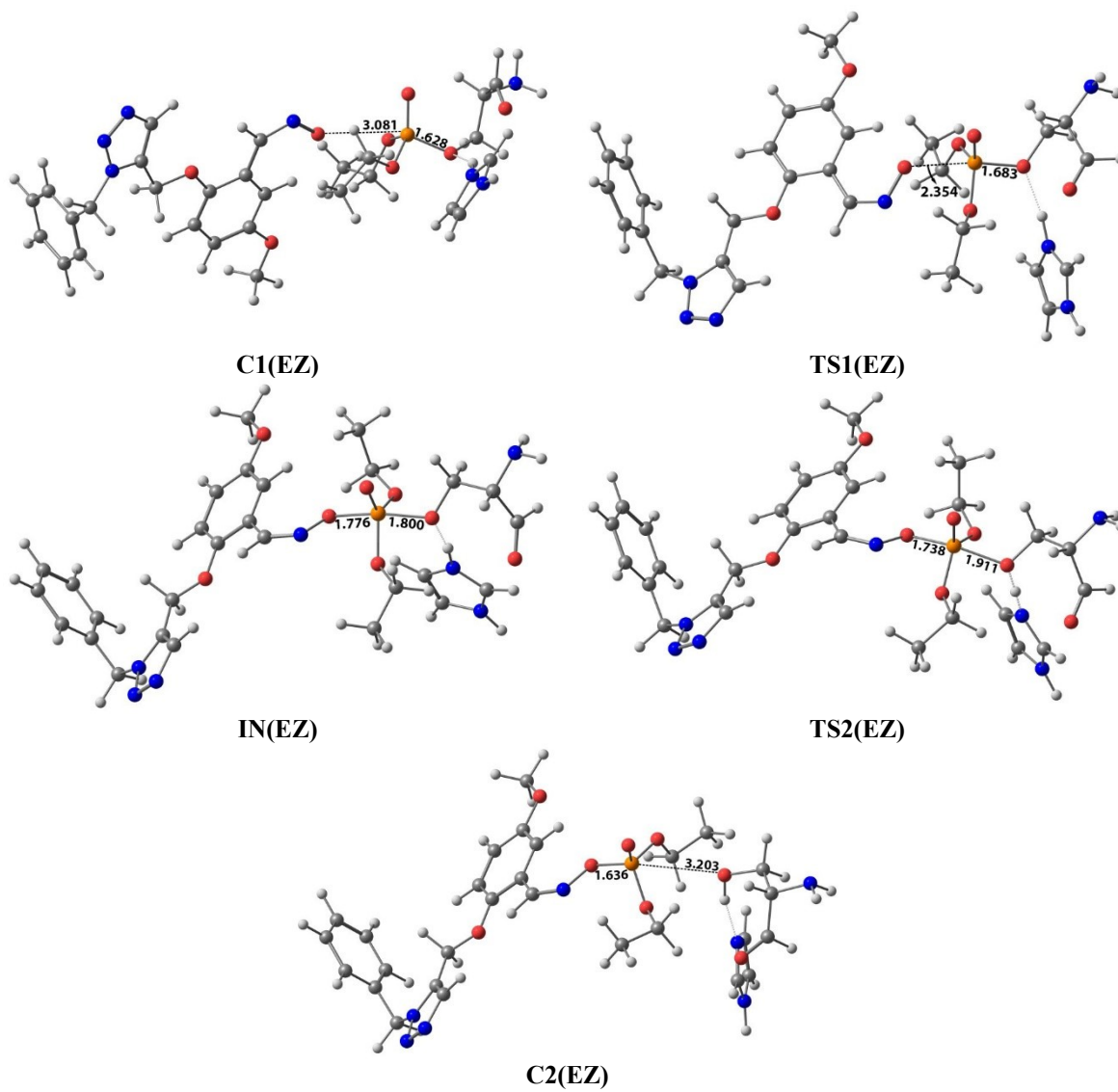
S10. The optimized structures of species involved in reactivating SON by DZ. The optimized structures at the theoretical M062X/6-31G* level and the selected bond lengths (Å) of species involved in reactivating SON by DZ in the aqueous phase.



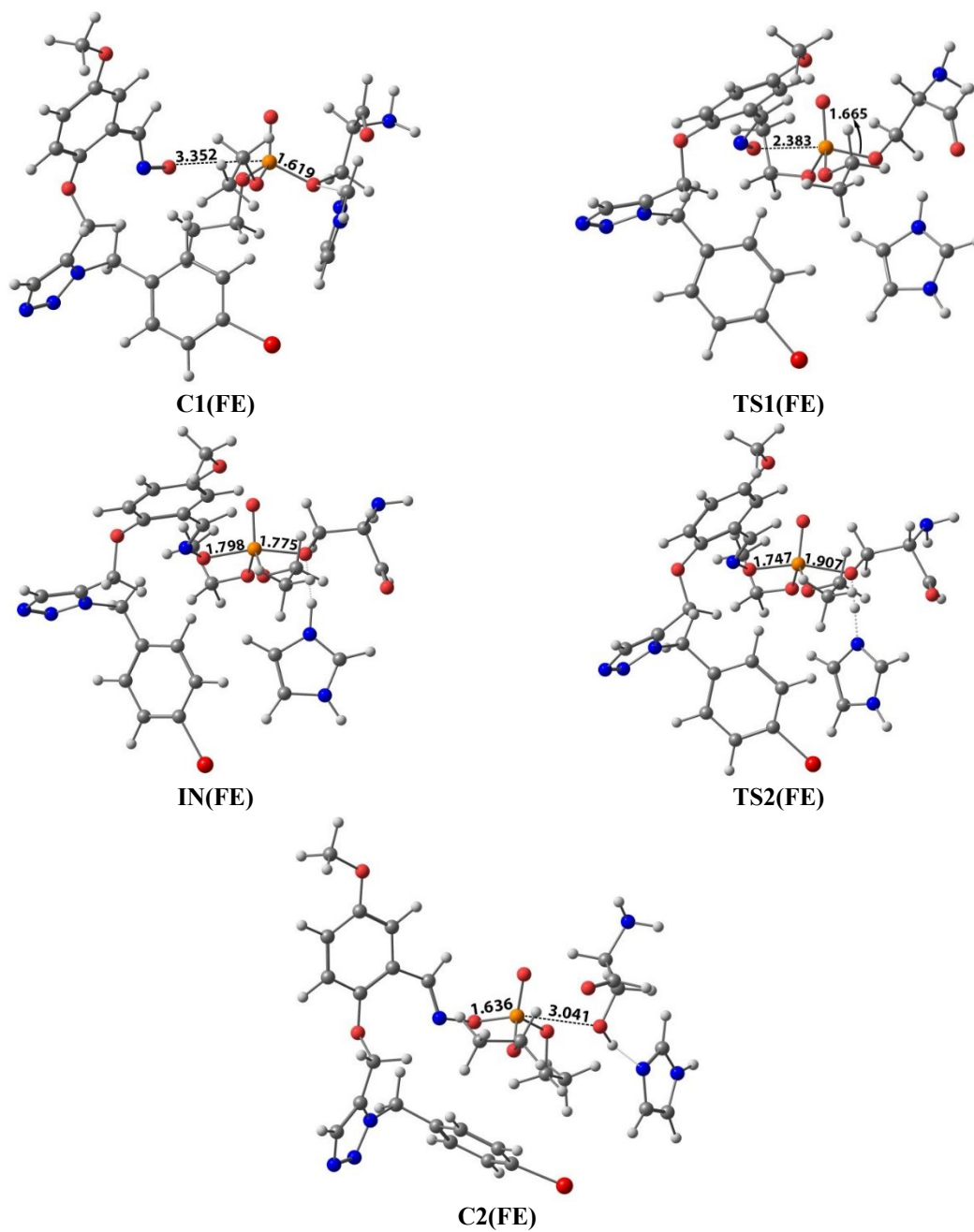
S11. The optimized structures of species involved in reactivating SON by EE
The optimized structures at the theoretical M062X/6-31G* level and the selected bond lengths (Å) of species involved in reactivating SON by EE in the aqueous phase.



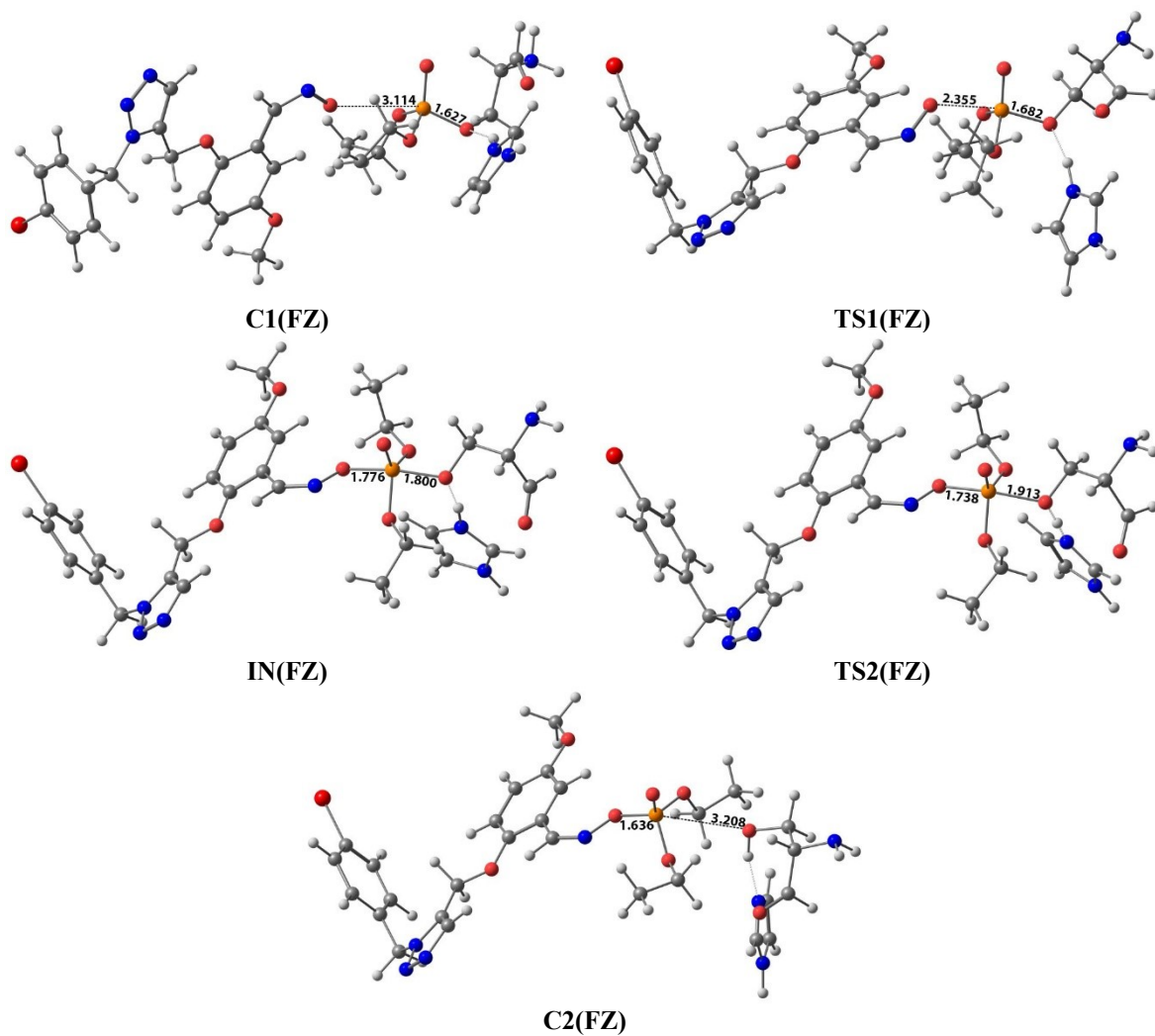
S12. The optimized structures of species involved in reactivating SON by EZ
The optimized structures at the theoretical M062X/6-31G* level and the selected bond lengths (Å) of species involved in reactivating SON by EZ in the aqueous phase.



S13. The optimized structures of species involved in reactivating SON by FE
The optimized structures at the theoretical M062X/6-31G* level and the selected bond lengths (Å) of species involved in reactivating SON by FE in the aqueous phase.

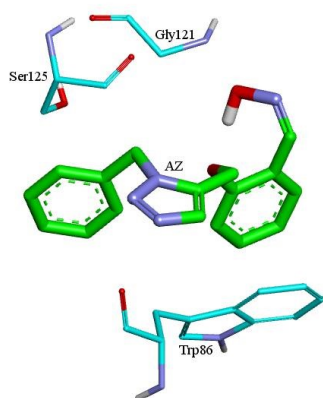


S14. The optimized structures of species involved in reactivating SON by FZ
The optimized structures at the theoretical M062X/6-31G* level and the selected bond lengths (Å) of species involved in reactivating SON by FZ in the aqueous phase.

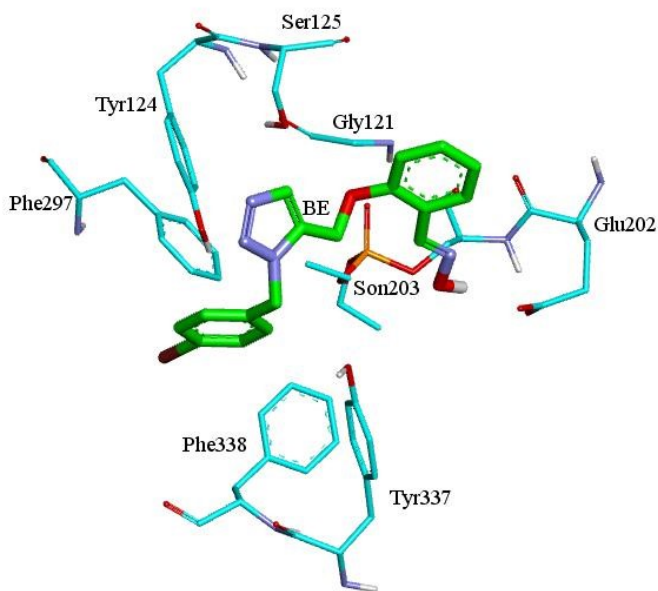
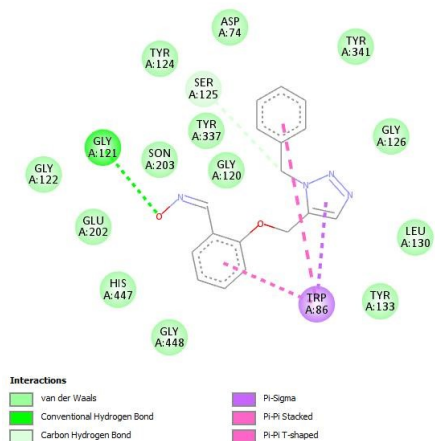


S15. The 2D and 3D structures of interactions

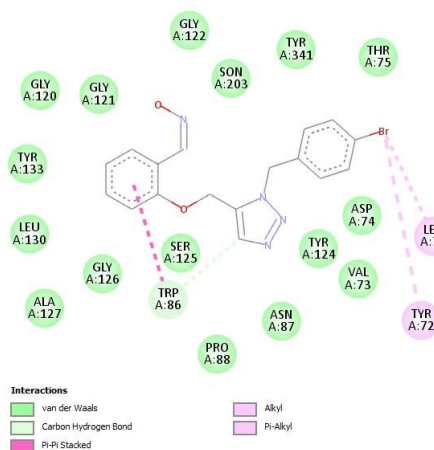
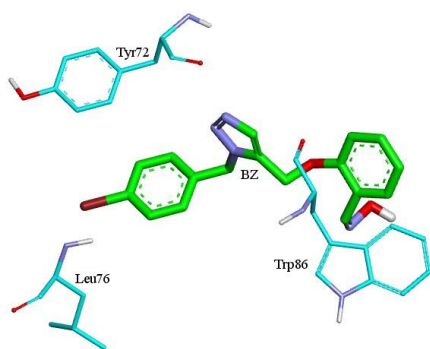
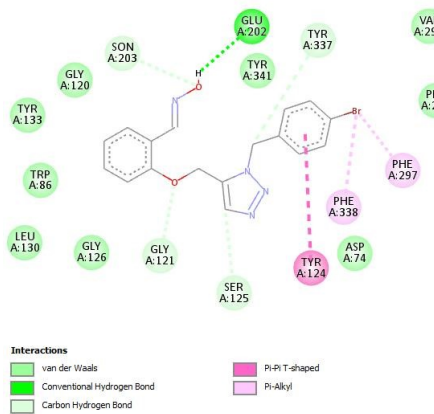
The 2D and 3D structures of interactions between the amino acids of the active site of enzyme AChE-POX and (a) AZ, (b) BE, (c) BZ, (d) CE, (e) CZ, (f) DE, (g) DZ, (h) EE, (i) EZ, (j) FE, and (k) FZ oxime.



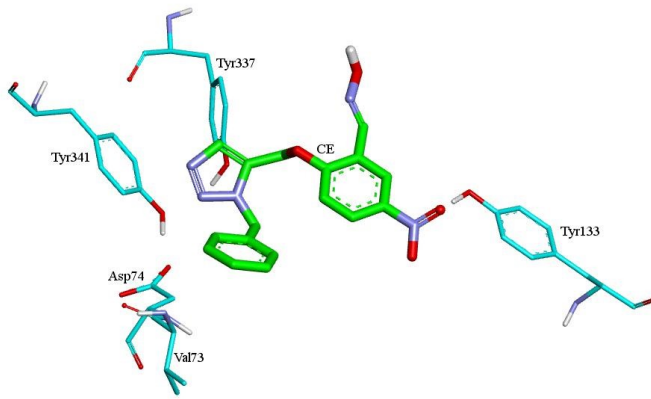
(a)



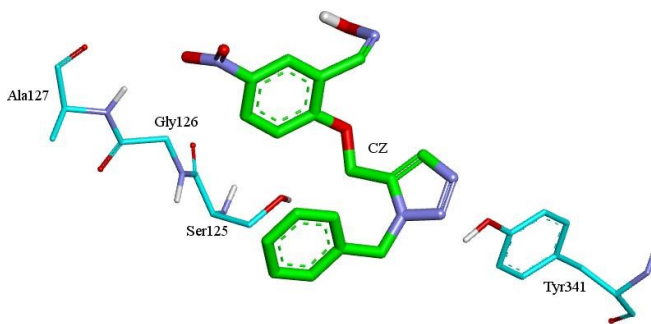
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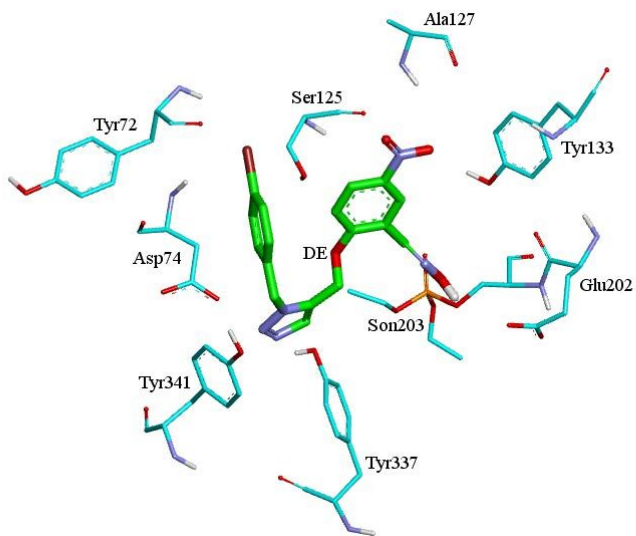
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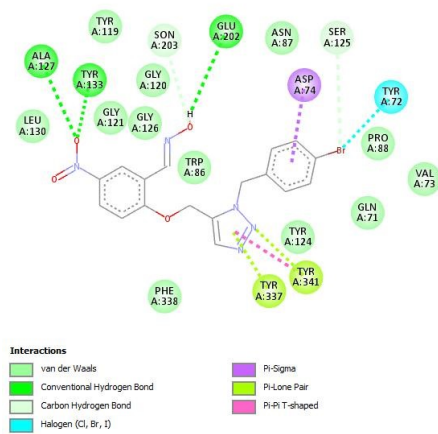
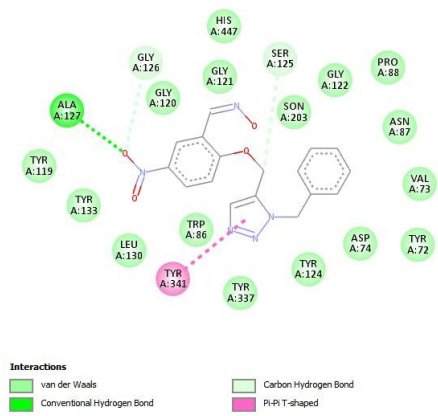
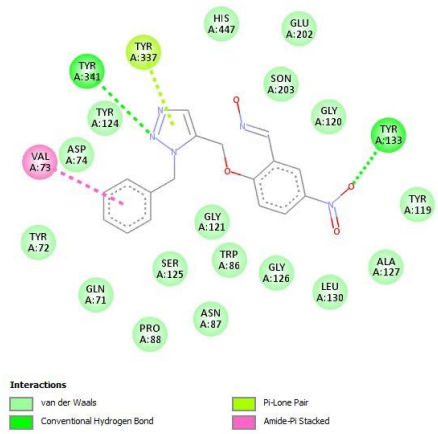
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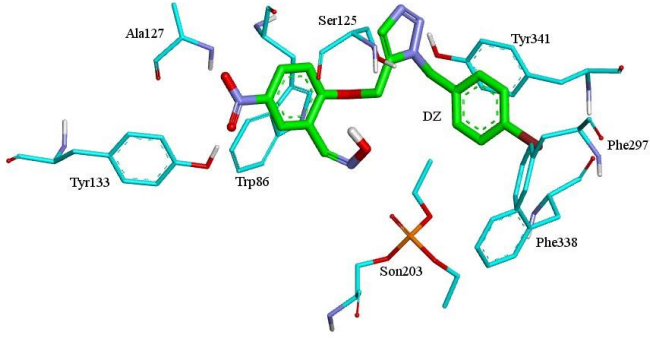


(e)

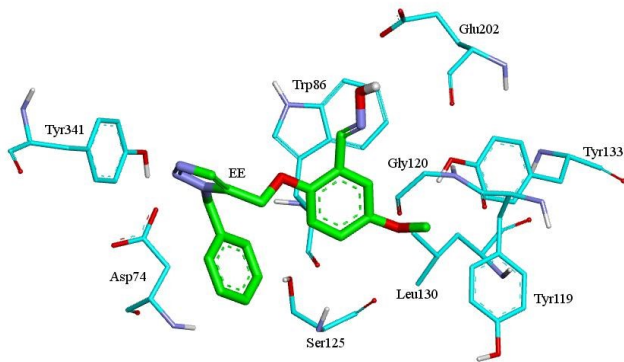
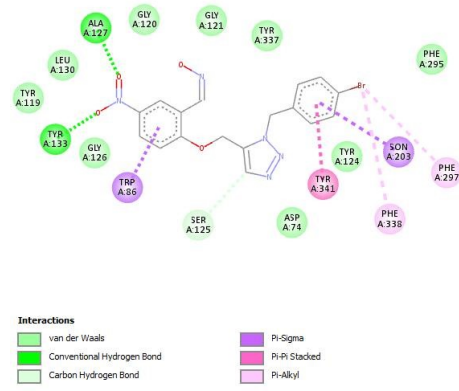


(f)

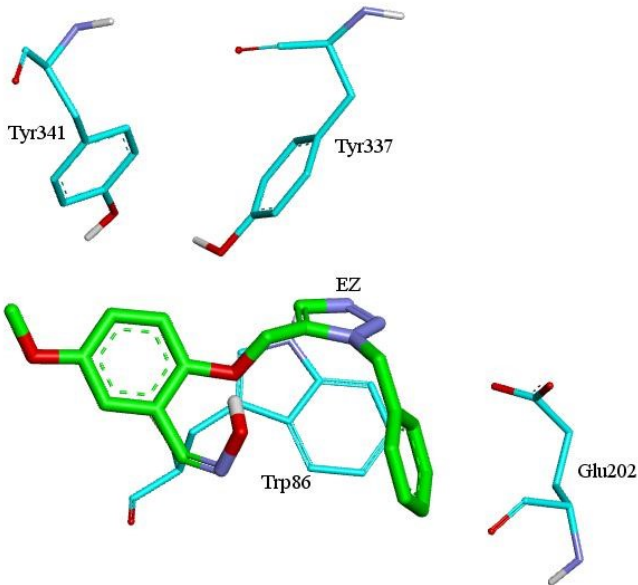
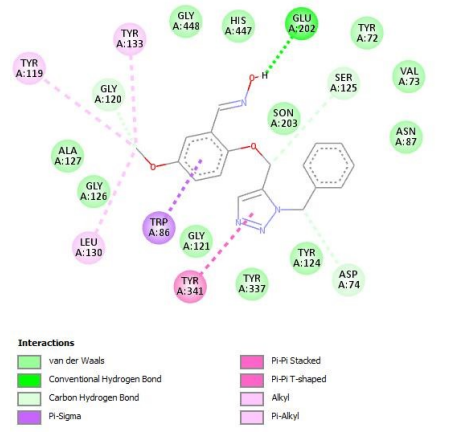




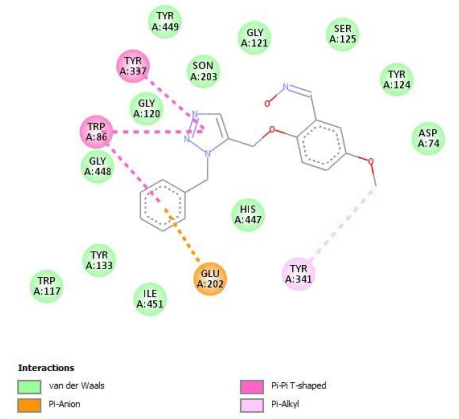
(g)

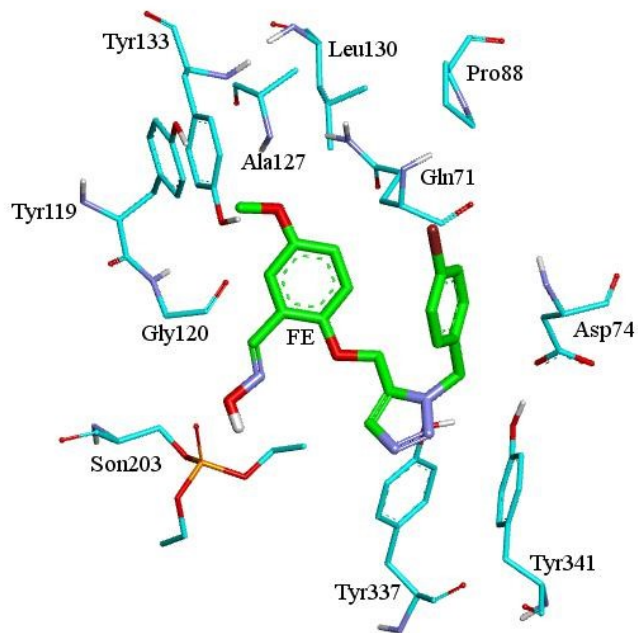


(h)

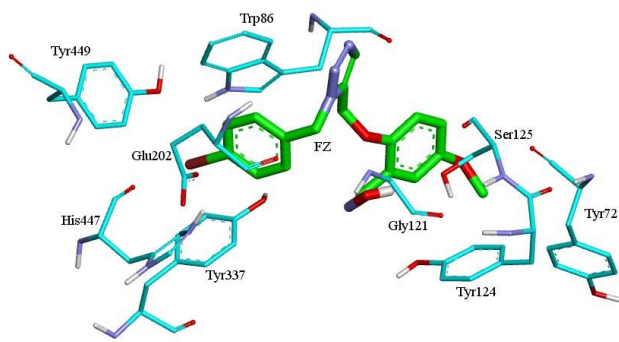
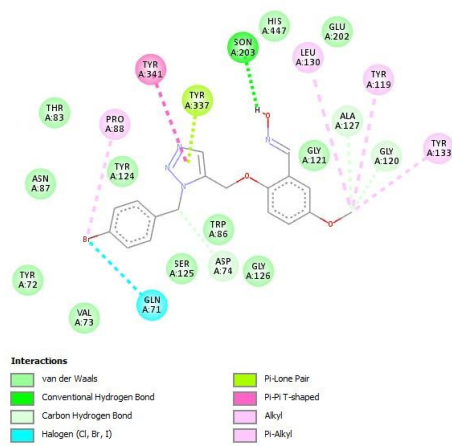


(i)

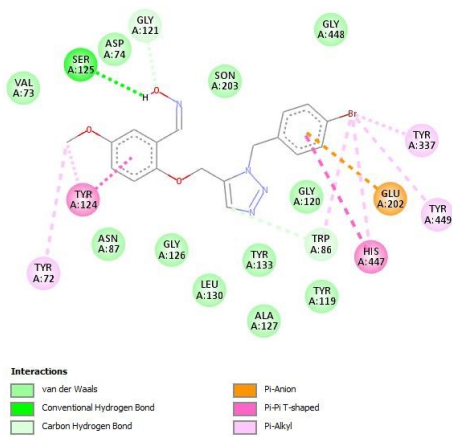




(j)

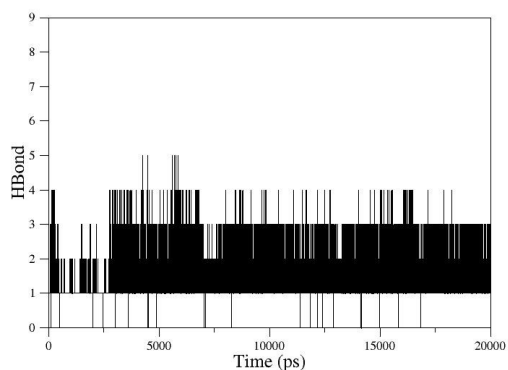


(k)

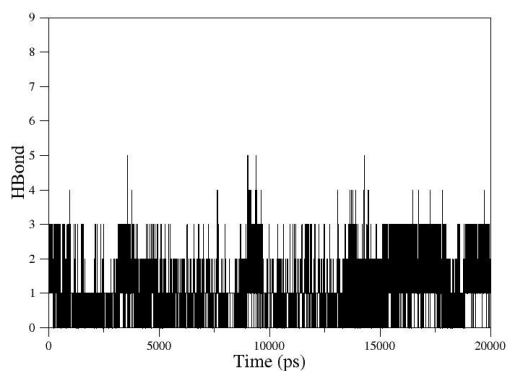
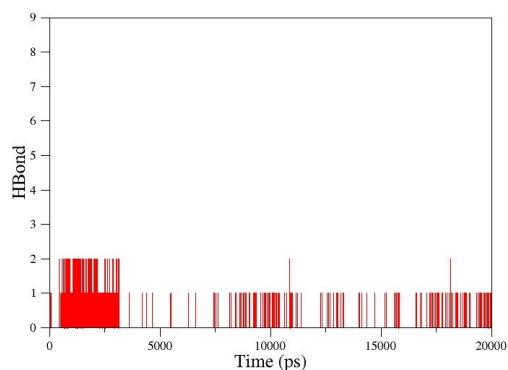


S16. The number of hydrogen bonds

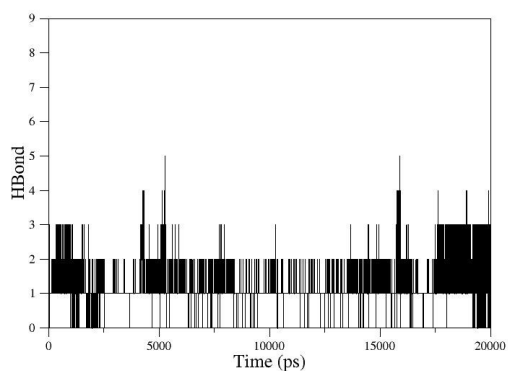
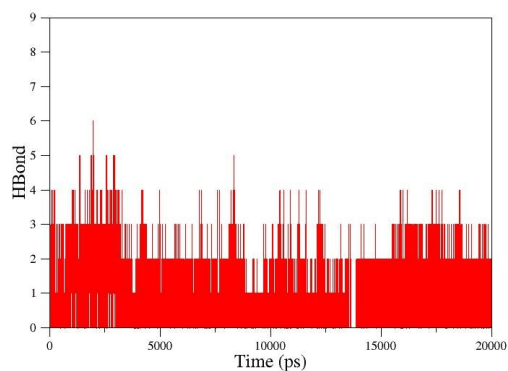
The number of hydrogen bonds formed between AChE-POX and oxime (black) and the number of hydrogen bonds formed between oxime and solvent (red) during simulation for oximes (a) 2-PAM, (b) AE, (c) AZ, (d) BE, (e) BZ, (f) CE, (g) CZ, (h) DE, (i) DZ, (j) EE, (k) EZ, (l) FE, and (m) FZ.



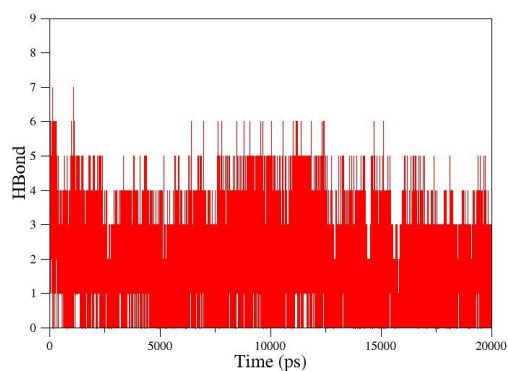
(a)

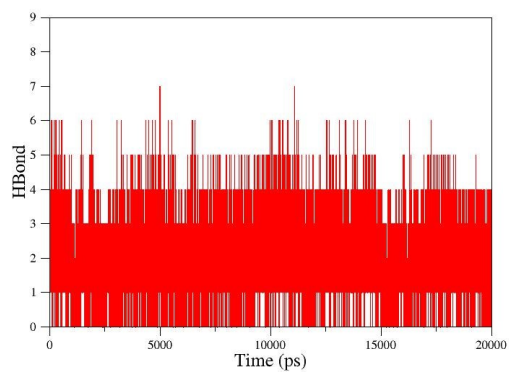
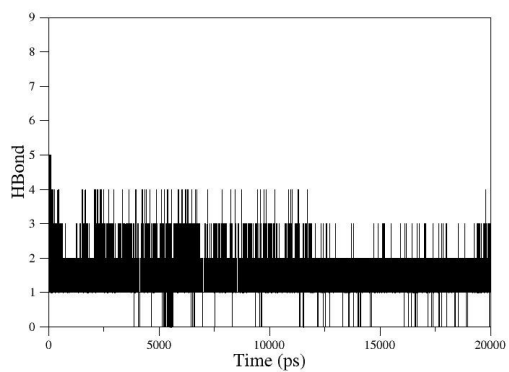


(b)

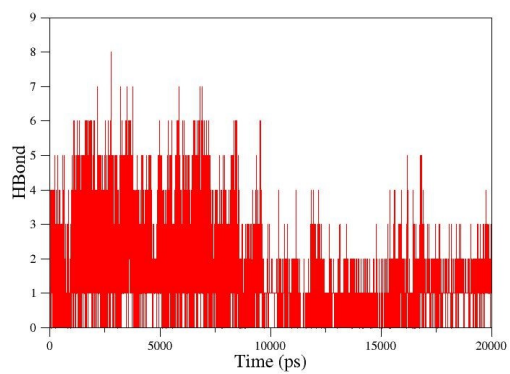
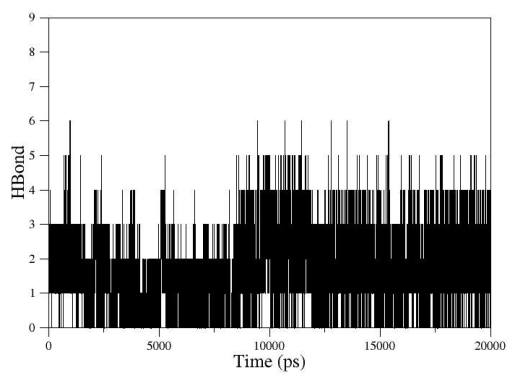


(c)

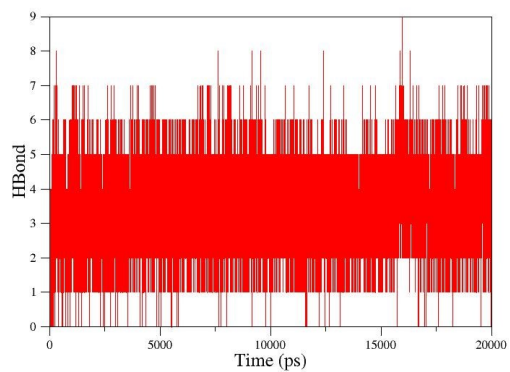
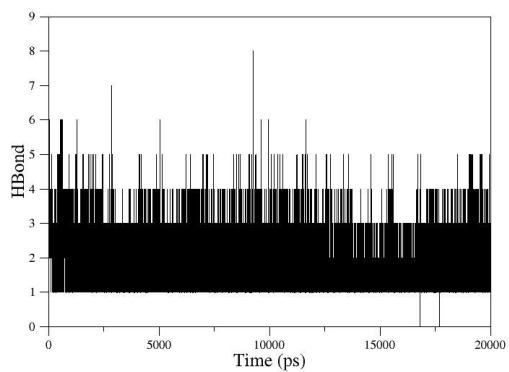




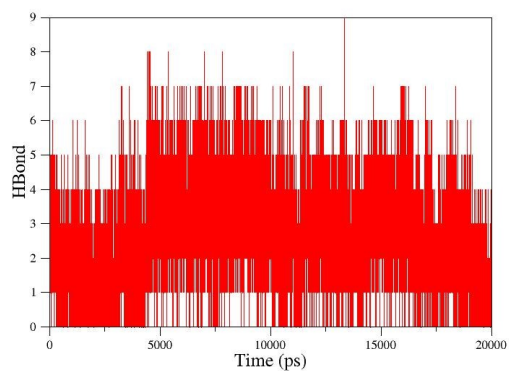
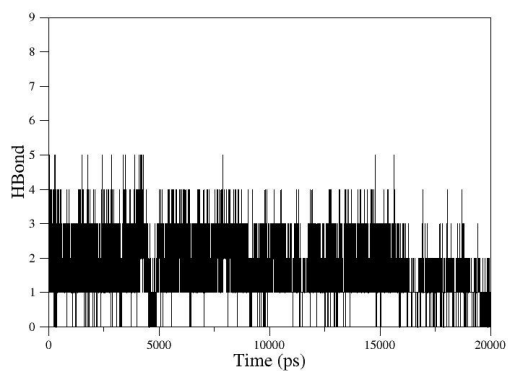
(d)



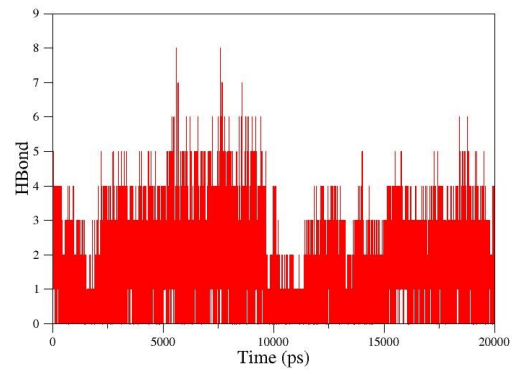
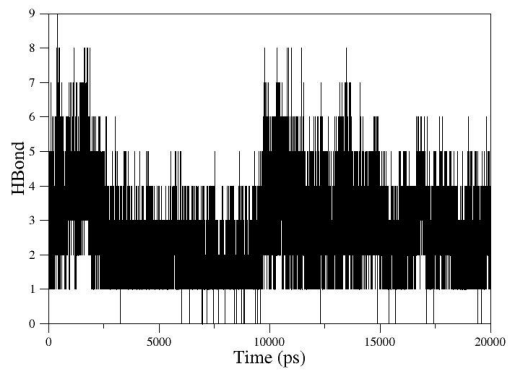
(e)



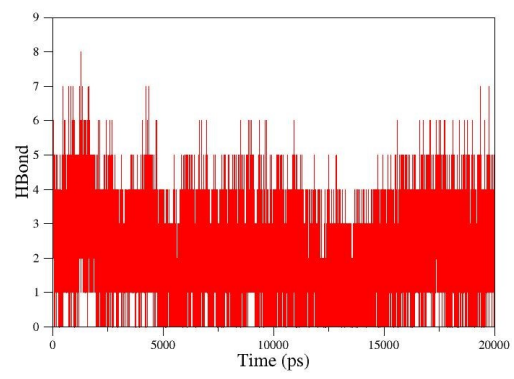
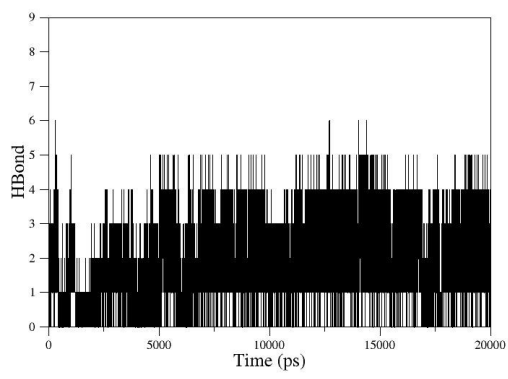
(f)



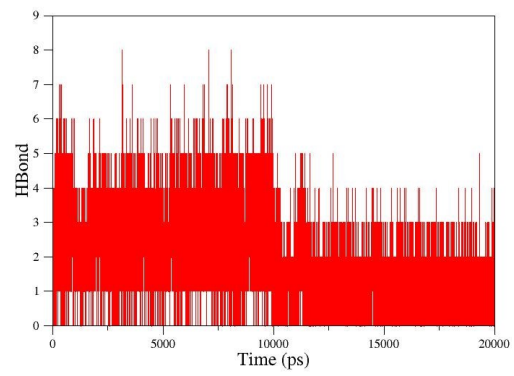
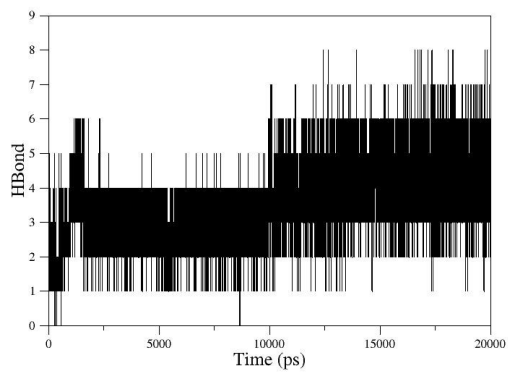
(g)



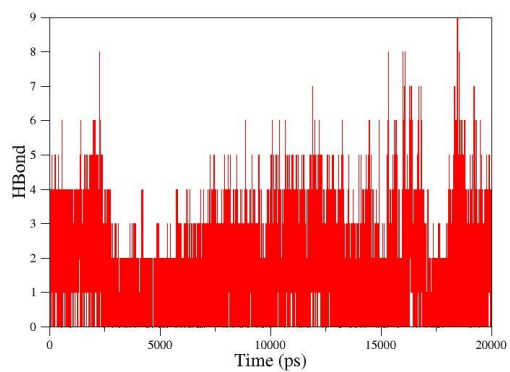
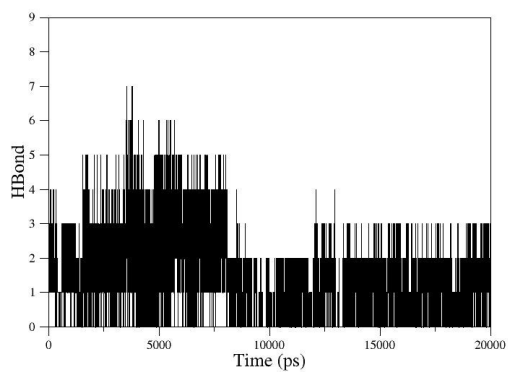
(h)



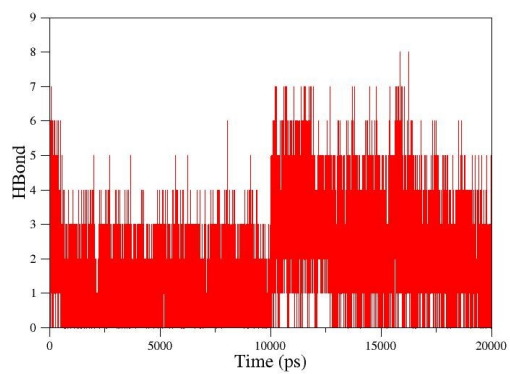
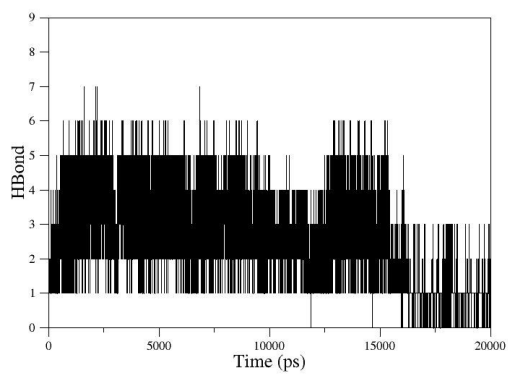
(i)



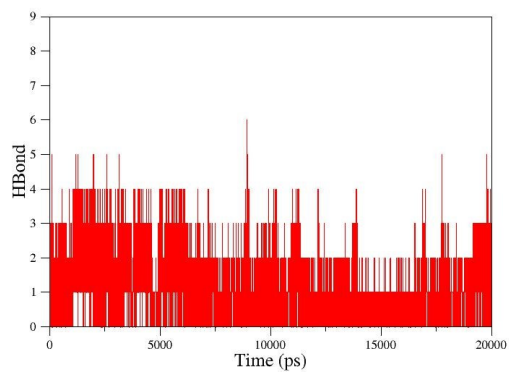
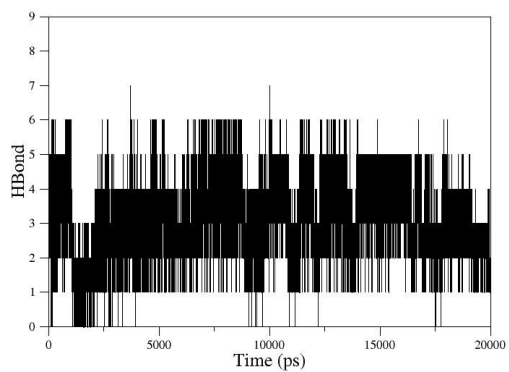
(j)



(k)



(l)



(m)

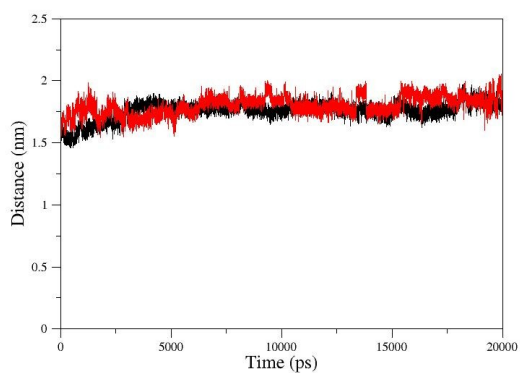
S17. The percentage of hydrogen bond occupation

The percentage of hydrogen bond occupation between the residues of the enzyme AChE-POX and different oximes.

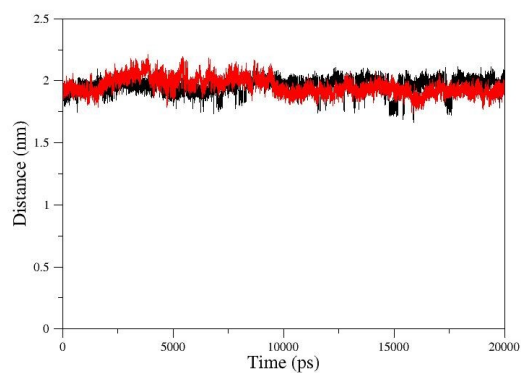
AChE-POX complexed by	Donor	Acceptor	Occupancy (%)
2-PAM	2-PAM (H1)	GLU202 (OE2)	53.2
	2-PAM (H1)	GLU202 (OE1)	53.4
	ALA127 (H)	2-PAM (O1)	50.3
AE	AE (H1)	SON203 (O3)	12.1
	AE (H1)	TRP86 (O)	17.1
	TYR133 (HH)	AE (O2)	44.2
	ALA127 (H)	AE (O2)	12.0
BE	BE (H1)	GLU202 (OE2)	54.9
	BE (H1)	GLU202 (OE1)	46.0
	GLY121 (H)	BE (N4)	21.6
CE	CE (H1)	GLU202 (OE2)	53.8
	CE (H1)	GLU202 (OE1)	64.6
	ALA127 (H)	CE (O1)	34.5
	ALA127 (H)	CE (O2)	18.1
	GLY121 (H)	CE (N5)	13.5
DE	DE (H1)	GLU202 (OE2)	46.0
	DE (H1)	GLU202 (OE1)	59.4
	TYR337 (HH)	DE (N3)	14.0
	TYR337 (HH)	DE (N2)	22.9
	ALA127 (H)	DE (O2)	10.2
	TYR124 (HH)	DE (N3)	19.3
	TYR124 (HH)	DE (N2)	22.7
	ASN87 (D21)	DE (O1)	27.1
EE	EE (H1)	GLU202 (OE2)	58.3
	EE (H1)	GLU202 (OE1)	63.9
	TYR337 (HH)	EE (N2)	28.3
	TYR337 (HH)	EE (N1)	45.6
	ALA127 (H)	EE (O1)	85.2
	GLY121 (H)	EE (N4)	73.0
FE	FE (H1)	HIS447 (NE2)	16.0
	FE (H1)	GLU202 (OE2)	38.6
	FE (H1)	GLU202 (OE1)	53.0
	TYR337 (HH)	FE (N2)	22.7
	TYR337 (HH)	FE (N1)	35.1
	ALA127 (H)	FE (O1)	28.6
	GLY121 (H)	FE (O3)	19.7
	GLY121 (H)	FE (N4)	38.1
AZ	AZ (H1)	GLU202 (OE2)	35.1
	AZ (H1)	GLU202 (OE1)	59.8
BZ	LYS348 (HZ1)	BZ (O2)	18.4
	LYS348 (HZ1)	BZ (N4)	17.1
	TYR341 (HH)	BZ (O2)	12.0
	ASN87 (D21)	BZ (N2)	28.0
	ASN87 (D21)	BZ (N1)	67.4
CZ	CZ (H1)	GLU202 (OE2)	35.4
	CZ (H1)	GLU202 (OE1)	57.7
	ALA127 (H)	CZ (O1)	18.7
	ALA127 (H)	CZ (O2)	48.5
DZ	TYR337 (HH)	DZ (O4)	59.2
	TYR337 (HH)	DZ (N5)	39.6
	ALA127 (H)	DZ (O1)	12.9
	TYR124 (HH)	DZ (N3)	41.9
	TYR124 (HH)	DZ (N2)	29.8
EZ	LYS348 (HZ1)	EZ (O3)	31.3
	TYR341 (HH)	EZ (O3)	29.7
	TYR341 (HH)	EZ (O2)	21.3
	TYR77 (H)	EZ (O3)	17.0
FZ	FZ (H1)	SON203 (O3)	85.6
	TYR337 (HH)	FZ (O3)	49.1
	TYR337 (HH)	FZ (N4)	40.2
	TYR133 (HH)	FZ (N2)	56.7
	TYR133 (HH)	FZ (N1)	69.7
	SER125 (HG)	FZ (O2)	11.4
ASN87 (D21)	FZ (O1)	10.9	

S18. COM distances between POX and oximes

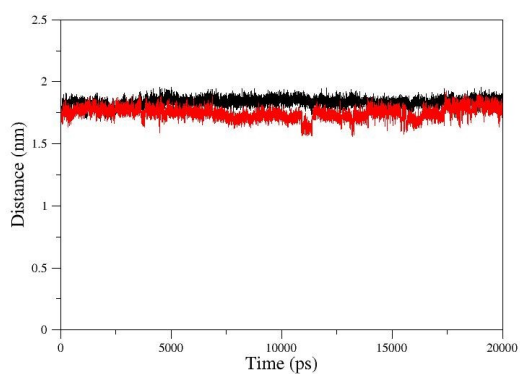
COM distances between POX and oximes during simulation for oximes (a) A, (b) B, (c) C, (d) D, (e) E, and (f) F. *E* isomers of oximes (black), *Z* isomers of oximes (red).



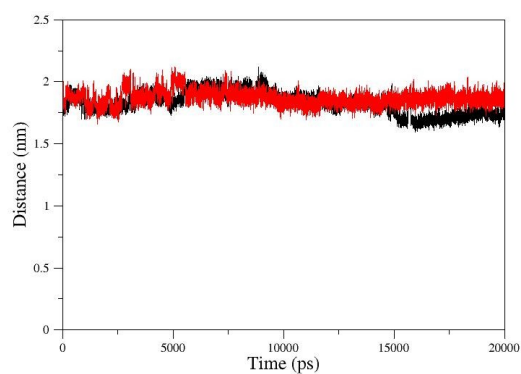
(a)



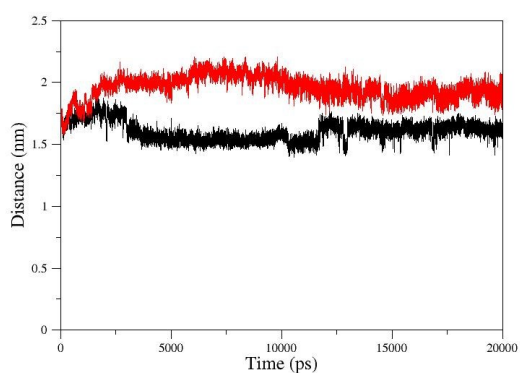
(b)



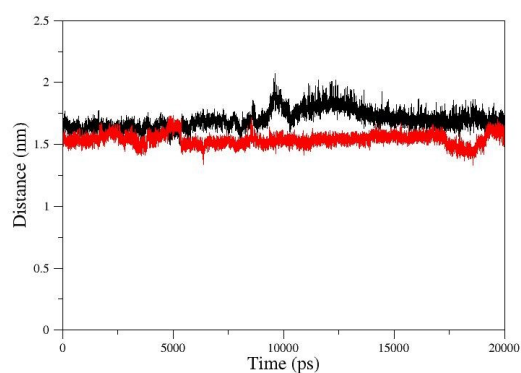
(c)



(d)



(e)



(f)

S19. M062X/6-31G* calculated cartesian coordinates of all optimized structures.

Paraoxon-inhibited AChE (SON)

N	3.22638900	-3.00883000	-0.73382000
C	2.15254200	-2.20947700	-0.15417900
C	0.87699100	-3.01601600	0.00134500
O	-0.21200800	-2.67587800	-0.41134200
C	1.95004300	-0.96847600	-1.01322700
O	0.91322100	-0.12417200	-0.47537800
C	0.73157100	2.87438200	-0.98000400
C	1.41485300	4.10693100	-1.52513500
C	-0.75204400	0.13671900	2.16827400
C	-2.17545600	0.52259200	2.49580300
O	1.60917200	2.28895900	0.01302300
O	-0.20318800	1.15721300	1.29426100
O	2.30274100	0.44969900	1.63757100
P	1.25686900	0.91483100	0.71136100
H	2.89130800	-0.41870600	-1.08688200
H	1.61655200	-1.23828800	-2.01778700
H	3.57419500	-3.68753700	-0.06168700
H	2.89518900	-3.53123200	-1.54268800
H	2.46437700	-1.89055300	0.84850200
H	1.00537900	-3.99631000	0.49750600
H	0.55804500	2.13256200	-1.76548400
H	-0.21643600	3.12137200	-0.49311000
H	1.59698700	4.82928900	-0.72600900
H	2.36789100	3.84192900	-1.98905500
H	0.77621100	4.57366800	-2.27924800
H	-2.19999900	1.49032800	3.00268800
H	-2.78318700	0.59121200	1.58870400
H	-2.61460200	-0.22916200	3.15632500
H	-0.12957400	0.08526500	3.06484900
H	-0.70383600	-0.83058900	1.65371800
C	-2.59903500	0.63058500	-1.16225400

N	-1.93561300	-0.53085500	-0.84050000
C	-3.92688000	0.38161400	-0.99707400
C	-2.81183400	-1.46477300	-0.48777800
N	-4.02543400	-0.92531000	-0.57505000
H	-4.79326400	1.00630600	-1.13754700
H	-2.57106700	-2.47317100	-0.19046500
H	-4.88767800	-1.41554100	-0.36463000
H	-2.08043300	1.52076400	-1.47674800
H	-0.92049300	-0.68015000	-0.84550200

2-PAM

C	2.57737300	-0.76549500	0.00044600
C	1.57740900	-1.76758200	-0.00022900
C	0.25772200	-1.41845600	-0.00047700
C	-0.14405800	-0.04977100	-0.00023900
C	2.17909500	0.53634800	0.00049600
H	3.63223200	-1.00609000	0.00086600
H	1.85981900	-2.81521700	-0.00043800
C	-1.49797700	0.34800400	0.00023100
H	2.87827600	1.36282200	0.00096000
H	-1.81675300	1.38553100	0.00122400
N	-2.43455400	-0.61724700	-0.00012000
O	-3.62439000	-0.22645200	0.00037500
H	-0.53142500	-2.15840300	-0.00077700
N	0.85888700	0.88748100	-0.00010500
C	0.50682200	2.31053200	-0.00046000
H	-0.07908200	2.54386800	-0.89172800
H	-0.07708100	2.54502100	0.89182700
H	1.42048400	2.90096100	-0.00197500

C1(2-PAM)

N	5.02721600	-2.53231200	-2.15103400
C	3.96997600	-1.61862200	-1.75636300
C	3.86980100	-1.65397600	-0.22221400

O	2.88247400	-0.74216500	0.27262200
C	4.15231200	-0.18944400	-2.24201000
O	3.30751300	0.67316100	-2.12357400
O	0.91309400	-1.93028900	-0.95124800
P	1.32331400	-1.19468000	0.25917300
C	1.11286500	-1.38607800	2.88263900
O	0.69482000	0.23956200	0.51338100
C	-0.25468500	0.78315600	-0.43983900
C	-0.98258900	1.92282700	0.23176100
H	5.00600800	-2.68520800	-3.15591100
H	3.01334500	-1.97390500	-2.15393000
H	3.64566900	-2.67813500	0.09003800
H	4.81520900	-1.35030800	0.23381300
H	5.12502700	0.03736700	-2.72276900
H	2.12395900	-1.03562400	3.11608900
H	0.42924900	-0.53786200	2.81980000
H	0.30940000	1.12067400	-1.31582300
H	-0.94171600	-0.00988000	-0.74122600
H	-1.70222400	2.35596300	-0.46877600
H	-0.28314000	2.70541100	0.54069700
H	-1.52422000	1.55732200	1.10806400
C	2.55114700	4.02745300	1.32527100
N	2.94175900	4.31574900	0.03582100
C	2.45781100	2.67212500	1.40308800
C	3.08640700	3.18634100	-0.65432600
N	2.79573700	2.18307000	0.16330800
H	2.17477700	2.02171400	2.21447100
H	3.38312600	3.09025800	-1.68656400
H	2.82086000	1.19379500	-0.09996200
H	2.37734900	4.79818100	2.05733000
H	5.94135800	-2.13838400	-1.93356300
H	3.09727200	5.24381300	-0.34089200
O	1.14448100	-2.03279100	1.58761900
C	0.61984200	-2.40764300	3.88032700

H	1.27485400	-3.28239100	3.90016100
H	0.59618600	-1.96594700	4.88013400
H	-0.39107100	-2.72069300	3.60843700
C	-6.93588400	1.03992500	-0.76730600
C	-6.31364400	1.23466100	0.48728600
C	-5.12949300	0.61271900	0.76860300
C	-4.50201400	-0.23862900	-0.18436700
C	-6.32057400	0.22430700	-1.66905200
H	-7.87216300	1.51747200	-1.02415100
H	-6.77461200	1.88018300	1.22752200
C	-3.27433500	-0.89634200	0.06843700
H	-6.72884100	0.02329700	-2.65144600
H	-2.78089900	-1.53832000	-0.65585600
N	-2.69736800	-0.70327000	1.26205100
O	-1.58629400	-1.26377900	1.43663100
H	-4.62628000	0.74211800	1.71747400
N	-5.13837700	-0.39716400	-1.38805900
C	-4.53277700	-1.25635000	-2.41106300
H	-3.54625200	-0.87035800	-2.67589900
H	-4.43742100	-2.27344900	-2.02648900
H	-5.17100700	-1.25757800	-3.29165000

TS1(2-PAM)

N	4.48004500	-3.58308400	-0.67149400
C	3.73874700	-2.37811100	-1.00602600
C	2.66001300	-2.15014000	0.05799900
O	1.86431200	-1.04709300	-0.34072300
C	4.58906800	-1.12565100	-1.10427200
O	4.27381100	-0.15157800	-1.75334200
O	-0.18314300	-1.94126800	0.84113800
P	0.54607000	-0.66855700	0.61053900
C	1.21999100	0.16308900	3.14326400
O	0.03524300	0.45033400	-0.43104000
C	-0.05777100	0.13466300	-1.83529400

C	-0.95866300	1.17424100	-2.46438800
H	5.15272400	-3.79534300	-1.40447100
H	3.23326300	-2.51260700	-1.96799300
H	2.05095400	-3.05537000	0.13335400
H	3.11897800	-1.95088200	1.03736400
H	5.52854800	-1.13585000	-0.51399300
H	2.19924900	0.44828800	3.53470200
H	0.51522600	0.97687200	3.30516400
H	0.94502900	0.14894200	-2.27258200
H	-0.46401400	-0.87727300	-1.95282100
H	-1.05861800	0.98346700	-3.53615700
H	-0.53645800	2.17340400	-2.32456100
H	-1.95197600	1.15055300	-2.00557700
C	2.37639500	3.95905400	0.14994400
N	3.54520400	3.80482200	-0.56353300
C	1.82564900	2.72063100	0.26084900
C	3.71189500	2.52400100	-0.88234300
N	2.67646700	1.85289400	-0.39103100
H	0.91764600	2.37743800	0.72990100
H	4.53285800	2.09337900	-1.43310500
H	2.55365500	0.83693700	-0.47985300
H	2.04640700	4.91978900	0.50794200
H	5.01833000	-3.44221700	0.18247200
H	4.18860400	4.54650100	-0.81429300
O	1.45157100	0.03627400	1.72456800
C	0.73812400	-1.12300900	3.78197700
H	1.41887900	-1.94808000	3.55067300
H	0.70874000	-0.99249500	4.86770800
H	-0.26121500	-1.37823500	3.42621000
C	-6.76039800	0.22673300	-0.72306100
C	-6.24814400	1.04480100	0.30048200
C	-4.93804300	0.91439300	0.68832400
C	-4.09093600	-0.03535100	0.07457100
C	-5.92265100	-0.68225800	-1.30564300

H	-7.78701700	0.29899700	-1.05724900
H	-6.88637400	1.77727400	0.78309100
C	-2.71528100	-0.21307100	0.44882300
H	-6.24029600	-1.34511800	-2.10003300
H	-2.09488700	-0.97787900	-0.00089700
N	-2.26194600	0.56684600	1.40684100
O	-1.04264800	0.45185800	1.77438100
H	-4.50732700	1.52483000	1.47063400
N	-4.62432500	-0.80787100	-0.91667000
C	-3.78329900	-1.80383900	-1.59891000
H	-2.94799900	-1.29974300	-2.08879500
H	-3.40798100	-2.52760600	-0.87464700
H	-4.38544400	-2.31412700	-2.34669800

IN(2-PAM)

N	4.20015900	-3.66906000	-0.60617100
C	3.49378100	-2.45686700	-0.99327500
C	2.52273700	-2.06574300	0.12859300
O	1.78201500	-0.94079000	-0.28107900
C	4.39702000	-1.27150900	-1.25954200
O	4.12640700	-0.36945400	-2.02363800
O	-0.33223800	-1.87937400	0.63394400
P	0.36677200	-0.55354100	0.64627600
C	1.11584000	0.05199400	3.22809100
O	0.04167400	0.62486100	-0.44041200
C	0.16472000	0.40517400	-1.85407500
C	-0.62454500	1.50062900	-2.53974900
H	4.83360700	-3.95893000	-1.34772300
H	2.90694600	-2.64338400	-1.89847200
H	1.85985200	-2.91534800	0.31937000
H	3.07996900	-1.84582500	1.05256800
H	5.33748600	-1.24983800	-0.66909200
H	2.08903100	0.30296100	3.65897400
H	0.42969100	0.88114300	3.40347300

H	1.21901400	0.42746400	-2.14488500
H	-0.22686200	-0.58845900	-2.10424600
H	-0.56608400	1.38377100	-3.62531400
H	-0.21997100	2.48125100	-2.27244000
H	-1.67612900	1.46727500	-2.23875300
C	2.79322200	3.80741200	0.34561000
N	3.84761400	3.55733900	-0.50517500
C	2.15051900	2.62113800	0.51777400
C	3.85489900	2.26959800	-0.84464700
N	2.83195400	1.68665300	-0.23102800
H	1.27780100	2.35507400	1.09085500
H	4.55509700	1.77843900	-1.50223900
H	2.57628500	0.68186600	-0.30643000
H	2.60076600	4.78893800	0.74538500
H	4.77969200	-3.49073800	0.21333200
H	4.52087800	4.24092400	-0.83045400
O	1.38437500	-0.06624900	1.82201900
C	0.58895800	-1.23892600	3.82440500
H	1.26795500	-2.06688700	3.59808400
H	0.51387100	-1.13885500	4.91126200
H	-0.39876000	-1.47476100	3.42298200
C	-6.78228500	0.34503400	-0.60865000
C	-6.21040400	1.09003600	0.42814300
C	-4.87214500	0.93169300	0.72292600
C	-4.08438000	0.02672200	-0.00039800
C	-5.98583400	-0.53321400	-1.29994900
H	-7.82645100	0.43997200	-0.87688100
H	-6.81216700	1.79103500	0.99598700
C	-2.66490000	-0.17339800	0.27651600
H	-6.35837000	-1.14546100	-2.11072200
H	-2.06578500	-0.82518200	-0.34495800
N	-2.20705600	0.43942200	1.31818600
O	-0.94198700	0.34058800	1.65780900
H	-4.38872600	1.49209900	1.51214500

N	-4.67286800	-0.68666400	-0.99799000
C	-3.88721300	-1.66454800	-1.77714800
H	-3.10043500	-1.14640000	-2.32624200
H	-3.45634400	-2.40336800	-1.10145600
H	-4.55397300	-2.15749500	-2.47989500

TS2(2-PAM)

N	3.91543500	-3.82346500	-0.28711200
C	3.19632300	-2.68830400	-0.86786900
C	2.73867500	-1.74095200	0.22913500
O	1.92860400	-0.71969600	-0.32953200
C	4.06598300	-1.98090500	-1.89147200
O	4.44804000	-0.83688400	-1.78837200
O	-0.29413500	-1.67572000	0.55359900
P	0.14706300	-0.28049000	0.80622800
C	1.09040300	0.07744800	3.29987200
O	-0.01269600	0.86125300	-0.30159800
C	0.04700700	0.60573600	-1.72217100
C	-0.93222600	1.54577400	-2.39085500
H	4.08219700	-4.53904200	-0.99127500
H	2.30916000	-3.07547600	-1.38388800
H	2.14565800	-2.30356400	0.95431900
H	3.60044900	-1.29790700	0.74370400
H	4.40309100	-2.61360500	-2.73741700
H	2.05985000	0.39167500	3.68931500
H	0.33611900	0.80901600	3.59056900
H	1.07044000	0.78998400	-2.05508700
H	-0.19566700	-0.44467800	-1.91014800
H	-0.89615800	1.40477500	-3.47428000
H	-0.67609400	2.58437100	-2.16586400
H	-1.95479500	1.35883300	-2.04986800
C	3.36742000	3.81039500	0.07592400
N	4.42614400	3.35691100	-0.67362200
C	2.56503700	2.72065600	0.26720600

C	4.24142300	2.04094700	-0.90931100
N	3.12212600	1.62442900	-0.35152500
H	1.63067800	2.64666500	0.80273300
H	4.92423900	1.43011300	-1.47936600
H	2.46543800	0.15231100	-0.37959600
H	3.28876100	4.83755300	0.39337300
H	4.83087900	-3.52386000	0.04554600
H	5.20989100	3.90983900	-0.99360200
O	1.26797500	0.13304200	1.86359000
C	0.73754600	-1.31655200	3.77720000
H	1.48949800	-2.03746400	3.44428100
H	0.70652100	-1.32780400	4.87017200
H	-0.24047600	-1.62662600	3.40023000
C	-6.83728600	0.37199100	-0.79357700
C	-6.28268300	1.27032400	0.11613200
C	-4.95642500	1.12690600	0.49098900
C	-4.19038200	0.08543100	-0.02607500
C	-6.04817800	-0.64403300	-1.28631100
H	-7.86532200	0.44927300	-1.12270100
H	-6.87785700	2.08082400	0.52109600
C	-2.77723800	-0.10335500	0.33630600
H	-6.41530400	-1.37759100	-1.99173500
H	-2.14063800	-0.73367100	-0.27478700
N	-2.38974600	0.49045900	1.40308900
O	-1.10119500	0.39871200	1.78972600
H	-4.48051900	1.81113200	1.18137700
N	-4.75954700	-0.78113800	-0.90481300
C	-3.97811000	-1.90806800	-1.46026300
H	-3.19967900	-1.52088300	-2.11865700
H	-3.54089400	-2.48106500	-0.64347700
H	-4.65276000	-2.54244500	-2.02898500

C2(2-PAM)

N	-3.17403400	3.45704200	2.34521500
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C	-2.63783800	2.92076800	1.09462600
C	-3.19177000	1.51979900	0.87023200
O	-2.77699500	1.07725800	-0.40216500
C	-3.00348900	3.78840300	-0.09210300
O	-2.20976900	4.30995600	-0.84191200
O	-0.14355000	0.91010700	1.26873500
P	-0.09328700	-0.13026600	0.23105200
C	-1.36490900	-2.20439400	-0.75579200
O	-0.01372200	0.32321800	-1.28047400
C	-0.07704100	1.72746900	-1.64585100
C	1.30383900	2.34377500	-1.60530700
H	-2.76386100	4.36842900	2.53739700
H	-1.54753700	2.86322500	1.16099900
H	-2.82576300	0.86900900	1.67614700
H	-4.29315800	1.55401800	0.93101900
H	-4.09615400	3.95662000	-0.21856700
H	-2.04608200	-1.72959400	-1.46542000
H	-0.40414800	-2.38639900	-1.24642100
H	-0.49283000	1.72837200	-2.65475700
H	-0.77598500	2.23578200	-0.98322400
H	1.24926400	3.38365600	-1.94032200
H	1.98870800	1.80043200	-2.26305600
H	1.70042200	2.32598300	-0.58574100
C	-5.54994500	-3.09062300	-0.74889900
N	-5.53877700	-2.75594900	0.58172700
C	-4.86227100	-2.08926800	-1.37850800
C	-4.86116000	-1.59278700	0.71211500
N	-4.43646700	-1.15978800	-0.45768800
H	-4.64759800	-1.98230200	-2.43193300
H	-4.70435000	-1.11107600	1.66672600
H	-3.28998500	0.25031100	-0.57598000
H	-6.03240300	-3.98381900	-1.11200300
H	-4.17918800	3.60724200	2.25709600
H	-5.96489300	-3.28164600	1.33324500

O	-1.17106700	-1.27586000	0.34423800
C	-1.93766900	-3.48067200	-0.18621800
H	-2.14711000	-4.18183600	-0.99848700
H	-1.22666200	-3.94298100	0.50342400
H	-2.86987500	-3.27737100	0.34731000
C	7.25887600	0.58366500	-0.29278200
C	6.13974400	1.24969700	-0.78220900
C	4.88242700	0.69211700	-0.59578800
C	4.74800500	-0.51355400	0.08193000
C	7.08320700	-0.61117700	0.37486700
H	8.25999700	0.97547700	-0.41807100
H	6.24412700	2.19138500	-1.30903000
C	3.43075400	-1.13769400	0.29384700
H	7.91022500	-1.17544700	0.78558000
H	3.33109700	-2.19066200	0.54541000
N	2.40731000	-0.39342200	0.14936200
O	1.24681800	-1.10770900	0.34431900
H	3.98593500	1.16972500	-0.97134200
N	5.85594500	-1.13983900	0.55706200
C	5.74159900	-2.41714900	1.29673300
H	5.04994300	-2.29076600	2.12867600
H	5.39639800	-3.19795000	0.61859300
H	6.72506400	-2.67614500	1.67991900

AE

C	-4.64709100	0.35899800	-1.47694400
C	-3.48956100	1.06903000	-1.16832800
C	-2.58853100	0.59517000	-0.21971500
C	-2.80591100	-0.62533300	0.45895300
C	-3.98603700	-1.31815900	0.12367300
C	-4.88937200	-0.84664700	-0.82105200
H	-5.34397500	0.74158600	-2.21564400
H	-3.26314500	2.01524900	-1.65194000
C	-1.94002000	-1.20409900	1.47963600

H	-4.18725200	-2.25779200	0.63301000
H	-5.78438700	-1.42028100	-1.04309200
H	-2.29163700	-2.11942200	1.96905700
O	-1.49211600	1.38981400	0.05304600
N	-0.78557300	-0.71180500	1.83170700
O	-0.13487000	-1.34982300	2.76364100
C	0.80783800	1.85817600	-0.21739400
C	1.05743400	3.17592700	-0.53639800
N	1.84142600	1.52803100	0.59420500
H	0.47945000	3.84190100	-1.16058700
N	2.20143400	3.56677600	0.07322100
N	2.67522700	2.55875400	0.74944800
C	-0.31095300	0.95251500	-0.61407200
H	-0.46426200	1.02081000	-1.69906200
H	-0.08407300	-0.08147000	-0.34343100
C	2.16784200	0.24276700	1.21421900
H	3.06093000	0.44858100	1.81105700
H	1.35638500	-0.07448700	1.87689400
C	2.44799200	-0.82473000	0.17888500
C	3.27305500	-0.55948900	-0.91670800
C	1.88587000	-2.09350600	0.33163700
C	3.53953500	-1.55634000	-1.85069200
H	3.70455800	0.43226700	-1.03646000
C	2.15910900	-3.09199200	-0.60290600
H	1.22747600	-2.26961200	1.18082100
C	2.98374800	-2.82649200	-1.69385100
H	4.18054700	-1.34320600	-2.70089200
H	1.71870100	-4.07755600	-0.48305200
H	3.18927400	-3.60357300	-2.42391000

C1(AE)

N	7.00652400	1.01650800	-2.42642100
C	5.81088100	1.01579100	-1.60208700
C	5.13690100	-0.35847600	-1.76316300

O	3.99912900	-0.51603000	-0.90985000
C	6.05323100	1.33288800	-0.13463400
O	5.16670500	1.47081000	0.68185900
O	2.77234800	1.55550100	-1.90568700
P	2.59980100	0.20792200	-1.33148300
C	1.48602900	-2.11787100	-1.91403500
O	1.87783900	0.06864600	0.07284500
C	1.41965100	1.28290000	0.72373500
C	0.55865000	0.88865000	1.89827300
H	7.37545700	1.95970500	-2.51486400
H	5.10964700	1.76962400	-1.97463500
H	4.85471900	-0.48987100	-2.81221700
H	5.83023500	-1.15729500	-1.48801500
H	7.11520900	1.44041000	0.16555800
H	2.29311700	-2.82686800	-2.12035600
H	1.29029900	-2.09952200	-0.83854500
H	2.30560700	1.84512700	1.03996600
H	0.84834000	1.86361600	-0.00026700
H	0.26450400	1.78811600	2.44721300
H	1.09939300	0.22613600	2.58394800
H	-0.34471000	0.38286200	1.54670400
C	3.06859800	-1.69929800	3.73665000
N	3.58391600	-0.47292400	4.09369700
C	3.25068300	-1.81278400	2.39206600
C	4.06683800	0.14439600	3.01614100
N	3.87282200	-0.65960100	1.97946500
H	2.99823000	-2.60299600	1.70360500
H	4.53450400	1.11573000	2.97941300
H	4.09692500	-0.42235300	1.00733300
H	2.63033600	-2.36966100	4.45715000
H	7.73939600	0.45388100	-1.99704000
H	3.60287300	-0.08980200	5.03201600
O	1.93664300	-0.81002300	-2.34080300
C	0.22213900	-2.43026300	-2.68158700

H	0.42690800	-2.50395900	-3.75342500
H	-0.20074000	-3.37890900	-2.33670500
H	-0.49004000	-1.62049100	-2.49808900
C	-4.50305400	4.77729700	1.24536900
C	-4.84250600	3.52167700	0.74944400
C	-3.90171000	2.73539400	0.08908800
C	-2.57170900	3.17154800	-0.08075400
C	-2.26531900	4.45425400	0.41020200
C	-3.20245000	5.24510300	1.06404500
H	-5.24613900	5.38303500	1.75411000
H	-5.85362100	3.13442500	0.84384700
C	-1.52306600	2.41528200	-0.76232400
H	-1.25171900	4.82476000	0.27502800
H	-2.91653200	6.22607500	1.43171000
H	-0.67269400	2.97759900	-1.16574700
O	-4.33894900	1.54548700	-0.45964400
N	-1.53283100	1.11868200	-0.86349500
O	-0.52291300	0.55863700	-1.47275700
C	-5.02001600	-0.69577000	-0.19686200
C	-6.34866800	-1.06095600	-0.22199600
N	-4.42680500	-1.60837300	-1.00198700
H	-7.18913000	-0.59813600	0.27438800
N	-6.48735800	-2.15371500	-1.01060700
N	-5.31419400	-2.48246500	-1.47511000
C	-4.30676200	0.44574100	0.44680600
H	-4.82607800	0.71215000	1.37521700
H	-3.26446700	0.18940900	0.66905800
C	-3.00083700	-1.78959700	-1.26212500
H	-2.94209700	-2.39666700	-2.16988500
H	-2.54882800	-0.81044700	-1.44693400
C	-2.31334700	-2.46477100	-0.09396600
C	-2.87488900	-3.58856500	0.51655600
C	-1.10352600	-1.94961900	0.37448200
C	-2.22931200	-4.19790500	1.58903900

H	-3.82185500	-3.98224800	0.15390100
C	-0.46185600	-2.56332100	1.45129700
H	-0.67664100	-1.07483700	-0.12285900
C	-1.01985500	-3.68522100	2.05982500
H	-2.67067300	-5.07132400	2.05962600
H	0.47333500	-2.14807900	1.81896300
H	-0.51932400	-4.15805200	2.89966000

TS1(AE)

N	-6.86158600	1.92576000	1.55056000
C	-5.83326300	1.49261100	0.61971900
C	-4.60046600	1.06104500	1.42271800
O	-3.56941300	0.69859200	0.51410100
C	-6.25239500	0.35699500	-0.29859800
O	-5.67494900	0.08204100	-1.32839000
O	-1.81976400	2.11617200	1.67225900
P	-1.99449100	0.79582500	1.02932100
C	-1.24180100	-0.95445600	3.00660700
O	-1.38397100	0.44012000	-0.40597900
C	-1.71833300	1.27542800	-1.53412300
C	-0.77244600	0.91137000	-2.65536900
H	-7.65396700	2.31276600	1.04368600
H	-5.53395900	2.33433600	-0.01377000
H	-4.28350700	1.90444500	2.04159900
H	-4.83669500	0.20878700	2.07339500
H	-7.12402800	-0.23972500	0.03985900
H	-1.77324100	-1.83381200	3.37769800
H	-0.24673300	-1.23556800	2.66647300
H	-2.76396300	1.09753000	-1.80798600
H	-1.61066700	2.32732900	-1.24603900
H	-0.98169200	1.52656700	-3.53477200
H	-0.89885100	-0.14048600	-2.92926200
H	0.26298200	1.07578800	-2.34227000
C	-2.39895900	-3.56122700	-1.57911600

N	-3.59232000	-3.45468400	-2.25920200
C	-2.30144400	-2.45093800	-0.79880000
C	-4.20774800	-2.32570000	-1.91494300
N	-3.43603800	-1.70548900	-1.03001700
H	-1.53839200	-2.12080400	-0.11181600
H	-5.15744200	-1.96751100	-2.27891000
H	-3.66141300	-0.80569500	-0.58101900
H	-1.73362700	-4.39821900	-1.71347300
H	-7.21691100	1.13066600	2.08006500
H	-3.95476400	-4.12590600	-2.92624400
O	-2.01299900	-0.56604500	1.84699100
C	-1.17567700	0.12861300	4.06191800
H	-2.17984100	0.47070000	4.33164500
H	-0.69677800	-0.27783500	4.95792800
H	-0.59225100	0.97255200	3.69306400
C	3.76152400	4.36429800	-2.40743500
C	4.28867800	3.41041100	-1.54086800
C	3.46028100	2.67120300	-0.70078100
C	2.06114400	2.85304300	-0.70917100
C	1.56022200	3.83090000	-1.58755100
C	2.38390100	4.57289800	-2.42598600
H	4.41827300	4.93793100	-3.05363100
H	5.35867400	3.23008600	-1.48548400
C	1.10247800	2.14228900	0.14153900
H	0.48548400	4.00093400	-1.60405600
H	1.95076600	5.31403100	-3.09085400
H	0.10616700	2.57956600	0.24027300
O	4.06718900	1.79457400	0.17591300
N	1.39445700	1.03465000	0.74670000
O	0.46295800	0.45140600	1.46655600
C	4.78251000	-0.39200100	0.71536600
C	6.08526700	-0.45440400	1.16231500
N	4.14189900	-1.30861700	1.48078000
H	6.94263500	0.11447700	0.83290200

N	6.16969200	-1.38482100	2.14224700
N	4.98832700	-1.90424500	2.32283600
C	4.14647200	0.46332700	-0.33062500
H	4.77046500	0.45617400	-1.23345600
H	3.14518400	0.09907000	-0.57415200
C	2.74513400	-1.74571600	1.43698700
H	2.65092100	-2.44695600	2.27082800
H	2.08162400	-0.89311700	1.60564900
C	2.42103300	-2.42168000	0.12343400
C	3.24057700	-3.44519000	-0.35822800
C	1.30477000	-2.02102200	-0.61422200
C	2.94842800	-4.07154900	-1.56545000
H	4.11320100	-3.74659300	0.21781900
C	1.01768000	-2.64906700	-1.82749900
H	0.68365000	-1.20975400	-0.23211700
C	1.83389900	-3.67280800	-2.30375600
H	3.58968200	-4.86724500	-1.93225200
H	0.15672500	-2.33154200	-2.40872000
H	1.60743500	-4.15515200	-3.24984400

IN(AE)

N	-6.45699000	1.81855400	2.16274300
C	-5.55664100	1.51714900	1.05800400
C	-4.22358100	1.00064300	1.61802300
O	-3.33026700	0.79346900	0.55412500
C	-6.08463300	0.47011500	0.10348500
O	-5.84183200	0.44362200	-1.08453300
O	-1.54910500	2.07646000	1.68292500
P	-1.59592800	0.77218400	0.93856700
C	-1.05673700	-1.53536300	2.38509600
O	-1.34332000	0.64530000	-0.67977200
C	-2.00058000	1.50901000	-1.61343400
C	-1.13095400	1.56444400	-2.85313400
H	-7.34142400	2.17512000	1.80749900

H	-5.35218100	2.42723000	0.48517100
H	-3.83313500	1.75273100	2.31016400
H	-4.38821400	0.06575900	2.17764400
H	-6.69559600	-0.32992300	0.57434500
H	-1.66761700	-2.42390300	2.57219700
H	-0.19943200	-1.82939300	1.77415000
H	-2.99985200	1.12241700	-1.83897700
H	-2.12425200	2.50487200	-1.17067700
H	-1.59097300	2.20389100	-3.61185100
H	-1.00539900	0.56146200	-3.27229300
H	-0.14121800	1.96441800	-2.60974800
C	-2.58993300	-3.31981700	-1.81872700
N	-3.87219400	-3.11230700	-2.27671100
C	-2.31881300	-2.29182600	-0.96928700
C	-4.36746900	-2.00062600	-1.73243100
N	-3.43790200	-1.49162900	-0.93395400
H	-1.43668000	-2.05153000	-0.39868700
H	-5.34386800	-1.57667700	-1.91007500
H	-3.51572200	-0.60601500	-0.36960100
H	-1.99606300	-4.16303100	-2.13130300
H	-6.67785000	0.96642200	2.67697700
H	-4.37194100	-3.70484100	-2.92891900
O	-1.92151700	-0.67733100	1.63074700
C	-0.61543800	-0.91396100	3.69591600
H	-1.48702500	-0.60404600	4.28043100
H	-0.05025400	-1.64577600	4.28153000
H	0.01913600	-0.04518500	3.51062900
C	3.95928300	4.66838200	-1.76388200
C	4.35666600	3.57563400	-0.99874800
C	3.41270600	2.75445400	-0.38742100
C	2.03704800	3.01178500	-0.53433400
C	1.66269000	4.12706400	-1.29848100
C	2.60258100	4.94504600	-1.91459300
H	4.70607100	5.30121800	-2.23269200

H	5.40734400	3.34407500	-0.85036900
C	0.94827000	2.22577900	0.07213900
H	0.60274500	4.34585900	-1.40701800
H	2.27796300	5.79690400	-2.50306000
H	-0.03493100	2.69418700	0.06856400
O	3.87572700	1.72043700	0.39549500
N	1.16369800	1.06822400	0.57270800
O	0.13987400	0.34724000	1.10247200
C	4.70090600	-0.49296000	0.57224200
C	6.01739200	-0.68640300	0.93131800
N	4.03803000	-1.43507900	1.28562800
H	6.89519100	-0.14666500	0.60699900
N	6.08487000	-1.71238900	1.81258800
N	4.87973500	-2.16475000	2.01685300
C	4.05709200	0.50402300	-0.33179000
H	4.71476300	0.68681700	-1.18969800
H	3.08943400	0.14036300	-0.69344100
C	2.61532400	-1.77291400	1.25830200
H	2.44778200	-2.38220500	2.15054300
H	2.03864900	-0.85035500	1.34015700
C	2.25117300	-2.53152000	-0.00073700
C	2.91209600	-3.72348300	-0.30915800
C	1.26444100	-2.04705900	-0.86144200
C	2.58740700	-4.42905300	-1.46299100
H	3.68575000	-4.09319500	0.36022000
C	0.94244400	-2.75570200	-2.02104400
H	0.75280900	-1.11569300	-0.62230900
C	1.59937900	-3.94554500	-2.32215700
H	3.10393300	-5.35562600	-1.69371700
H	0.17939100	-2.37017100	-2.69167900
H	1.34768000	-4.49398400	-3.22467400

TS2(AE)

N	-6.38530900	1.77836000	2.11535500
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C	-5.46978200	1.57467800	1.00181300
C	-4.25667900	0.77169300	1.49199400
O	-3.30843000	0.65824100	0.45297900
C	-6.07206000	0.82496200	-0.16806500
O	-5.72381900	0.96614400	-1.31985600
O	-1.62982100	2.06508500	1.62321000
P	-1.46914800	0.72822900	0.97052700
C	-1.03933200	-1.47887500	2.55455200
O	-1.18037400	0.55901700	-0.62050000
C	-1.78214100	1.41979300	-1.60103000
C	-0.81631300	1.51720000	-2.76355600
H	-7.18612400	2.32932700	1.81447900
H	-5.10392900	2.53988700	0.63769900
H	-3.81341100	1.30610300	2.33569100
H	-4.56953500	-0.22661400	1.83375500
H	-6.84691000	0.07555200	0.10348700
H	-1.63047000	-2.38647700	2.70452800
H	-0.10858300	-1.74848500	2.05119800
H	-2.74257800	0.99779600	-1.91121200
H	-1.97426000	2.40240900	-1.15523400
H	-1.24009900	2.14657300	-3.55109800
H	-0.62089900	0.52418500	-3.17883200
H	0.13506700	1.95219200	-2.44189100
C	-2.95395300	-3.37044700	-1.75297700
N	-4.09968500	-2.91307300	-2.35999600
C	-2.62180600	-2.42477100	-0.82800500
C	-4.43635500	-1.73372800	-1.81775400
N	-3.55685400	-1.41640700	-0.88094800
H	-1.78659900	-2.38306700	-0.14618200
H	-5.28631600	-1.13737500	-2.11358600
H	-3.47889400	-0.35986300	-0.20555100
H	-2.48913400	-4.30253200	-2.03104800
H	-6.75708500	0.88291300	2.43104000
H	-4.60810500	-3.38083200	-3.09950200

O	-1.85196700	-0.68596500	1.67170900
C	-0.78651200	-0.78267200	3.87676700
H	-1.73520000	-0.50077700	4.34330300
H	-0.25486700	-1.45711600	4.55468300
H	-0.18084000	0.11396500	3.72907100
C	3.99434400	4.71831600	-1.65673000
C	4.40750900	3.57463400	-0.97945300
C	3.48010100	2.74428500	-0.35612900
C	2.10663300	3.04675700	-0.40136200
C	1.71554200	4.20753900	-1.08453000
C	2.63922600	5.03528000	-1.71147700
H	4.72879400	5.35789300	-2.13569100
H	5.45783100	3.30694200	-0.91311200
C	1.03317100	2.25757500	0.22619200
H	0.65719600	4.45543900	-1.11959900
H	2.30343700	5.92468600	-2.23429000
H	0.04553800	2.71891900	0.23110300
O	3.95943700	1.65306300	0.33138000
N	1.25594700	1.10873000	0.74077400
O	0.21534200	0.40369500	1.28824200
C	4.74161700	-0.58173100	0.31267800
C	6.08410900	-0.84599100	0.47726400
N	4.13879800	-1.50708600	1.09763500
H	6.93314500	-0.34258400	0.03834700
N	6.22297200	-1.89433900	1.32304200
N	5.03746500	-2.29256300	1.68965200
C	4.02853700	0.46973300	-0.46830100
H	4.59344200	0.68057900	-1.38349300
H	3.01743700	0.14530200	-0.73956800
C	2.71098700	-1.78680900	1.25064200
H	2.62483200	-2.35040600	2.18319500
H	2.18778300	-0.83510400	1.35600300
C	2.17954100	-2.57973500	0.07501300
C	2.74871100	-3.81792200	-0.23582100

C	1.13892100	-2.08216000	-0.71124600
C	2.28362400	-4.55306500	-1.32051600
H	3.56358900	-4.19831600	0.37602500
C	0.67794200	-2.81984500	-1.80375500
H	0.68705700	-1.12126100	-0.47086100
C	1.24644400	-4.05295900	-2.10952300
H	2.73003600	-5.51517600	-1.55276900
H	-0.12926900	-2.42437400	-2.41363400
H	0.88672300	-4.62373300	-2.96040600

C2(AE)

N	4.83975500	4.08642900	0.87605000
C	3.96648500	2.96906600	1.23572000
C	4.43958200	1.70944900	0.52316700
O	3.70648700	0.61798700	1.02899100
C	3.96945600	2.71564000	2.72943800
O	2.99952500	2.78906400	3.44923300
O	1.55885800	2.10347800	-0.72614400
P	1.24481800	0.66290600	-0.74426800
C	2.23127200	-1.69890500	-1.28907200
O	0.88009000	-0.01747800	0.63800500
C	0.88387900	0.70929400	1.88921500
C	-0.54604600	0.92567400	2.33435100
H	4.50127400	4.94504800	1.30502100
H	2.94290800	3.19240400	0.92165100
H	4.29415500	1.84250200	-0.55785500
H	5.51908400	1.57505300	0.70999400
H	4.97292700	2.48958700	3.15425400
H	2.71017800	-1.94660700	-0.33813900
H	1.17852200	-1.99684500	-1.24580000
H	1.44530400	0.08864800	2.59005100
H	1.42622500	1.64633800	1.76106400
H	-0.56017800	1.42839800	3.30589600
H	-1.06618800	-0.03291800	2.42801200

H	-1.08507000	1.54663600	1.61122100
C	6.24847700	-3.15978400	-1.09253100
N	6.61036600	-2.03370100	-1.78783500
C	5.42777200	-2.71710700	-0.09094400
C	6.01135200	-0.97250600	-1.20074500
N	5.28665500	-1.35063600	-0.16756500
H	4.93090700	-3.29512000	0.67479100
H	6.13075400	0.03946900	-1.56063400
H	4.15060300	-0.18980200	0.67446300
H	6.59839800	-4.14151500	-1.36839800
H	5.77657600	3.92929400	1.24785900
H	7.21812700	-1.99969500	-2.59531100
O	2.31530300	-0.26017100	-1.45537200
C	2.93509600	-2.34271100	-2.46042800
H	2.93829600	-3.42867900	-2.33429900
H	2.42295700	-2.09877600	-3.39489700
H	3.97015900	-1.99594800	-2.52192400
C	-4.79507500	4.47515400	-0.63809100
C	-4.93436800	3.09589600	-0.51845100
C	-3.87354500	2.25294000	-0.83970200
C	-2.65482100	2.78839700	-1.28507800
C	-2.54458700	4.17816200	-1.43090300
C	-3.59806800	5.02045300	-1.10026700
H	-5.62844100	5.12215900	-0.38399900
H	-5.86901000	2.65090300	-0.19003100
C	-1.47357600	1.98455000	-1.61959700
H	-1.60971600	4.59371600	-1.79671400
H	-3.48942500	6.09407300	-1.20898500
H	-0.71896700	2.44715900	-2.25811200
O	-4.06393200	0.89658300	-0.78828300
N	-1.27977300	0.80899500	-1.15710200
O	-0.04988600	0.28460500	-1.66836700
C	-4.91817100	-0.87549000	0.51940800
C	-6.15844600	-1.12150600	1.06444200

N	-4.64004900	-2.01065500	-0.16293700
H	-6.77093900	-0.47942700	1.68018400
N	-6.55200400	-2.36749300	0.70194500
N	-5.62447200	-2.89915200	-0.04198800
C	-4.02507700	0.31684600	0.52093600
H	-4.38427800	1.03180600	1.26743700
H	-2.98747700	0.04692700	0.75323700
C	-3.40143400	-2.36162300	-0.85634800
H	-3.68518800	-3.04402600	-1.66064900
H	-3.00158600	-1.44275600	-1.29492700
C	-2.40363700	-2.99140600	0.09011900
C	-2.65936000	-4.24066800	0.66182200
C	-1.23012600	-2.31276100	0.41394200
C	-1.74543400	-4.80287900	1.54813100
H	-3.57789000	-4.76695900	0.41410200
C	-0.31226400	-2.87759500	1.30026900
H	-1.03181000	-1.33800900	-0.02331500
C	-0.56953300	-4.12200400	1.86841800
H	-1.94769400	-5.77427900	1.98892100
H	0.59870000	-2.33557400	1.53822700
H	0.14183600	-4.56328300	2.55980600

AZ

C	-2.44200700	-2.83187500	-0.58644700
C	-1.50614100	-1.79277500	-0.54019400
C	-1.92288000	-0.49873600	-0.25167800
C	-3.28590800	-0.18659200	0.00608900
C	-4.19492200	-1.25826000	-0.05154500
C	-3.78034800	-2.55928300	-0.34392700
H	-2.10915800	-3.84017600	-0.81286400
H	-0.46106100	-2.01278600	-0.73032400
C	-3.65184200	1.19384800	0.30701300
H	-5.23255800	-1.02665200	0.14302900
H	-4.51445900	-3.35954800	-0.38053300

O	-1.05374900	0.56491400	-0.19796900
C	1.02827700	1.59683000	-0.23254700
C	0.63936900	2.80747500	0.29261600
N	2.31701500	1.79827800	-0.58973400
H	-0.31861800	3.09674300	0.69672400
N	1.69428500	3.66095800	0.23172600
N	2.70685200	3.04552700	-0.29854300
C	0.31219500	0.29683300	-0.39873800
H	0.49074600	-0.11867700	-1.40194300
H	0.67934100	-0.43835400	0.33247300
N	-4.82720400	1.69927100	0.61540500
O	-5.86708800	0.92637300	0.68232800
H	-2.85223200	1.92735600	0.28106700
C	3.24803500	0.84958800	-1.19293800
H	2.90274900	0.60468400	-2.20189500
H	4.19506700	1.38831900	-1.27695900
C	3.38108200	-0.39787100	-0.34949500
C	3.17007500	-1.65801800	-0.90690800
C	3.68766200	-0.28693300	1.00937900
C	3.26888100	-2.80163000	-0.11445900
H	2.92124500	-1.74635800	-1.96168100
C	3.78174400	-1.42641900	1.80110700
H	3.84159000	0.69759200	1.44560000
C	3.57154900	-2.68664300	1.23945600
H	3.10170500	-3.77919700	-0.55561000
H	4.01685700	-1.33312800	2.85673000
H	3.63992200	-3.57558300	1.85863100

C1(AZ)

N	8.28771900	-1.64705200	-2.10068800
C	7.04161700	-0.97444200	-1.73545200
C	7.21719600	0.53062500	-1.80083600
O	7.26662800	1.25897600	-0.83159400
C	6.64033500	-1.45476600	-0.34401700

O	5.55878500	-0.70558300	0.22391800
C	2.97296600	-2.75330800	0.53283400
C	2.23584100	-3.95925800	-0.00066300
C	2.47437200	1.25164900	0.32911500
C	1.35945400	1.20639400	1.34597800
O	3.66250600	-2.14216800	-0.58350500
O	3.36676200	0.14348100	0.61399100
O	4.20537000	0.01038000	-1.87039100
P	4.12315400	-0.62913800	-0.54038700
H	6.37586200	-2.51524300	-0.38272400
H	7.47560700	-1.32451400	0.34837300
H	8.47996700	-1.53847400	-3.09337200
H	9.07445600	-1.24227300	-1.59577300
H	6.28050600	-1.25078800	-2.47110600
H	7.39075000	0.93724100	-2.81473100
H	3.72142100	-3.02283900	1.28614700
H	2.27343400	-2.02123700	0.93945900
H	1.50562500	-3.62201100	-0.74016600
H	2.92607900	-4.67145200	-0.46123800
H	1.70937800	-4.46276800	0.81590200
H	0.82017900	0.26198100	1.23006600
H	1.75563500	1.28855000	2.36296400
H	0.66769900	2.03610000	1.17409300
H	2.08364300	1.15308000	-0.68279500
H	3.07144300	2.16683400	0.41316500
C	4.96441900	1.86763100	2.55081300
N	5.76711200	1.84874600	1.43403500
C	4.87240900	3.16753800	2.94276500
C	6.15854700	3.08117100	1.13978700
N	5.62401200	3.89662000	2.04666300
H	4.35011200	3.63232800	3.76215100
H	6.78852200	3.35803500	0.30967600
H	5.75457300	4.90130800	2.06530000
H	4.52700800	0.96749100	2.95023000

H	6.01416200	1.01976500	0.88027300
C	-2.94165300	-2.51981400	2.08976000
C	-3.62371800	-1.50886100	1.40385100
C	-2.96522200	-0.76864400	0.42871000
C	-1.60311300	-1.00513100	0.09977600
C	-0.95414400	-2.03165900	0.80905400
C	-1.61242200	-2.77724200	1.78959200
H	-3.46319400	-3.09196900	2.85086700
H	-4.66369100	-1.31534900	1.64393600
C	-0.97693400	-0.18545500	-0.93648500
H	0.07934900	-2.22358200	0.55663400
H	-1.07614800	-3.56323800	2.31415200
O	-3.57923900	0.23762700	-0.27578200
C	-5.39596300	1.50234300	-0.99396200
C	-4.82272400	2.01890300	-2.13315200
N	-6.57285800	2.16179700	-0.89641500
H	-3.87349000	1.77704900	-2.58623600
N	-5.66787700	2.94392400	-2.65783900
N	-6.72515000	3.02412600	-1.90905800
C	-4.94964800	0.44783200	-0.03511900
H	-5.12435300	0.76677400	1.00327200
H	-5.52002800	-0.47886200	-0.19520400
N	0.25467100	-0.20705800	-1.38391300
O	1.10493200	-1.05951600	-0.87993200
H	-1.60542600	0.56017600	-1.41289300
C	-7.60314800	2.03229000	0.13105100
H	-7.21785800	2.43698100	1.07169300
H	-8.42631200	2.66791800	-0.20396200
C	-8.03028100	0.59237400	0.29937700
C	-7.94446100	-0.03097100	1.54337300
C	-8.47558200	-0.13552600	-0.80723700
C	-8.29846700	-1.37270500	1.68303300
H	-7.59097200	0.53094300	2.40455400
C	-8.82639600	-1.47437200	-0.66947700

H	-8.53492300	0.34906000	-1.77934700
C	-8.73648700	-2.09569500	0.57692300
H	-8.22394500	-1.85132000	2.65444200
H	-9.16694500	-2.03536500	-1.53410700
H	-9.00555300	-3.14195900	0.68265300

TS1(AZ)

N	7.54501400	-3.18436000	-0.56456200
C	6.72624600	-1.99224000	-0.71697400
C	5.76832500	-1.90619400	0.48566000
O	4.94405700	-0.75548400	0.42608000
C	7.51136400	-0.69932500	-0.81487100
O	7.04590400	0.34295100	-1.22624200
O	3.79043800	-1.54112900	-1.68848600
P	3.48521200	-0.87403500	-0.40206000
C	1.91527100	-1.08324300	1.70685900
O	3.23244200	0.69802700	-0.24692500
C	3.16332400	1.48487400	-1.45924900
C	2.63174700	2.84992200	-1.09199000
H	8.11218300	-3.33144100	-1.39599400
H	6.10582500	-2.07529500	-1.61388600
H	5.17138700	-2.82383000	0.51149400
H	6.34065700	-1.84692100	1.41818300
H	8.56226600	-0.74546800	-0.46016000
H	2.53144400	-0.33627100	2.22127400
H	1.08163500	-0.58127200	1.21064900
H	4.17537800	1.54369900	-1.87905500
H	2.50229100	0.97179500	-2.15758100
H	2.55075200	3.46671800	-1.99174400
H	3.29319900	3.35863700	-0.38404000
H	1.64053200	2.73389200	-0.64907600
C	5.39736600	3.81383400	1.82894600
N	6.43268000	3.92600600	0.92717100
C	4.91209200	2.54945900	1.69540800

C	6.58169900	2.77791600	0.26752500
N	5.66535800	1.93465900	0.72344400
H	4.09829800	2.04321900	2.18746800
H	7.31114100	2.56108200	-0.49645900
H	5.52637400	0.96079600	0.40812300
H	5.10334200	4.63023500	2.46706000
H	8.19490000	-3.07171400	0.21261600
H	7.00243300	4.75119200	0.78001700
O	2.71115100	-1.73282600	0.70035700
C	1.43974700	-2.14771700	2.67072200
H	2.28846000	-2.65128900	3.14144500
H	0.82819800	-1.68991600	3.45331400
H	0.83239300	-2.89058900	2.14630200
C	-2.89692700	-3.40988900	0.50849500
C	-3.54649000	-2.17929200	0.38207400
C	-2.82680800	-1.05656700	-0.01611200
C	-1.43808900	-1.12375800	-0.29679900
C	-0.82116500	-2.37833300	-0.16272900
C	-1.53931600	-3.50656300	0.23832800
H	-3.46595300	-4.28156400	0.81679600
H	-4.60788100	-2.11687600	0.59546500
C	-0.73402000	0.11510700	-0.65144900
H	0.23760300	-2.43609900	-0.37789000
H	-1.02943000	-4.46072500	0.33541400
O	-3.40250500	0.17947300	-0.16040000
C	-5.16062600	1.70567900	-0.15586900
C	-4.54879300	2.70464700	-0.87724000
N	-6.31218500	2.27261600	0.27055000
H	-3.60237600	2.68607700	-1.39568400
N	-5.34821200	3.80280400	-0.85307200
N	-6.41375500	3.53523300	-0.16152300
C	-4.77596000	0.29113000	0.12936100
H	-4.97800500	0.03520000	1.17986200
H	-5.36481900	-0.39447100	-0.49701400

N	0.50393900	0.29136300	-1.01426100
O	1.26388500	-0.77375800	-1.18587200
H	-1.30284700	1.03624200	-0.56814000
C	-7.36315600	1.68157300	1.09511400
H	-6.97422200	1.53020400	2.10650700
H	-8.15269800	2.43557900	1.14103500
C	-7.85478900	0.37877300	0.50711900
C	-7.82304400	-0.79342500	1.26167300
C	-8.30798600	0.33602900	-0.81399200
C	-8.23876400	-2.00123200	0.70221500
H	-7.46417600	-0.76441200	2.28760900
C	-8.72128800	-0.86860000	-1.37335700
H	-8.32401700	1.24890600	-1.40504300
C	-8.68548700	-2.04016000	-0.61563700
H	-8.20822000	-2.90941100	1.29578800
H	-9.06921600	-0.89572800	-2.40115000
H	-9.00470300	-2.98036700	-1.05431100

IN(AZ)

N	-8.15222500	0.91136300	-1.74240500
C	-7.11597300	-0.00744400	-1.28913400
C	-5.80174400	0.76474400	-1.10439700
O	-4.79115500	-0.12909700	-0.72673400
C	-7.43130700	-0.68296300	0.02504900
O	-7.09717400	-1.81225200	0.31497100
O	-3.22112600	0.81435200	-2.39696400
P	-3.09254500	0.42381700	-0.95376400
C	-2.73021400	2.59664300	0.69618100
O	-2.66658700	-1.07852800	-0.45503200
C	-3.28923300	-2.25567900	-0.97712400
C	-2.29389900	-3.38929700	-0.82968000
H	-9.03274800	0.41615000	-1.86474600
H	-6.95273000	-0.78538600	-2.04140500
H	-5.55783500	1.24784000	-2.05640800

H	-5.93808000	1.55274200	-0.34494800
H	-7.97199600	-0.04713800	0.75970100
H	-3.24860300	2.94305200	1.59563600
H	-1.70278200	2.34393800	0.96563500
H	-4.21303100	-2.46529600	-0.42750900
H	-3.55738700	-2.09775000	-2.02714700
H	-2.72143000	-4.32211400	-1.20817500
H	-2.03295200	-3.52984300	0.22354700
H	-1.37927400	-3.16913900	-1.38699600
C	-3.45018000	-1.25808400	3.75580700
N	-4.70380900	-1.82642100	3.81264500
C	-3.34186300	-0.69714100	2.52108100
C	-5.33841600	-1.62395100	2.65791600
N	-4.52753100	-0.93763000	1.86331400
H	-2.53617100	-0.16348000	2.04483700
H	-6.32970500	-1.96548900	2.40148200
H	-4.73584000	-0.62951600	0.87471600
H	-2.76303700	-1.30441000	4.58399900
H	-8.32069400	1.62340700	-1.03238900
H	-5.09282000	-2.32712200	4.60267400
O	-3.44588000	1.42187700	0.30579400
C	-2.77530800	3.66468500	-0.38104800
H	-3.81255400	3.92115000	-0.61793000
H	-2.26217800	4.56967000	-0.03986000
H	-2.29218600	3.30741400	-1.29490300
C	2.68046200	3.34092200	1.06246800
C	3.29238700	2.12213100	0.76846500
C	2.61924300	1.19011000	-0.02076700
C	1.32815700	1.46041200	-0.51602000
C	0.74841600	2.69440000	-0.21336100
C	1.41356400	3.63348000	0.57080100
H	3.20976300	4.06127200	1.67838200
H	4.28290600	1.91577200	1.15829900
C	0.68558400	0.46781200	-1.40019500

H	-0.23149700	2.91322000	-0.61903000
H	0.94409300	4.58717700	0.78938200
O	3.13627800	-0.02780600	-0.35732200
C	4.83116200	-1.61385600	-0.56263400
C	4.25600000	-2.36857000	-1.55850500
N	5.92266700	-2.32836800	-0.20341900
H	3.35980100	-2.17356300	-2.12720800
N	5.01583400	-3.47802200	-1.74951100
N	6.02280200	-3.44742200	-0.93097400
C	4.46359300	-0.29816200	0.04086800
H	4.54059900	-0.33624800	1.13665900
H	5.14165700	0.49010000	-0.31557400
N	-0.55599300	0.18583100	-1.54165900
O	-1.39268600	0.87504300	-0.71109400
H	1.34169000	-0.12418900	-2.03401000
C	6.91235300	-2.02553900	0.82787000
H	6.44707400	-2.14391100	1.81098600
H	7.68334800	-2.79200400	0.71912200
C	7.47092000	-0.63126000	0.66061400
C	7.40029000	0.28812400	1.70612000
C	8.02645000	-0.24437400	-0.56193600
C	7.87976400	1.58644200	1.53406800
H	6.96114500	-0.00870000	2.65549600
C	8.50192100	1.05125600	-0.73537700
H	8.07398000	-0.95962700	-1.38003800
C	8.42775500	1.96937200	0.31292000
H	7.81753700	2.29713600	2.35209100
H	8.92918700	1.34726700	-1.68834000
H	8.79604600	2.98105500	0.17524500

TS2(AZ)

N	-7.96094500	1.21174500	-1.83743100
C	-6.98850600	0.19297600	-1.46468900
C	-5.73812000	0.87406000	-0.88982600

O	-4.77173200	-0.09775900	-0.57681000
C	-7.49005800	-0.78354700	-0.42343700
O	-7.18166300	-1.95457400	-0.37740900
O	-3.14840400	0.74531800	-2.26983000
P	-2.94527400	0.41208100	-0.82636500
C	-2.59586400	2.63255900	0.71447300
O	-2.63862700	-1.09177000	-0.29448200
C	-3.24353400	-2.23320800	-0.91889800
C	-2.21434500	-3.34465800	-0.92700300
H	-8.79506900	0.77630800	-2.22500400
H	-6.68725300	-0.37779600	-2.34854500
H	-5.34677500	1.56332800	-1.64361300
H	-6.00679800	1.45768600	0.00601500
H	-8.14817800	-0.33890700	0.35527900
H	-3.09033400	3.01020400	1.61395200
H	-1.55697300	2.40384600	0.95859400
H	-4.13879600	-2.51735200	-0.35620500
H	-3.55628300	-1.97399200	-1.93482200
H	-2.63150800	-4.24310300	-1.39068900
H	-1.90912800	-3.59147100	0.09377900
H	-1.32943300	-3.03358200	-1.48852200
C	-4.45688100	-1.05606700	3.94267100
N	-5.46711900	-1.92590000	3.60397900
C	-4.14179600	-0.38630700	2.79806900
C	-5.74779900	-1.78285300	2.30239400
N	-4.95776400	-0.85073300	1.79189600
H	-3.40554100	0.37853600	2.61106800
H	-6.50086800	-2.33741600	1.76207900
H	-4.89500700	-0.49923800	0.64708500
H	-4.06482200	-0.99601200	4.94444400
H	-8.26454400	1.72342000	-1.00935600
H	-5.92964300	-2.57234300	4.23070600
O	-3.30642900	1.42463100	0.40371300
C	-2.69671200	3.64583000	-0.41040400

H	-3.74551300	3.87448000	-0.62278800
H	-2.18763600	4.57255300	-0.12728300
H	-2.23870900	3.25758400	-1.32494300
C	2.81511000	3.37001500	0.92002800
C	3.41462500	2.12950200	0.70259100
C	2.73091500	1.15670000	-0.02669200
C	1.44080500	1.40850500	-0.53248900
C	0.87314900	2.66510600	-0.30836300
C	1.55020300	3.64489000	0.41256500
H	3.35226100	4.12251900	1.48879000
H	4.40335600	1.93744800	1.10411100
C	0.78461300	0.36676400	-1.34768000
H	-0.10591800	2.86971800	-0.72386600
H	1.09165400	4.61538200	0.57150600
O	3.23498800	-0.08346200	-0.28994000
C	4.92687100	-1.67922700	-0.43635400
C	4.33281600	-2.48022100	-1.38384300
N	6.02796400	-2.37403600	-0.06784000
H	3.42387100	-2.31382300	-1.94129100
N	5.09152400	-3.59574600	-1.53960800
N	6.11546600	-3.52556100	-0.74497500
C	4.56629300	-0.33634400	0.10863300
H	4.65270600	-0.32106800	1.20401500
H	5.24093600	0.43305900	-0.29204700
N	-0.45787400	0.07650600	-1.44665400
O	-1.26898800	0.82114500	-0.62548400
H	1.42695800	-0.25983200	-1.96194000
C	7.03903800	-2.02383500	0.92798000
H	6.59967700	-2.11605800	1.92569000
H	7.81778700	-2.78314000	0.82456600
C	7.57231800	-0.62826500	0.70105100
C	7.50144900	0.32830100	1.71274000
C	8.09830900	-0.27654700	-0.54492000
C	7.94937200	1.62889800	1.48316400

H	7.08498900	0.05901000	2.68035800
C	8.54210900	1.02129800	-0.77588000
H	8.14676100	-1.02094200	-1.33659000
C	8.46591600	1.97708800	0.23814200
H	7.88558000	2.36864000	2.27494500
H	8.94559500	1.28959700	-1.74723300
H	8.80800100	2.99091500	0.05544800

C2(AZ)

N	-8.99146400	-0.48090000	-1.11724600
C	-7.53212700	-0.54902400	-1.07934900
C	-6.99698400	0.63602400	-0.26517500
O	-5.59353200	0.71080700	-0.28714000
C	-7.04682600	-1.84161600	-0.45788200
O	-6.23689700	-2.59388100	-0.95327300
O	-2.99938100	1.59245400	-2.62972400
P	-2.57635400	1.34716300	-1.24017500
C	-3.11447800	2.12110900	1.22467600
O	-2.82113600	-0.10923400	-0.66485600
C	-3.49122400	-1.12025800	-1.45817100
C	-2.52012800	-1.79160600	-2.40423700
H	-9.36560700	-1.25563600	-1.66124800
H	-7.13421900	-0.48718100	-2.09756200
H	-7.40577600	1.55126200	-0.70398200
H	-7.37704000	0.56241000	0.76717700
H	-7.51306400	-2.07730600	0.52341800
H	-3.29090100	1.05573800	1.39980400
H	-2.11105500	2.38167800	1.57527100
H	-3.89303800	-1.81895200	-0.72406800
H	-4.33178800	-0.66012100	-1.97974300
H	-3.03229700	-2.59724900	-2.93865800
H	-1.67663100	-2.21650700	-1.85379700
H	-2.13404400	-1.07481900	-3.13345600
C	-4.55358900	-1.57142700	3.92941800

N	-4.57041700	-2.71465100	3.17039800
C	-4.86112000	-0.55976800	3.06169100
C	-4.87917300	-2.36993500	1.90105000
N	-5.06016200	-1.06785400	1.79764700
H	-4.95950300	0.49645000	3.26874700
H	-4.98180900	-3.08806300	1.09881700
H	-5.26372500	0.05910600	0.37845200
H	-4.33249000	-1.58585600	4.98450000
H	-9.36861500	-0.58508300	-0.17532300
H	-4.38875400	-3.65288200	3.50107000
O	-3.16800200	2.37694200	-0.19712100
C	-4.18349700	2.96536900	1.87960700
H	-4.13510500	2.84909900	2.96611800
H	-4.04073600	4.02252100	1.64068200
H	-5.16710400	2.64604000	1.52510900
C	3.33695600	3.53455200	0.96882700
C	3.80430500	2.24400000	0.73025100
C	3.02459700	1.36087700	-0.01534400
C	1.77131600	1.76236600	-0.52674900
C	1.33032900	3.06585800	-0.27223100
C	2.10657700	3.94974600	0.47048800
H	3.94881600	4.21575100	1.55166800
H	4.76688800	1.94378300	1.12729700
C	1.05259500	0.79543800	-1.37215700
H	0.38026800	3.39044700	-0.67589300
H	1.75183400	4.95808200	0.65348600
O	3.39170100	0.07807900	-0.28473600
C	4.85462500	-1.73875400	-0.32460400
C	4.16428200	-2.51159500	-1.22920000
N	5.85210800	-2.54832100	0.09984000
H	3.28826800	-2.26413100	-1.80844500
N	4.77038900	-3.72466500	-1.30705300
N	5.79084400	-3.74002100	-0.50547300
C	4.67448200	-0.33361900	0.14648000

H	4.74732200	-0.27847200	1.24140100
H	5.44958500	0.31981900	-0.27725500
N	-0.19150500	0.65365100	-1.62286000
O	-0.98942700	1.58456000	-0.92761400
H	1.65753500	0.05136600	-1.88446500
C	6.90225200	-2.26550100	1.07583100
H	6.45184100	-2.19327700	2.07022500
H	7.55405600	-3.14213700	1.05815200
C	7.64690600	-0.99724200	0.72812600
C	7.75116900	0.03868300	1.65526400
C	8.20542200	-0.84374800	-0.54392500
C	8.40775500	1.22157300	1.31628700
H	7.31110700	-0.07589600	2.64288000
C	8.85774100	0.33671200	-0.88346800
H	8.11586800	-1.64870700	-1.26988100
C	8.95864000	1.37227300	0.04656700
H	8.48289200	2.02415000	2.04315700
H	9.28711300	0.45147400	-1.87371500
H	9.46522900	2.29423300	-0.22080700

BE

C	-4.49808200	-2.50980600	-1.74404200
C	-4.02288900	-1.20514000	-1.63884000
C	-3.31831300	-0.78638000	-0.51434400
C	-3.05000900	-1.66702800	0.55779900
C	-3.54341800	-2.97926800	0.41911300
C	-4.24997700	-3.40009700	-0.70090900
H	-5.05034800	-2.82212400	-2.62452700
H	-4.19563700	-0.47605500	-2.42561100
C	-2.34130100	-1.32969000	1.78747700
H	-3.36049800	-3.68101100	1.22965500
H	-4.60970700	-4.42329100	-0.75658500
H	-2.27401700	-2.11124800	2.55259100
O	-2.92632900	0.53774100	-0.47963800

N	-1.78922400	-0.17318000	2.02233000
O	-1.19666900	-0.02619900	3.17519800
C	-1.24250500	2.17505300	-0.73000000
C	-1.61819500	3.23553700	-1.52652100
N	-0.49355100	2.75697200	0.23823900
H	-2.23040300	3.22989100	-2.41658300
N	-1.08737000	4.37443600	-1.02159300
N	-0.39931900	4.07413200	0.04281900
C	-1.55770600	0.71918400	-0.83163200
H	-1.40466100	0.38824500	-1.86707300
H	-0.91609700	0.13633300	-0.16598700
C	0.23979100	2.14412600	1.34573600
H	0.66858400	2.98933900	1.89160400
H	-0.44457500	1.59895300	2.00327800
C	1.33073100	1.22215200	0.84745900
C	2.17230400	1.61136200	-0.19646300
C	1.50399500	-0.02726300	1.44524500
C	3.18328500	0.76775700	-0.64410300
H	2.03589900	2.58173900	-0.66842600
C	2.51684400	-0.87982000	1.00929700
H	0.82217400	-0.32427800	2.24117500
C	3.34215400	-0.47117400	-0.03105500
H	3.83688900	1.06505200	-1.45659800
H	2.65509200	-1.85462700	1.46443700
Br	4.70735100	-1.63808000	-0.64753400

C1(BE)

N	-6.97349500	-2.29515100	-1.97453400
C	-5.74738400	-2.09399100	-1.22312000
C	-5.04191000	-0.86298700	-1.81857200
O	-3.87538100	-0.48041400	-1.08126200
C	-5.94332000	-1.95360300	0.27983700
O	-5.03711900	-1.81135900	1.07299400
O	-2.72609200	-2.82839200	-1.22615000

P	-2.52199700	-1.36817500	-1.25272100
C	-1.56000000	0.51044900	-2.83983900
O	-1.70793300	-0.71663500	-0.05601400
C	-1.17488600	-1.62149300	0.95051300
C	-0.29235400	-0.82770600	1.88083500
H	-7.36999900	-3.20883000	-1.77116500
H	-5.08706000	-2.95604900	-1.36739900
H	-4.78426100	-1.07484500	-2.86076700
H	-5.70624600	0.00401900	-1.79560600
H	-6.99413300	-2.00058200	0.63075900
H	-2.40262800	0.99185500	-3.34446000
H	-1.40271800	0.99658000	-1.87342000
H	-2.02461500	-2.06869400	1.47811500
H	-0.60618900	-2.39842900	0.44002500
H	0.04636600	-1.47734100	2.69342800
H	-0.83268300	0.02031400	2.31765700
H	0.58440100	-0.45818000	1.34204800
C	-2.82951100	2.09922700	2.96751400
N	-3.23530700	0.98355500	3.66508400
C	-3.13269900	1.86244100	1.66118900
C	-3.76116300	0.09201800	2.82592600
N	-3.70588800	0.61417700	1.60729500
H	-2.99682000	2.47317400	0.78291300
H	-4.16651900	-0.87487700	3.07941800
H	-3.97749000	0.11874400	0.75090600
H	-2.36348400	2.94384200	3.44742400
H	-7.67413200	-1.60454400	-1.70973100
H	-3.15348800	0.84992000	4.66673700
O	-1.91763700	-0.87585000	-2.62795300
C	-0.29567900	0.53338000	-3.66932100
H	-0.47878800	0.11087500	-4.66143100
H	0.05595600	1.56323500	-3.78597600
H	0.46520300	-0.06281800	-3.15581200
C	5.07453100	-4.17276700	2.56259200

C	5.27111900	-3.11114600	1.68452300
C	4.26259700	-2.70498000	0.81427100
C	3.00417700	-3.34073700	0.80214700
C	2.84268400	-4.42259900	1.68850100
C	3.84711800	-4.83352100	2.55604400
H	5.86999400	-4.48285900	3.23259700
H	6.22140200	-2.58555900	1.64073500
C	1.89079300	-2.99975900	-0.08081800
H	1.88776100	-4.94319800	1.68970500
H	3.67134100	-5.66987800	3.22602600
H	1.11341600	-3.75940200	-0.22155700
O	4.56838500	-1.69480200	-0.07786800
N	1.75599600	-1.84610400	-0.66563600
O	0.69441100	-1.68142800	-1.41094900
C	4.97791900	0.59425900	-0.47859500
C	6.23677800	1.15371700	-0.50248900
N	4.39003400	1.09450900	-1.59069900
H	7.05158000	1.02090100	0.19411400
N	6.33998300	1.95256400	-1.59220700
N	5.21206900	1.91524000	-2.24467200
C	4.33042500	-0.38772700	0.43867600
H	4.78037400	-0.29128000	1.43374700
H	3.24931700	-0.21695300	0.50824200
C	2.99987200	0.94674000	-2.00971100
H	2.97704400	1.19787300	-3.07360000
H	2.70433000	-0.09864800	-1.87155200
C	2.09090600	1.84876100	-1.20170000
C	2.41055300	3.19057700	-0.97847500
C	0.91905900	1.31803300	-0.66561200
C	1.56479400	4.00481000	-0.23039700
H	3.32961900	3.60481000	-1.38589700
C	0.06901000	2.12332200	0.08958800
H	0.66456300	0.26981800	-0.85163900
C	0.39937800	3.45442000	0.29511700

H	1.80768500	5.04704900	-0.05479700
H	-0.83247100	1.69607500	0.51472000
Br	-0.76418100	4.54946200	1.32970700

TS1(BE)

N	6.01958600	-3.48455500	0.58585200
C	4.89020900	-2.69909700	0.09455500
C	4.46372000	-1.67924500	1.13940600
O	3.34376500	-0.95224000	0.65984400
C	5.22827600	-2.04344600	-1.23263300
O	5.14300400	-0.85686700	-1.47786900
O	1.85578600	-2.85312900	1.36223000
P	1.81055900	-1.38644100	1.13396900
C	0.99518200	-0.33291100	3.54477600
O	1.11552700	-0.72321800	-0.15319300
C	1.48286800	-1.20611400	-1.45751500
C	0.45042300	-0.70017700	-2.44109000
H	6.18272600	-4.29297400	-0.00972200
H	4.04382800	-3.37744700	-0.07447500
H	4.23987100	-2.19805600	2.07519600
H	5.26995100	-0.95884500	1.31999700
H	5.63589800	-2.73321300	-1.99665600
H	1.44234800	0.47603100	4.12761600
H	-0.04004100	-0.09337000	3.31017200
H	2.48588600	-0.84326900	-1.70420600
H	1.50806500	-2.30248400	-1.44345300
H	0.68368500	-1.06688100	-3.44457800
H	0.44438200	0.39322800	-2.46360100
H	-0.54509400	-1.05265200	-2.15681200
C	2.96854100	3.37364800	0.22312300
N	3.49860200	3.53799800	-1.03759400
C	3.15596900	2.06574400	0.55175400
C	3.99896300	2.38128600	-1.46871700
N	3.79565700	1.48077000	-0.51630700

H	2.87378900	1.49067900	1.42140100
H	4.47906500	2.20929800	-2.41861700
H	4.07244000	0.49140100	-0.56320800
H	2.48897000	4.18331000	0.74821800
H	6.87372600	-2.92959500	0.56986100
H	3.49394900	4.40064100	-1.56986900
O	1.75145600	-0.31575400	2.31679800
C	1.10418900	-1.65241500	4.27963500
H	2.15309000	-1.91973800	4.44185300
H	0.61562500	-1.56237200	5.25455400
H	0.61578200	-2.43946100	3.70488500
C	-3.63492300	-4.34820000	-3.14303000
C	-4.18718700	-3.48514200	-2.20058600
C	-3.40798800	-2.94284300	-1.18183400
C	-2.03436100	-3.24616700	-1.07464900
C	-1.50569800	-4.12026300	-2.04179800
C	-2.28022500	-4.66338200	-3.05985600
H	-4.25489900	-4.76574300	-3.92975100
H	-5.23976900	-3.21826600	-2.22918700
C	-1.11756300	-2.75388700	-0.04269800
H	-0.44959400	-4.37311500	-1.97867400
H	-0.11509700	-3.18910000	-0.02773700
O	-4.04894300	-2.12723600	-0.27071700
N	-1.44108300	-1.85145300	0.82489200
O	-0.52230800	-1.47297800	1.69313200
C	-4.77581100	0.03619100	0.36093500
C	-6.13253000	0.27921800	0.37141500
N	-4.33555500	0.66291000	1.47913400
H	-6.88404900	-0.04246700	-0.33472900
N	-6.43631100	1.02769500	1.45852000
N	-5.33881800	1.26177600	2.12120500
C	-3.91850900	-0.74102300	-0.58202600
H	-4.26705700	-0.56495500	-1.60692000
H	-2.86946700	-0.43876700	-0.49832700

C	-2.96467900	0.82847300	1.95950100
H	-3.06218500	1.17146800	2.99253000
H	-2.45948400	-0.14152200	1.94209700
C	-2.19989800	1.82453700	1.11473900
C	-2.70016700	3.10588000	0.87029000
C	-0.97696700	1.44302300	0.56642800
C	-1.97891500	4.00814700	0.09374400
H	-3.65896600	3.40350500	1.28828500
C	-0.25526200	2.32929400	-0.22974900
H	-0.58578500	0.44933200	0.77137100
C	-0.76109200	3.60324000	-0.44693000
H	-2.35562100	5.00784200	-0.09210700
H	0.68614900	2.01945500	-0.67030200
Br	0.23675400	4.82621200	-1.50959000
H	-1.82711900	-5.33351900	-3.78382000

IN(BE)

N	6.74763100	-2.42827700	1.46467300
C	5.76150700	-1.88263400	0.54194800
C	4.43502500	-1.67452300	1.28753600
O	3.46822000	-1.20849200	0.38201000
C	6.15757500	-0.55629000	-0.06692400
O	5.82942500	-0.18697700	-1.17452300
O	1.85473200	-2.93671800	1.09211400
P	1.75899500	-1.46587900	0.80175500
C	1.14202200	0.14791700	2.96474900
O	1.40976900	-0.85923800	-0.68469300
C	2.07589600	-1.33352100	-1.86022500
C	1.14573600	-1.08139100	-3.02935200
H	7.63023900	-2.58576800	0.98326800
H	5.58307800	-2.59062800	-0.27359200
H	4.13409900	-2.63596100	1.71452900
H	4.57764900	-0.95699100	2.11182800
H	6.75307600	0.10700500	0.59695400

H	1.67562200	0.99065600	3.41461800
H	0.20275900	0.51623000	2.54582300
H	3.03108300	-0.81257800	-1.98393000
H	2.29516800	-2.40310700	-1.75319100
H	1.61008900	-1.41236500	-3.96260900
H	0.92191600	-0.01335700	-3.11178600
H	0.20395600	-1.62314700	-2.89422400
C	2.30218600	3.33401100	-0.59561800
N	3.56539800	3.38897400	-1.14292200
C	2.17400400	2.08712000	-0.06496900
C	4.18520000	2.22318000	-0.95831000
N	3.35472500	1.42272200	-0.30242700
H	1.35490100	1.60589400	0.44408400
H	5.17823900	1.96334700	-1.29133800
H	3.52726400	0.41832500	-0.03498300
H	1.61121300	4.16072000	-0.65895100
H	6.94181500	-1.75523200	2.20538200
H	3.97032500	4.18575800	-1.61986800
O	2.00932600	-0.28508500	1.90898400
C	0.90456100	-0.93809600	3.99598800
H	1.85937100	-1.30742700	4.38264900
H	0.32465500	-0.53729800	4.83306300
H	0.35448500	-1.77038700	3.55219400
C	-3.58850700	-4.85210500	-2.83922700
C	-4.04186200	-4.03068300	-1.81127200
C	-3.14268600	-3.34371800	-0.99988800
C	-1.75539900	-3.46394800	-1.20543200
C	-1.32414300	-4.30555500	-2.24176600
C	-2.21956000	-4.98871000	-3.05611000
H	-4.30096200	-5.38319400	-3.46230300
H	-5.10274200	-3.91229300	-1.61102900
C	-0.70432900	-2.80503100	-0.41018500
H	-0.25449400	-4.41706500	-2.40434000
H	-1.85001100	-5.62872200	-3.85054900

H	0.31085400	-3.16108800	-0.57956600
O	-3.66315900	-2.58035800	0.02250100
N	-0.98189100	-1.88443900	0.43408200
O	0.00650400	-1.27470900	1.14033100
C	-4.66057200	-0.54534600	0.73079100
C	-6.00425300	-0.44142700	1.01820900
N	-4.06874400	0.13028400	1.74580200
H	-6.84724300	-0.84194400	0.47416000
N	-6.15436800	0.27779900	2.15619700
N	-4.97470500	0.62497000	2.58735500
C	-3.93228300	-1.23487500	-0.37354800
H	-4.56538900	-1.23480200	-1.26818800
H	-2.99142100	-0.72401400	-0.60584000
C	-2.65056200	0.43302200	1.93883500
H	-2.53802400	0.65054400	3.00363000
H	-2.07686600	-0.45991900	1.68751200
C	-2.22402000	1.61246800	1.09124000
C	-2.71646900	2.88837400	1.37934800
C	-1.35937800	1.43904800	0.00981300
C	-2.34358300	3.98566000	0.61173100
H	-3.39741800	3.02445200	2.21584900
C	-0.99771500	2.52705400	-0.78498400
H	-0.94829600	0.45569300	-0.20901400
C	-1.48286100	3.78720100	-0.46403000
H	-2.71142300	4.97905100	0.84350300
H	-0.33443000	2.39354500	-1.63342100
Br	-0.94474600	5.27741100	-1.50771000

TS2(BE)

N	6.05431800	-3.57069600	0.80428600
C	4.98083200	-2.94827400	0.04365200
C	3.94085100	-2.37752900	1.01913700
O	2.90734400	-1.76483600	0.28115100
C	5.43421700	-1.82478600	-0.87117400

O	4.89164800	-1.53722300	-1.91486300
O	1.14359600	-3.35228500	1.05988700
P	1.12093100	-1.86182300	0.92812300
C	1.08107100	-0.45423400	3.27918000
O	0.77113600	-1.12935500	-0.48240300
C	1.18814300	-1.66712400	-1.74675400
C	0.17110400	-1.21723700	-2.77503200
H	6.72686200	-4.00326500	0.17511100
H	4.47960900	-3.69950600	-0.57528300
H	3.53189000	-3.19712100	1.61519600
H	4.41091700	-1.64808700	1.69661200
H	6.30127900	-1.23646500	-0.49992600
H	1.78186500	0.26060800	3.71973400
H	0.14803900	0.06390300	3.05304600
H	2.19352100	-1.30612500	-1.98236600
H	1.23451900	-2.76034700	-1.67946100
H	0.45717000	-1.57494700	-3.76805500
H	0.11518700	-0.12468000	-2.80118500
H	-0.82211400	-1.60927100	-2.53411900
C	3.46521200	2.83046600	0.29294900
N	3.78137900	2.54847900	-1.01488000
C	3.22958500	1.62418200	0.88486800
C	3.74132400	1.22006900	-1.19452700
N	3.40769400	0.63593200	-0.05485000
H	2.93963000	1.39152000	1.89666300
H	3.97231300	0.71257100	-2.11928200
H	3.16601000	-0.58736500	0.10381400
H	3.41439500	3.84158100	0.66283300
H	6.56660700	-2.86290300	1.32965600
H	3.98819300	3.23092700	-1.73363100
O	1.72146900	-0.85325100	2.05488200
C	0.86459700	-1.62546500	4.21695400
H	1.81050600	-2.14434700	4.39854000
H	0.47762900	-1.26558200	5.17474200

H	0.14762900	-2.33204500	3.79336800
C	-4.92027400	-3.95020000	-2.49468500
C	-5.10234500	-2.88510600	-1.61751500
C	-4.05670300	-2.44048300	-0.81343000
C	-2.79612700	-3.06241700	-0.87009000
C	-2.63597100	-4.13002500	-1.76594000
C	-3.67722300	-4.57354400	-2.57247600
H	-5.74514500	-4.28671400	-3.11447000
H	-6.05942700	-2.37894200	-1.53495200
C	-1.62098800	-2.70131400	-0.06006200
H	-1.66555400	-4.61708200	-1.82283700
H	-3.51885300	-5.40156200	-3.25534300
H	-0.73396600	-3.31907400	-0.20872900
O	-4.31544300	-1.39534200	0.04368500
N	-1.63886900	-1.74158600	0.78534000
O	-0.48855300	-1.47204100	1.48828000
C	-4.57599100	0.93734300	0.35479800
C	-5.81495700	1.53991100	0.35388600
N	-3.95394700	1.49658900	1.42013400
H	-6.64358900	1.38483800	-0.32151100
N	-5.87500200	2.41774700	1.38362900
N	-4.73949800	2.38880200	2.02236400
C	-3.98752300	-0.12111500	-0.51507200
H	-4.42302700	-0.03688200	-1.51696600
H	-2.89832000	-0.01732700	-0.59241600
C	-2.56908100	1.32786800	1.85522600
H	-2.55282600	1.61022700	2.91046600
H	-2.31082400	0.26934900	1.76123300
C	-1.63092500	2.18774700	1.03559900
C	-1.77579000	3.57720800	1.01305600
C	-0.62289200	1.59007400	0.28234500
C	-0.91995500	4.36240000	0.24843700
H	-2.56609900	4.04913100	1.59153500
C	0.24056000	2.36297600	-0.49261900

H	-0.50149600	0.51229700	0.29523000
C	0.07884700	3.74158600	-0.49793800
H	-1.02635700	5.44137200	0.22748700
H	1.02268600	1.88916000	-1.07999100
Br	1.23449900	4.81569800	-1.55458100

C2(BE)

N	2.53026200	6.02528900	-0.00863400
C	2.11389000	4.77383300	0.62429100
C	2.95572500	3.62719600	0.07901100
O	2.66729400	2.47441600	0.83462700
C	2.27815300	4.82122400	2.12927100
O	1.38225300	4.68319700	2.93103700
O	0.02490400	2.87430600	-0.86025400
P	0.25637400	1.42277100	-0.74079200
C	1.98121700	-0.47776800	-1.19249000
O	0.18306000	0.80479900	0.71754200
C	0.01970300	1.65501200	1.87945700
C	-1.42022500	1.60877300	2.34179500
H	1.94222200	6.79141700	0.31247200
H	1.06198600	4.58175400	0.39586600
H	2.72446500	3.49527700	-0.98675400
H	4.02293100	3.89548500	0.16686900
H	3.31436500	5.04035300	2.47151200
H	2.40686000	-0.52253400	-0.18544200
H	1.09504400	-1.11755300	-1.23300600
H	0.70362100	1.25560100	2.63056500
H	0.33749000	2.66822300	1.63516200
H	-1.54233500	2.23607800	3.22986500
H	-1.71581800	0.58728000	2.59884100
H	-2.08822800	1.98254400	1.55834700
C	6.01122600	-0.98059800	-0.36169200
N	6.41169100	0.05299200	-1.17084700
C	5.02933300	-0.45507000	0.43310300

C	5.67310500	1.14058400	-0.85313100
N	4.82340400	0.86678300	0.11630500
H	4.45046000	-0.95425900	1.19620800
H	5.79002000	2.09360400	-1.34865600
H	3.37539500	1.81903700	0.61875800
H	6.44709800	-1.96486900	-0.42794400
H	3.48276300	6.25714000	0.27356600
H	7.13092100	0.01302500	-1.88063900
O	1.57472900	0.89206100	-1.43919700
C	2.99391400	-0.87983500	-2.23709900
H	3.37608800	-1.87463900	-1.98694200
H	2.54029900	-0.90845500	-3.23135800
H	3.83434800	-0.17992100	-2.24511900
C	-6.83952600	2.54759500	-0.58915600
C	-6.39668100	1.25414200	-0.32836000
C	-5.08711900	0.88632400	-0.62273700
C	-4.20001000	1.81983400	-1.18642500
C	-4.67259700	3.10915700	-1.46560900
C	-5.97614000	3.47986300	-1.16130600
H	-7.86326000	2.82144500	-0.35532600
H	-7.06047200	0.50568400	0.09300900
C	-2.80323700	1.53435500	-1.53617500
H	-3.99578400	3.82698700	-1.92059500
H	-6.31857100	4.48593200	-1.37759900
H	-2.32118500	2.19579400	-2.25840800
O	-4.71599700	-0.42067500	-0.41590400
N	-2.14094500	0.58040200	-1.00408900
O	-0.83040700	0.51744400	-1.55947000
C	-4.16238800	-2.17075200	1.08036300
C	-4.77379500	-3.01467200	1.97963000
N	-3.42371000	-3.00678100	0.31069200
H	-5.45684600	-2.77433300	2.78083300
N	-4.38147200	-4.28657500	1.71778800
N	-3.56761300	-4.27292900	0.70336500

C	-4.22175200	-0.69264900	0.89907200
H	-4.89571600	-0.27220500	1.65308800
H	-3.23157900	-0.23598000	1.00808300
C	-2.54066600	-2.68727400	-0.80801300
H	-2.85271200	-3.29258000	-1.66191100
H	-2.70824400	-1.63371800	-1.04569000
C	-1.09052000	-2.94490500	-0.47138400
C	-0.29141200	-3.68769300	-1.33906900
C	-0.52971300	-2.42873700	0.69960600
C	1.05401600	-3.91149400	-1.05381600
H	-0.71705900	-4.09849800	-2.25015400
C	0.80677400	-2.65537200	1.00833400
H	-1.13743200	-1.83676800	1.37959200
C	1.58495600	-3.38991200	0.11875300
H	1.67805100	-4.48243900	-1.73257600
H	1.24442700	-2.24484200	1.91194800
Br	3.43072500	-3.63160700	0.47454200

BZ

C	1.97615200	-3.05047700	0.95239500
C	1.57621400	-1.72261500	0.76761800
C	2.48464800	-0.78594800	0.28890600
C	3.82947400	-1.13076500	-0.01882400
C	4.19177100	-2.47520400	0.18129600
C	3.28029000	-3.41997500	0.65770500
H	1.26026900	-3.77595900	1.32631000
H	0.55539900	-1.44179700	1.00316600
C	4.73214100	-0.09439200	-0.51075000
H	5.21219100	-2.74369300	-0.05253900
H	3.60035900	-4.44883100	0.79750300
O	2.15076100	0.53212700	0.08372600
C	0.70815600	2.35468300	-0.00678100
C	1.47618200	3.16490500	-0.81072700
N	-0.30127000	3.16116600	0.39406000

H	2.38543200	2.92791400	-1.34138200
N	0.90161200	4.39505300	-0.85598000
N	-0.17323500	4.38718100	-0.12903100
C	0.82908000	0.91513300	0.37309500
H	0.60058900	0.77055200	1.43970700
H	0.11164000	0.31092900	-0.20182900
N	6.00011400	-0.18430400	-0.85216900
O	6.61206900	-1.32531100	-0.76957300
H	4.31923700	0.90391200	-0.61444800
C	-1.41625500	2.85080000	1.28294100
H	-1.03153900	2.69636200	2.29528100
H	-2.04077600	3.74722500	1.28769900
C	-2.18130400	1.63681300	0.80953800
C	-2.39009400	0.55622900	1.66448600
C	-2.66478000	1.57893200	-0.49997700
C	-3.07825800	-0.57336000	1.22699700
H	-2.01050500	0.58767500	2.68224200
C	-3.35099500	0.45797400	-0.95269000
H	-2.49786600	2.41453100	-1.17537400
C	-3.55053400	-0.60709500	-0.07866000
H	-3.24120200	-1.41440400	1.89153700
H	-3.72747300	0.41049100	-1.96832600
Br	-4.49429300	-2.13848300	-0.67829500

C1(BZ)

N	8.94281800	-2.57972000	-1.92425400
C	7.82776700	-1.68150000	-1.62786100
C	8.25232100	-0.23635500	-1.80835700
O	8.43273500	0.54259400	-0.89595100
C	7.35616800	-1.97314300	-0.20695900
O	6.40577500	-1.01602700	0.27868600
C	3.59913300	-2.69711500	0.60767500
C	2.70470300	-3.80712900	0.10765100
C	3.59397000	1.33384600	0.24964100

C	2.47718100	1.46582500	1.25699700
O	4.34517800	-2.20451100	-0.52985800
O	4.35085500	0.14256200	0.59350000
O	5.19477800	-0.19374000	-1.86780300
P	5.00904300	-0.76849000	-0.51899800
H	6.92543400	-2.97720500	-0.16031700
H	8.20075600	-1.91668200	0.48377600
H	9.14636700	-2.58855000	-2.92053100
H	9.78826400	-2.27036300	-1.44744000
H	7.02915600	-1.88620000	-2.34739300
H	8.48285600	0.05726900	-2.84961200
H	4.31596500	-3.04746200	1.35844700
H	3.01090900	-1.86973100	1.00868300
H	2.02676700	-3.39682000	-0.64477600
H	3.29310600	-4.61845800	-0.32975800
H	2.11523100	-4.21104900	0.93650000
H	1.83206600	0.58558700	1.18037700
H	2.87521800	1.55236200	2.27293100
H	1.88705600	2.36018500	1.03717200
H	3.20024300	1.23256600	-0.76039700
H	4.29447100	2.17474700	0.29791900
C	6.20208700	1.81979500	2.37065300
N	7.00921000	1.55342800	1.28898800
C	6.36917100	3.13721000	2.66724800
C	7.65206400	2.65521700	0.92530700
N	7.27471000	3.62842800	1.75208700
H	5.93313600	3.75936500	3.43082100
H	8.34772500	2.73446400	0.10516100
H	7.60887700	4.58418800	1.70660000
H	5.57967500	1.06017000	2.81456000
H	7.09749600	0.64808200	0.81072300
C	-2.17733500	-1.90129300	2.14802400
C	-2.78164400	-0.83680900	1.47027700
C	-2.07426500	-0.14774500	0.49165600

C	-0.74068400	-0.49636000	0.14568100
C	-0.16913900	-1.56999900	0.85096400
C	-0.87494100	-2.26183400	1.83772300
H	-2.73685000	-2.43289100	2.91154600
H	-3.80116000	-0.56339300	1.71934100
C	-0.05840700	0.25970700	-0.90320100
H	0.84408600	-1.84016300	0.59053100
H	-0.39650400	-3.08672000	2.35852500
O	-2.60799700	0.91167800	-0.20081600
C	-4.29021600	2.38697000	-0.83906100
C	-3.67150400	2.90759100	-1.95182400
N	-5.40118400	3.14592800	-0.70149500
H	-2.74738500	2.60486100	-2.41993600
N	-4.42865100	3.93193300	-2.42417900
N	-5.47513500	4.06918600	-1.66896100
C	-3.94672800	1.25063900	0.06698700
H	-4.07774600	1.54331900	1.11969500
H	-4.61020500	0.39413200	-0.12369600
N	1.15842900	0.12155000	-1.37094500
O	1.93498600	-0.80481000	-0.87703900
H	-0.62158000	1.05902600	-1.37436400
C	-6.45551200	3.03077100	0.29982300
H	-6.03448800	3.23981600	1.28756100
H	-7.17311400	3.81883900	0.05943700
C	-7.09075200	1.65953700	0.26166900
C	-7.17798200	0.88015700	1.41342600
C	-7.56443800	1.14986000	-0.95005300
C	-7.72957900	-0.39923600	1.36556800
H	-6.80439500	1.26411400	2.35895400
C	-8.11384300	-0.12420000	-1.01489900
H	-7.49296700	1.75030100	-1.85373400
C	-8.18671800	-0.88652700	0.14818300
H	-7.79042000	-1.00916900	2.25981100
H	-8.47749400	-0.52438300	-1.95454700

Br	-8.90866700	-2.63660600	0.05429500
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TS1(BZ)

N	8.20442600	-3.63073500	-0.64570400
C	7.40611100	-2.42615700	-0.80858800
C	6.59383100	-2.20859500	0.48244200
O	5.83228400	-1.01431600	0.44323300
C	8.20995100	-1.17713200	-1.11035700
O	7.72788000	-0.15112500	-1.54356200
O	4.45915900	-1.86505200	-1.50724900
P	4.31153300	-1.05946300	-0.27398900
C	2.84486800	-0.91547900	1.91797400
O	4.20341300	0.53538200	-0.24817800
C	4.19875200	1.21089400	-1.52695000
C	3.88886200	2.66804500	-1.27721400
H	8.64708400	-3.88142700	-1.52636900
H	6.68485000	-2.56075900	-1.61937600
H	5.95401000	-3.08458900	0.63276100
H	7.27017400	-2.12971900	1.34051900
H	9.29645600	-1.23816000	-0.89091500
H	3.54838700	-0.18530800	2.33473600
H	2.03691500	-0.38698700	1.40737700
H	5.18755600	1.07754400	-1.98329700
H	3.43773400	0.74288700	-2.15125500
H	3.86002400	3.20616200	-2.22894200
H	4.64563000	3.13649400	-0.63962600
H	2.91173200	2.74725300	-0.79583200
C	6.68929100	3.62142600	1.42584800
N	7.54088200	3.61991900	0.34327900
C	6.18669600	2.35984700	1.51583200
C	7.56583200	2.40716400	-0.20855700
N	6.75024900	1.63289700	0.49451800
H	5.47734600	1.92505800	2.20036900
H	8.13979000	2.09844300	-1.06774300

H	6.53209500	0.64298900	0.29378200
H	6.51744400	4.50431100	2.01866300
H	8.95812600	-3.46989600	0.02143400
H	8.07508900	4.41403000	0.00996900
O	3.53369000	-1.72694800	0.94938500
C	2.32160000	-1.83964100	2.99517000
H	3.14251400	-2.37992800	3.47439500
H	1.79535300	-1.25807800	3.75720600
H	1.62160900	-2.56322900	2.56819200
C	-2.30271100	-2.75231700	1.12752900
C	-2.81705500	-1.47772100	0.87574600
C	-1.98984600	-0.49156000	0.34727800
C	-0.62492400	-0.74277800	0.05403200
C	-0.14602600	-2.03693600	0.31419000
C	-0.97160200	-3.02810200	0.84870200
H	-2.95538200	-3.51647200	1.53825600
H	-3.85932500	-1.27474100	1.09584800
C	0.19922900	0.36462900	-0.44611200
H	0.89264200	-2.23584600	0.08536100
H	-0.56576500	-4.01734300	1.04009500
O	-2.43024600	0.77898200	0.07718400
C	-4.00593200	2.48370900	-0.06905400
C	-3.29148900	3.32948100	-0.88519100
N	-5.08273500	3.21790100	0.29466500
H	-2.35704200	3.15166800	-1.39487900
N	-3.96101700	4.50816200	-0.97370500
N	-5.04383200	4.43513800	-0.26230900
C	-3.77838400	1.07066800	0.35759800
H	-3.99296400	0.94630400	1.42926300
H	-4.44705800	0.39416200	-0.19483300
N	1.43264000	0.35635500	-0.86444500
O	2.05575800	-0.80246600	-0.94816600
H	-0.25835400	1.34927500	-0.44028800
C	-6.18645100	2.83921400	1.17165700

H	-5.80960800	2.73457500	2.19326600
H	-6.87942000	3.68350600	1.14651700
C	-6.83918100	1.55824600	0.70584300
C	-6.93931700	0.46123000	1.55944400
C	-7.31008400	1.45252100	-0.60522000
C	-7.49776200	-0.73632300	1.11585900
H	-6.57013200	0.53081500	2.57928400
C	-7.86853100	0.26532000	-1.06327500
H	-7.22946200	2.30221600	-1.27866300
C	-7.95192600	-0.81917500	-0.19396400
H	-7.56749300	-1.59278100	1.77684200
H	-8.23075700	0.17891500	-2.08140700
Br	-8.68644000	-2.45015300	-0.82143200

IN(BZ)

N	8.95262100	-1.31910000	-1.74120600
C	7.97789900	-0.34837500	-1.26123700
C	6.61747100	-1.03960200	-1.08413300
O	5.67263900	-0.09164800	-0.66977400
C	8.33888000	0.27712800	0.06662000
O	8.06313100	1.41348400	0.38855400
O	4.07068300	-0.73805600	-2.44411600
P	3.93619100	-0.47510300	-0.97311200
C	3.34375100	-2.74619100	0.46085600
O	3.63378000	1.00603200	-0.33866000
C	4.34295500	2.16710900	-0.78017200
C	3.44791000	3.36254400	-0.52231900
H	9.86018500	-0.87516700	-1.86397400
H	7.85850700	0.45471300	-1.99508900
H	6.33238300	-1.47835300	-2.04622300
H	6.70938800	-1.85500200	-0.34757600
H	8.85208700	-0.40389200	0.78023300
H	3.81988000	-3.23024000	1.31908400
H	2.34541300	-2.41887300	0.75914300

H	5.29134000	2.25422400	-0.23924200
H	4.57827700	2.07223600	-1.84592000
H	3.94595500	4.28477900	-0.83489600
H	3.21433200	3.43902800	0.54381100
H	2.51030300	3.26263500	-1.07598400
C	4.49680100	0.68349800	3.91090400
N	5.75109000	1.25080800	3.95708000
C	4.33564600	0.21992600	2.64169700
C	6.33504700	1.14027200	2.76330500
N	5.49135400	0.51385200	1.95386900
H	3.51306200	-0.28359200	2.16145900
H	7.31514100	1.50262000	2.49208100
H	5.65496200	0.28506000	0.93087700
H	3.84669900	0.66278200	4.76943100
H	9.08493100	-2.05251600	-1.04538800
H	6.17396400	1.68949900	4.76622400
O	4.17499200	-1.61419100	0.18844600
C	3.28673500	-3.70339100	-0.71552000
H	4.29500300	-4.03212700	-0.98595200
H	2.69174400	-4.58494900	-0.45617500
H	2.83702900	-3.21703000	-1.58530400
C	-2.16534400	-2.80969800	0.84528100
C	-2.62126000	-1.51627600	0.59170500
C	-1.83211000	-0.64576500	-0.15924600
C	-0.57631800	-1.05203800	-0.65355500
C	-0.15402800	-2.35754000	-0.39296500
C	-0.93801600	-3.23637100	0.35105900
H	-2.78418800	-3.48073200	1.43266900
H	-3.58223500	-1.20486900	0.98507200
C	0.19299100	-0.10355100	-1.48311800
H	0.79652200	-2.68144100	-0.79824500
H	-0.58987500	-4.24697700	0.53852200
O	-2.19601200	0.63699100	-0.45416500
C	-3.68574400	2.42524100	-0.59342900

C	-3.03454000	3.13115100	-1.57798200
N	-4.67338400	3.26038800	-0.19518300
H	-2.17849000	2.84321100	-2.16839400
N	-3.65053500	4.33323600	-1.72330300
N	-4.64052900	4.40522500	-0.88823600
C	-3.47799900	1.05527200	-0.03625300
H	-3.54368200	1.06409700	1.06088200
H	-4.24963500	0.36916600	-0.41308200
N	1.46072800	0.03816400	-1.59735000
O	2.19940900	-0.79248900	-0.80436100
H	-0.37982600	0.59382100	-2.08986000
C	-5.66869600	3.06479700	0.85574500
H	-5.17149100	3.11201400	1.82915900
H	-6.34589300	3.91851800	0.77552000
C	-6.39606800	1.75102600	0.68983000
C	-6.41315800	0.81861600	1.72540500
C	-7.02627400	1.44506300	-0.51903900
C	-7.04617800	-0.41230900	1.56392400
H	-5.92046300	1.04384700	2.66749100
C	-7.65993900	0.22060000	-0.69710700
H	-7.01169400	2.16464500	-1.33403300
C	-7.65858100	-0.69686900	0.35012100
H	-7.05421900	-1.14017600	2.36765900
H	-8.14572400	-0.02113500	-1.63583400
Br	-8.50205500	-2.37679700	0.10997700

TS2(BZ)

N	8.87818500	-1.43169600	-1.85683600
C	7.88641800	-0.42362400	-1.50807100
C	6.66688200	-1.10971300	-0.87470700
O	5.69342700	-0.14267500	-0.57050400
C	8.38343300	0.61473700	-0.52495700
O	8.03491100	1.77524800	-0.51843000
O	4.08847200	-1.02833500	-2.25227900

P	3.87140200	-0.62648400	-0.82815700
C	3.40916400	-2.74044200	0.83230000
O	3.58647700	0.90647600	-0.36805600
C	4.21840000	2.00590300	-1.03825500
C	3.19596000	3.11827700	-1.15164700
H	9.68877100	-0.99330800	-2.28852000
H	7.54831200	0.09721200	-2.40957500
H	6.26863800	-1.83201200	-1.59253200
H	6.97156900	-1.65370200	0.03455100
H	9.08133900	0.22770500	0.24987100
H	3.90191700	-3.10716800	1.73742600
H	2.39489100	-2.42998700	1.08986500
H	5.09527000	2.31897200	-0.46207800
H	4.56624800	1.68517700	-2.02473600
H	3.63379100	3.98508200	-1.65495800
H	2.85484200	3.42897800	-0.16011400
H	2.33034300	2.77451200	-1.72430800
C	5.51305600	0.90076500	3.94078500
N	6.44208600	1.82734500	3.52783500
C	5.18630100	0.17979000	2.83115200
C	6.66507900	1.66729300	2.21712400
N	5.91487800	0.67109100	1.77225300
H	4.49410900	-0.63622500	2.70146100
H	7.34958900	2.25499700	1.62316100
H	5.82513500	0.28987300	0.64174400
H	5.17787800	0.84319200	4.96317000
H	9.21777200	-1.89216100	-1.01290100
H	6.89008700	2.52083100	4.11360100
O	4.18932700	-1.59873900	0.44668600
C	3.40985100	-3.81302600	-0.24048000
H	4.43553900	-4.11026400	-0.47905200
H	2.86440800	-4.69462100	0.11074600
H	2.93483300	-3.44657100	-1.15498300
C	-2.10937900	-2.93175000	1.24952700

C	-2.58306900	-1.66602500	0.90592100
C	-1.81707300	-0.85208600	0.07266000
C	-0.57477400	-1.29255600	-0.42500500
C	-0.13110400	-2.56807900	-0.06944600
C	-0.88836600	-3.38754500	0.76457800
H	-2.70932200	-3.55986800	1.90043500
H	-3.53891100	-1.33167600	1.29254300
C	0.15356400	-0.41203400	-1.36002100
H	0.81272200	-2.91840100	-0.47013400
H	-0.52672300	-4.37616600	1.02748500
O	-2.18704200	0.40615800	-0.30310600
C	-3.60119400	2.25133500	-0.41479900
C	-2.94175400	2.93229300	-1.41140700
N	-4.54235000	3.12563700	0.00792200
H	-2.10854100	2.61292200	-2.01821700
N	-3.51168100	4.15873300	-1.54147000
N	-4.48019200	4.26916800	-0.68524000
C	-3.43885200	0.87842300	0.14802500
H	-3.47020800	0.90387400	1.24680200
H	-4.24815300	0.21919200	-0.19696400
N	1.41315100	-0.24851400	-1.51127700
O	2.17892900	-0.98143200	-0.63846000
H	-0.44697600	0.20465000	-2.02464800
C	-5.54356400	2.94338900	1.05295700
H	-5.03752000	2.83530300	2.01675400
H	-6.11729300	3.87313900	1.07047800
C	-6.42238600	1.74726500	0.76536500
C	-6.60650000	0.75074000	1.72211800
C	-7.03980300	1.62423300	-0.48204400
C	-7.40077000	-0.36128800	1.44610700
H	-6.12505200	0.83361600	2.69289100
C	-7.83092400	0.52024700	-0.77372700
H	-6.89340700	2.39390600	-1.23577800
C	-8.00098000	-0.46270500	0.19800900

H	-7.54231200	-1.13790200	2.18906800
H	-8.30758500	0.41912000	-1.74212700
Br	-9.06735100	-1.97668100	-0.20627300

C2(BZ)

N	10.02521400	-0.05498600	-0.96365000
C	8.57802600	0.13969200	-0.99843900
C	7.90213300	-0.98835300	-0.20622800
O	6.50070300	-0.93050000	-0.28557800
C	8.16525000	1.47040700	-0.40680700
O	7.40587100	2.25825800	-0.92614500
O	3.90140400	-1.64142100	-2.67834700
P	3.47438400	-1.37113900	-1.29467000
C	3.91942000	-2.17823700	1.17641600
O	3.79317900	0.06934900	-0.71645300
C	4.54514600	1.03601800	-1.49156600
C	3.63636500	1.77169500	-2.45187500
H	10.49303100	0.68299700	-1.48568100
H	8.22446900	0.10246300	-2.03408000
H	8.24272700	-1.93907900	-0.62775700
H	8.24433100	-0.94582100	0.84087500
H	8.62797200	1.69427000	0.57904200
H	4.14741800	-1.12366000	1.35760200
H	2.89656200	-2.38629200	1.50553400
H	4.97837800	1.70490800	-0.74723500
H	5.36317600	0.52432900	-2.00041900
H	4.20714600	2.54462000	-2.97504200
H	2.81173700	2.24766200	-1.91473200
H	3.21922400	1.08225900	-3.19041600
C	5.57202600	1.43213300	3.92996300
N	5.70809400	2.55952100	3.15949900
C	5.78788000	0.38531200	3.07644200
C	5.99554800	2.17173300	1.89765400
N	6.04970500	0.85691700	1.80983700

H	5.77889900	-0.67283700	3.29618200
H	6.17473600	2.86726800	1.08886100
H	6.20521000	-0.26562300	0.38362000
H	5.34260700	1.47979400	4.98228500
H	10.36164300	0.01688600	-0.00346700
H	5.61678700	3.51474500	3.47849700
O	3.98887200	-2.43438100	-0.24451000
C	4.92816000	-3.07899000	1.85148400
H	4.86111000	-2.96422100	2.93719200
H	4.73536800	-4.12642200	1.60485500
H	5.93526100	-2.81132800	1.52073900
C	-2.51068400	-3.04839900	1.10566800
C	-2.89962500	-1.74359800	0.80996500
C	-2.08631900	-0.95484600	-0.00247100
C	-0.87651200	-1.46435600	-0.52259800
C	-0.51537200	-2.78040300	-0.21085900
C	-1.32609900	-3.57079900	0.59749800
H	-3.14767800	-3.65663100	1.73993000
H	-3.82787200	-1.35889900	1.21555500
C	-0.11282000	-0.58795400	-1.42528500
H	0.40002500	-3.18742600	-0.61947900
H	-1.03393200	-4.58996300	0.82546900
O	-2.37695200	0.33372600	-0.33189500
C	-3.70251100	2.25053700	-0.41259500
C	-3.03126500	2.91012100	-1.41571100
N	-4.58948700	3.16583900	0.04071200
H	-2.23074100	2.55794600	-2.04765400
N	-3.54081200	4.16519300	-1.51865400
N	-4.48403800	4.31321100	-0.64019900
C	-3.60385200	0.86332300	0.12972300
H	-3.62895100	0.87288100	1.22848700
H	-4.44376200	0.24871800	-0.22306100
N	1.13193100	-0.54891000	-1.70919600
O	1.87340900	-1.51406000	-0.99925500

H	-0.67375300	0.17947800	-1.95260000
C	-5.57668600	3.02162400	1.10554400
H	-5.05615500	2.89138000	2.05888900
H	-6.11208000	3.97368700	1.13528000
C	-6.50654500	1.86102600	0.83406000
C	-6.69933300	0.86442000	1.78907500
C	-7.15757600	1.76615500	-0.39852000
C	-7.53244700	-0.22156400	1.52471400
H	-6.19236900	0.92549100	2.74845600
C	-7.98856400	0.68854400	-0.67829700
H	-7.00524500	2.53590600	-1.15102500
C	-8.16383300	-0.29667600	0.29020100
H	-7.67891100	-0.99920400	2.26563300
H	-8.49060800	0.60867300	-1.63580200
Br	-9.27706000	-1.77995900	-0.10109700

CE

C	3.81689500	-1.15297400	-1.06853200
C	2.53761300	-1.67049100	-0.91652700
C	1.63229900	-1.11844200	-0.01244500
C	1.96990500	-0.00133400	0.79497900
C	3.26679200	0.51235200	0.62508300
C	4.14738400	-0.05512000	-0.28273900
H	4.52834100	-1.57285900	-1.76712000
H	2.21337700	-2.52744700	-1.49803700
C	1.12044800	0.62750000	1.79122800
H	3.58796400	1.36288400	1.21536300
H	1.55862100	1.43956700	2.37991000
O	0.41004500	-1.73218900	0.08893900
N	-0.11957100	0.28082200	2.01692600
O	-0.74311500	0.93304200	2.94703900
C	-1.91280300	-1.75648100	-0.33382300
C	-2.33631900	-3.00650100	-0.73206800
N	-2.95171400	-1.28799400	0.39943100

H	-1.81629800	-3.73825800	-1.33301600
N	-3.57837700	-3.22598400	-0.24017700
N	-3.94719600	-2.17575200	0.43666700
C	-0.63331800	-1.03509300	-0.59780500
H	-0.41886100	-1.04969300	-1.67367500
H	-0.68958800	-0.00174300	-0.25013900
C	-3.12318300	0.00572300	1.06328200
H	-4.11308400	-0.05638100	1.52415300
H	-2.36919100	0.12937000	1.84738800
C	-3.05859600	1.15610900	0.08315000
C	-3.77248000	1.11388900	-1.11696500
C	-2.28695700	2.27838200	0.39005100
C	-3.72066000	2.18721500	-2.00128000
H	-4.36795700	0.23552700	-1.35748300
C	-2.24134100	3.35512100	-0.49504400
H	-1.71915700	2.28170700	1.31853000
C	-2.95565100	3.31190200	-1.69017000
H	-4.27780500	2.14821300	-2.93243700
H	-1.63911600	4.22596600	-0.25355900
H	-2.91463400	4.14888200	-2.38057400
N	5.48410500	0.52475100	-0.41533400
O	5.76798000	1.49245200	0.27251200
O	6.25590200	0.01329900	-1.21151000

C1(CE)

N	7.02835300	1.72699400	-2.39878000
C	5.81623500	1.56478500	-1.61579500
C	5.43094900	0.07532700	-1.66083600
O	4.30474800	-0.22443700	-0.82966100
C	5.91762100	2.05373900	-0.17981000
O	4.97346900	2.11020100	0.57980400
O	2.73670600	1.44841700	-2.06745400
P	2.81226900	0.15365800	-1.36581000
C	2.22515800	-2.39630000	-1.73818700

O	2.05775500	0.00027100	0.02129500
C	1.36261700	1.16616700	0.53741600
C	0.53540000	0.73431200	1.72273700
H	7.21408000	2.71273700	-2.56437600
H	5.00130100	2.12760500	-2.08215500
H	5.23046200	-0.20293900	-2.69972000
H	6.25154200	-0.54259400	-1.28794600
H	6.92695800	2.36952600	0.15330700
H	3.16530800	-2.94020400	-1.86717000
H	1.99990700	-2.31876200	-0.67106200
H	2.11828100	1.90908300	0.81704700
H	0.73060000	1.56458700	-0.25614400
H	0.05730700	1.61235100	2.16686900
H	1.15538100	0.25352000	2.48828800
H	-0.24249200	0.03635900	1.40181200
C	3.44045100	-1.12026000	3.89877600
N	3.66247800	0.21875000	4.13119300
C	3.70290900	-1.32661700	2.57845200
C	4.04831200	0.81482700	3.00392500
N	4.07811300	-0.11232600	2.05624400
H	3.66264500	-2.21887100	1.97492900
H	4.29877600	1.85573900	2.87372500
H	4.29096300	0.06769700	1.06953300
H	3.12338700	-1.79304900	4.67822000
H	7.83313200	1.35754700	-1.89495400
H	3.55859500	0.69002700	5.02273600
O	2.41538000	-1.06865400	-2.28441100
C	1.07537800	-3.03379200	-2.48451600
H	1.32483400	-3.16605700	-3.54113100
H	0.84672200	-4.01252700	-2.05143400
H	0.20383700	-2.37861500	-2.39395200
C	-5.10790500	3.51672700	0.51928400
C	-5.16712000	2.16600600	0.20594100
C	-4.07282700	1.50347400	-0.34892800

C	-2.84735200	2.16809100	-0.59223800
C	-2.81002800	3.53927300	-0.29461000
C	-3.91508700	4.17671800	0.24800900
H	-5.95078000	4.04548800	0.94462200
H	-6.08096000	1.60166400	0.36419200
C	-1.65797300	1.55258700	-1.16267400
H	-1.90430400	4.10571100	-0.47949700
H	-0.91097600	2.21231800	-1.61592700
O	-4.25062800	0.19565700	-0.72323700
N	-1.42793100	0.27022400	-1.10088800
O	-0.31394200	-0.15391900	-1.61499800
C	-4.50980500	-2.07946300	-0.15978300
C	-5.74784000	-2.68322400	-0.11823600
N	-3.75024900	-2.96240600	-0.85059600
H	-6.66424000	-2.32339000	0.32649500
N	-5.67433000	-3.87474400	-0.75814400
N	-4.45661900	-4.03804400	-1.19439800
C	-4.02621400	-0.75437700	0.32245000
H	-4.59658600	-0.46658200	1.21278700
H	-2.95696500	-0.77972900	0.56020700
C	-2.31309700	-2.91221900	-1.10722800
H	-2.13657400	-3.60947300	-1.93106600
H	-2.04742200	-1.89955800	-1.42498800
C	-1.51964600	-3.29411300	0.12454700
C	-1.86800000	-4.40961100	0.89029900
C	-0.42183400	-2.51456000	0.49104000
C	-1.11773500	-4.74818900	2.01336900
H	-2.73049300	-5.00948500	0.60838000
C	0.32583800	-2.85801900	1.61785500
H	-0.16306800	-1.64597700	-0.11874100
C	-0.01692700	-3.97251400	2.37958100
H	-1.39268200	-5.61647700	2.60448400
H	1.17115900	-2.23702200	1.90303800
H	0.56509000	-4.23498800	3.25806600

N	-3.82090900	5.60574000	0.54942100
O	-2.77588200	6.18357500	0.29720300
O	-4.79485300	6.15357800	1.04086700

TS1(CE)

N	6.67234000	2.09093600	-2.05701600
C	5.68355900	1.70398800	-1.06486700
C	4.63489900	0.80946000	-1.73709200
O	3.63114900	0.49829100	-0.78174200
C	6.25333700	0.97599300	0.14036800
O	5.67675400	0.88091400	1.20255300
O	1.77828500	1.25591700	-2.32081300
P	2.07284000	0.22720300	-1.29825700
C	1.63450900	-2.14532500	-2.61380300
O	1.46752200	0.26813500	0.18553600
C	1.68818300	1.44323300	0.99338500
C	0.77070300	1.33991800	2.19010500
H	7.32817200	2.75835500	-1.65797700
H	5.16401700	2.59541000	-0.69727300
H	4.20295300	1.35789100	-2.57773600
H	5.09090700	-0.11754800	-2.10966800
H	7.24364900	0.49956100	-0.01101800
H	2.29751900	-3.00958900	-2.69726700
H	0.67899600	-2.45281800	-2.19209700
H	2.74235700	1.48045800	1.28765600
H	1.46681600	2.33578200	0.39694400
H	0.87910700	2.22528900	2.82246600
H	1.02260800	0.45605000	2.78365500
H	-0.27040300	1.26162600	1.86184300
C	2.98146300	-2.99321900	2.53957100
N	4.11068100	-2.50200600	3.15713000
C	2.77771200	-2.21774000	1.44041000
C	4.58512000	-1.46500900	2.47015900
N	3.78596600	-1.28069200	1.42578900

H	2.01645400	-2.24034500	0.67656500
H	5.45492900	-0.87306700	2.70643100
H	3.90663500	-0.55035700	0.70831100
H	2.43138400	-3.83199900	2.93338900
H	7.22174400	1.28179200	-2.34363100
H	4.52356900	-2.86509300	4.00838800
O	2.30081400	-1.30844100	-1.64277400
C	1.45384900	-1.46579400	-3.95453600
H	2.41044400	-1.08946600	-4.33012000
H	1.06173700	-2.19281600	-4.67201000
H	0.75096100	-0.63771200	-3.85938400
C	-4.26982500	3.92442100	0.68598500
C	-4.59586600	2.68295700	0.15853600
C	-3.61506200	1.83403800	-0.35287000
C	-2.24657100	2.19621000	-0.34789800
C	-1.93280900	3.45664300	0.17897900
C	-2.92718100	4.28214000	0.68182900
H	-5.02056200	4.59495700	1.08323700
H	-5.62804700	2.35010800	0.11918800
C	-1.14885100	1.39483900	-0.88636300
H	-0.90167800	3.79298000	0.19757800
H	-0.20422800	1.90837000	-1.07220600
O	-4.03681700	0.65507800	-0.90973800
N	-1.27790000	0.12917900	-1.13745500
O	-0.24390500	-0.52212700	-1.60621400
C	-4.47798800	-1.66136400	-0.71866000
C	-5.73722600	-2.03085800	-1.14069200
N	-3.69247400	-2.68626500	-1.13040800
H	-6.67278400	-1.50287800	-1.02669800
N	-5.65636300	-3.23065000	-1.76263700
N	-4.41424900	-3.62460900	-1.74399600
C	-4.00487300	-0.44559100	0.00501300
H	-4.68133600	-0.23399900	0.84213500
H	-2.98757200	-0.58381900	0.37860600

C	-2.25896400	-2.89886500	-0.92479300
H	-2.03798600	-3.82448300	-1.46366700
H	-1.69479000	-2.07732000	-1.37489300
C	-1.92209100	-3.03096300	0.54416100
C	-2.67757000	-3.86679100	1.37009100
C	-0.85269800	-2.30928600	1.07830400
C	-2.36605700	-3.98790200	2.72095500
H	-3.51543900	-4.41946900	0.94955400
C	-0.54615400	-2.43140700	2.43417900
H	-0.28548200	-1.64550900	0.42503800
C	-1.29753700	-3.26863000	3.25598000
H	-2.95831500	-4.63902300	3.35663700
H	0.27745700	-1.86111300	2.85376600
H	-1.05717800	-3.35530600	4.31130500
N	-2.54524900	5.58494800	1.22826400
O	-1.36469000	5.89387600	1.21386400
O	-3.42718000	6.30093000	1.67439000

IN(CE)

N	6.27221700	2.32589200	-2.47723500
C	5.39152600	2.06453700	-1.34705100
C	4.22595900	1.18152700	-1.81325900
O	3.34342200	0.98201200	-0.73810100
C	6.06573300	1.35876800	-0.19217800
O	5.77051600	1.52208100	0.97278100
O	1.39528400	1.56325700	-2.13881200
P	1.68983500	0.49354800	-1.12630900
C	1.73759600	-2.11680300	-2.06614800
O	1.36507800	0.64319900	0.47601800
C	1.76994300	1.79415500	1.22582100
C	0.85696200	1.87601900	2.43210000
H	7.05301800	2.91040800	-2.18723100
H	4.97674700	3.00544400	-0.97184700
H	3.72085400	1.69357700	-2.63723500

H	4.61115200	0.21874300	-2.18534800
H	6.84811900	0.62406100	-0.48000300
H	2.52481400	-2.87621600	-2.03474500
H	0.90678100	-2.45475100	-1.44192100
H	2.81988200	1.69809600	1.52054200
H	1.68311300	2.69104900	0.59990400
H	1.12737700	2.73203600	3.05638000
H	0.94221600	0.96468500	3.03205900
H	-0.18581400	1.98549900	2.11727100
C	3.35882900	-2.62557700	2.46897000
N	4.53764400	-2.04480700	2.88149200
C	2.92459200	-1.89219000	1.40796800
C	4.81530600	-0.99568900	2.10754500
N	3.84724500	-0.89103100	1.20586100
H	2.04762000	-1.98314200	0.78785800
H	5.66591300	-0.33735000	2.19609400
H	3.77106700	-0.15206200	0.46407400
H	2.94160200	-3.49096200	2.95718500
H	6.67704000	1.45276700	-2.81364600
H	5.11201100	-2.35466700	3.65632900
O	2.35028000	-0.96251900	-1.47690400
C	1.29496100	-1.87116900	-3.49498500
H	2.13790000	-1.51972600	-4.09780300
H	0.92108400	-2.80170100	-3.93312200
H	0.49941100	-1.12401900	-3.52387100
C	-4.75711200	3.55155800	0.52085200
C	-4.84538000	2.26169600	0.01846200
C	-3.70172300	1.55769900	-0.36081700
C	-2.41989000	2.13574300	-0.24017300
C	-2.34121400	3.43969600	0.25678100
C	-3.49273000	4.11543600	0.63015100
H	-5.63582300	4.11068900	0.81598900
H	-5.80861700	1.77728600	-0.10262900
C	-1.14904700	1.50006100	-0.62911400

H	-1.37822900	3.92959000	0.35377500
H	-0.28738700	2.16136500	-0.69584400
O	-3.87840300	0.31381000	-0.89971200
N	-1.09150600	0.24662200	-0.88111200
O	0.08284700	-0.33278900	-1.21725000
C	-4.22458100	-2.01245700	-0.61622300
C	-5.45084900	-2.55310500	-0.93680000
N	-3.34190000	-2.91108900	-1.11652000
H	-6.43783000	-2.16265000	-0.73568200
N	-5.25533700	-3.72351300	-1.58898300
N	-3.97304300	-3.93508400	-1.68799500
C	-3.85245900	-0.74248500	0.06951200
H	-4.58511800	-0.52979700	0.85586300
H	-2.85399400	-0.80846700	0.51334900
C	-1.88316800	-2.92050700	-1.00830900
H	-1.54297100	-3.63288000	-1.76447500
H	-1.51198100	-1.92618300	-1.26059400
C	-1.43559900	-3.33566900	0.37768600
C	-1.82991500	-4.57457400	0.88988800
C	-0.63929800	-2.49044800	1.15333500
C	-1.42869800	-4.96969900	2.16158900
H	-2.45654000	-5.22643600	0.28523200
C	-0.24119300	-2.88781800	2.43175300
H	-0.33149700	-1.52465700	0.75460300
C	-0.63168600	-4.12505900	2.93607500
H	-1.73782900	-5.93501300	2.55045600
H	0.37210200	-2.22305500	3.03407500
H	-0.32109800	-4.43106300	3.93035700
N	-3.36928200	5.47737200	1.15313700
O	-2.25153800	5.95472500	1.25270300
O	-4.39199600	6.06420800	1.46404400

TS2(CE)

N	-6.10456500	3.07897700	1.57919000
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C	-5.05561800	2.66767600	0.65782000
C	-4.18349800	1.60516500	1.33987000
O	-3.16350500	1.19878000	0.45101400
C	-5.56499700	2.08518600	-0.64693500
O	-5.00163800	2.20922400	-1.71185600
O	-1.30412900	2.02012100	1.91487800
P	-1.46973600	0.72227000	1.19219200
C	-1.94822300	-1.39460900	2.85549300
O	-1.03809800	0.53926900	-0.36059300
C	-1.25745000	1.55974700	-1.34806200
C	-0.15707900	1.42684600	-2.38079200
H	-6.67240700	3.81271000	1.16163200
H	-4.41744800	3.52274900	0.41341700
H	-3.73512400	2.04091100	2.23593000
H	-4.79561600	0.73988300	1.63556200
H	-6.49740300	1.48549800	-0.56269500
H	-2.79121000	-2.08502200	2.94811400
H	-1.06117400	-1.96081200	2.56779300
H	-2.24557400	1.42176600	-1.79611100
H	-1.24166100	2.54397600	-0.86655000
H	-0.29668200	2.16872700	-3.17197400
H	-0.17530700	0.42921300	-2.82906000
H	0.82568200	1.58338000	-1.92559000
C	-4.30772000	-2.88885900	-1.41306800
N	-4.64538500	-2.05207800	-2.45010300
C	-3.85684100	-2.07724700	-0.41352900
C	-4.40923800	-0.78489400	-2.07790600
N	-3.92803300	-0.77248400	-0.84483300
H	-3.47885600	-2.32395100	0.56540500
H	-4.61089300	0.08510500	-2.68548000
H	-3.53929800	0.25343400	-0.19389700
H	-4.40933300	-3.95937500	-1.48422200
H	-6.73344300	2.29875200	1.76649500
H	-5.02266800	-2.33656600	-3.34532500

O	-2.33627400	-0.52266200	1.77792700
C	-1.73561500	-0.64059200	4.15324500
H	-2.62663800	-0.05752700	4.40414500
H	-1.54640000	-1.35039000	4.96375100
H	-0.88099200	0.03498600	4.07296100
C	5.25189900	2.85462400	-0.57978000
C	5.16871400	1.55436700	-0.10492500
C	3.95817500	1.03348900	0.35293900
C	2.78495700	1.81764200	0.35127700
C	2.87703300	3.12668100	-0.12903900
C	4.09094700	3.61693000	-0.58529600
H	6.18399000	3.27059700	-0.94061200
H	6.04414100	0.91460600	-0.07727200
C	1.45980900	1.38901600	0.83202500
H	2.00059100	3.76532000	-0.14697800
H	0.68681000	2.15796500	0.84105100
O	3.96692500	-0.24699900	0.82822500
N	1.24315000	0.19372400	1.23211600
O	-0.01330500	-0.13932800	1.65265900
C	3.82532000	-2.57515200	0.42276700
C	4.97608000	-3.31203400	0.59845100
N	2.85808100	-3.36855800	0.94269400
H	5.99247300	-3.05771200	0.33551400
N	4.65494400	-4.48734300	1.18998800
N	3.36720600	-4.51664300	1.38685600
C	3.59238200	-1.22174000	-0.15555000
H	4.21971100	-1.09251200	-1.04447500
H	2.54153200	-1.08512000	-0.43311200
C	1.41435200	-3.16024600	0.94558500
H	1.01378700	-3.92367700	1.61804900
H	1.20524200	-2.17337800	1.36720900
C	0.82516100	-3.27821200	-0.44481800
C	1.33996400	-4.18438800	-1.37524600
C	-0.25565900	-2.46975700	-0.79493800

C	0.77582400	-4.27757500	-2.64455800
H	2.18606200	-4.81305800	-1.10725100
C	-0.81625800	-2.56084600	-2.06790800
H	-0.64682200	-1.75423000	-0.07886400
C	-0.30209900	-3.46421400	-2.99539900
H	1.18121500	-4.98302700	-3.36337500
H	-1.64800800	-1.91194100	-2.33252600
H	-0.73474000	-3.53419900	-3.98870800
N	4.14997000	4.99079600	-1.08819500
O	3.12119400	5.64504500	-1.09172800
O	5.22670200	5.40806400	-1.47929700

C2(CE)

N	3.98816400	4.85906600	0.64080500
C	3.42734000	3.57938200	1.07567500
C	4.17595400	2.44102700	0.39636000
O	3.74223200	1.22936500	0.96959700
C	3.53282000	3.40726000	2.57716100
O	2.59379900	3.29299400	3.33168500
O	1.27445900	2.02998900	-0.72808400
P	1.32857900	0.55793600	-0.67357900
C	2.82852300	-1.52663400	-1.18821000
O	1.19271500	-0.12662400	0.74828200
C	1.02298200	0.64359800	1.96274000
C	-0.40346400	0.48850300	2.44529600
H	3.45235700	5.62675800	1.04007200
H	2.37245000	3.53040400	0.79246600
H	3.97699600	2.48437200	-0.68332300
H	5.25979700	2.58097000	0.55114400
H	4.57355000	3.44034500	2.97031300
H	3.36508900	-1.61290600	-0.23976200
H	1.87999000	-2.06791600	-1.11097700
H	1.74584500	0.23839500	2.67265700
H	1.28622300	1.68396600	1.76976200

H	-0.53523200	1.02062500	3.39185200
H	-0.64251100	-0.56804100	2.60371700
H	-1.10564500	0.89868900	1.71204100
C	7.08829300	-1.93161500	-1.03187300
N	7.15262300	-0.79355100	-1.79586600
C	6.19833000	-1.64535900	-0.03270900
C	6.31954800	0.12118900	-1.24949800
N	5.72447400	-0.36200400	-0.17787500
H	5.87069200	-2.28204500	0.77634900
H	6.18119600	1.10871300	-1.66606100
H	4.36239400	0.53617400	0.63649500
H	7.66520200	-2.81205900	-1.26494600
H	4.94016200	4.96005200	0.99305300
H	7.72218600	-0.65877700	-2.62060700
O	2.55523600	-0.11709800	-1.40620000
C	3.65290000	-2.02410300	-2.35187800
H	3.92375200	-3.07021800	-2.18560500
H	3.08445500	-1.95209800	-3.28280400
H	4.57077400	-1.43843400	-2.45010100
C	-5.39800300	2.78754600	-0.10187400
C	-5.20856200	1.41448300	-0.09061900
C	-4.00210200	0.86325400	-0.52636800
C	-2.95784300	1.69184300	-0.97598900
C	-3.16249600	3.07142200	-1.01842100
C	-4.36695000	3.59198100	-0.57358600
H	-6.32830300	3.23214800	0.22915300
H	-6.00105000	0.74882900	0.23493200
C	-1.64216500	1.19139200	-1.40366000
H	-2.38624900	3.73741900	-1.37824800
H	-1.05108800	1.81849500	-2.07206000
O	-3.87396300	-0.48930000	-0.59295300
N	-1.16910100	0.09238500	-0.95969400
O	0.11790800	-0.15579300	-1.51992700
C	-4.22718400	-2.56317100	0.48122800

C	-5.36348100	-3.21335500	0.90717500
N	-3.59617600	-3.48734100	-0.27984600
H	-6.16408600	-2.84618600	1.53223300
N	-5.35660800	-4.47171500	0.40240700
N	-4.28080600	-4.62805200	-0.31579200
C	-3.72712700	-1.17313200	0.66205400
H	-4.31320100	-0.67583400	1.44039100
H	-2.66694600	-1.15236100	0.94281500
C	-2.28184900	-3.38930400	-0.91497700
H	-2.32717400	-4.01848200	-1.80637000
H	-2.14395800	-2.34862300	-1.22215400
C	-1.18350600	-3.83112900	0.02593500
C	-1.06193400	-5.17500200	0.38797600
C	-0.29636600	-2.89309100	0.55147000
C	-0.05897400	-5.57305100	1.26640900
H	-1.75772200	-5.90512500	-0.01779900
C	0.71300800	-3.29224900	1.42772200
H	-0.38741900	-1.84762800	0.27176400
C	0.83157200	-4.63203700	1.78714300
H	0.03260400	-6.61892000	1.54301900
H	1.40323400	-2.54906300	1.81788100
H	1.61589500	-4.94743600	2.46847000
N	-4.56216000	5.04277000	-0.61092500
O	-3.65339700	5.73062900	-1.04261500
O	-5.62416300	5.48308100	-0.20687000

CZ

C	-2.36708500	-1.77850500	-0.35297700
C	-1.19304300	-1.02972400	-0.36626100
C	-1.23894300	0.34937600	-0.17051600
C	-2.46461400	1.04720000	0.04281100
C	-3.63205900	0.27122200	0.05346000
C	-3.55983500	-1.10643500	-0.14247800
H	-2.35080200	-2.85019200	-0.50198000

H	-0.25121200	-1.53991700	-0.52972200
C	-2.44041500	2.48770000	0.23063400
H	-4.57442800	0.77074600	0.21577700
O	-0.12219200	1.12614000	-0.17036800
C	2.16966300	1.54195500	-0.19993900
C	2.13239600	2.82216200	0.30252200
N	3.46293400	1.37082800	-0.55718200
H	1.29369900	3.37131800	0.70239900
N	3.38205800	3.34852200	0.22697100
N	4.18265900	2.46680700	-0.28932500
C	1.12421800	0.48488400	-0.33920600
H	1.18364800	0.00274600	-1.32525600
H	1.26429100	-0.29367600	0.42352700
N	-3.45039100	3.30469000	0.46042200
O	-4.64872100	2.83044500	0.54931000
H	-1.47535800	2.97827700	0.17224600
C	4.09167900	0.19916000	-1.16179300
H	3.72675900	0.09143000	-2.18755500
H	5.15843200	0.43251400	-1.19994600
C	3.81151900	-1.04956900	-0.35774500
C	3.23630300	-2.16585300	-0.96329500
C	4.09380000	-1.07593600	1.01067300
C	2.94368000	-3.30180800	-0.20881400
H	3.00763300	-2.14491700	-2.02607700
C	3.79903100	-2.20719200	1.76444000
H	4.53479300	-0.20151300	1.48397600
C	3.22124600	-3.32199900	1.15534800
H	2.49197900	-4.16510700	-0.68714100
H	4.01743600	-2.21956500	2.82759400
H	2.98574300	-4.20230100	1.74497100
N	-4.79815800	-1.87727000	-0.12620500
O	-4.73166300	-3.08701000	-0.29710400
O	-5.85137100	-1.28516300	0.05606600

C1(CZ)

N	-8.39236100	1.07191700	-2.27538500
C	-7.17243700	0.40974100	-1.81646200
C	-7.46213800	-1.03061700	-1.43883900
O	-7.47934900	-1.44976900	-0.30034600
C	-6.61194100	1.21605800	-0.64888700
O	-5.53241000	0.55654100	0.02800200
C	-2.96578800	2.42477900	-0.66917400
C	-2.19684200	3.28309800	-1.64553300
C	-2.53337900	-1.50332000	0.45116300
C	-1.37449700	-1.27280300	1.38988500
O	-3.69441200	1.44201800	-1.44570900
O	-3.34187200	-0.29691900	0.45870200
O	-4.47125100	-0.95988900	-1.80426600
P	-4.21470300	0.09524100	-0.80130100
H	-6.28087300	2.19527300	-1.00560400
H	-7.38413500	1.35763800	0.11050900
H	-8.68077200	0.71029800	-3.18118000
H	-9.15854000	0.90178000	-1.62588700
H	-6.46285000	0.39847400	-2.64975500
H	-7.75403100	-1.68533100	-2.28090300
H	-3.69241500	3.00417000	-0.08870100
H	-2.29083500	1.89694400	0.00627800
H	-1.48339200	2.65028900	-2.17878300
H	-2.87323200	3.75931700	-2.36112800
H	-1.65154600	4.05832100	-1.10143200
H	-0.78770200	-0.42546900	1.02397000
H	-1.72741200	-1.06796100	2.40538800
H	-0.73836400	-2.16217100	1.41522900
H	-2.18313700	-1.69490100	-0.56198900
H	-3.17741400	-2.32436600	0.78582500
C	-4.86780700	-1.36779400	2.89431000
N	-5.77819900	-1.58123600	1.88570200
C	-4.75240300	-2.54350000	3.56987400

C	-6.21140100	-2.83420600	1.92714200
N	-5.59855800	-3.43438200	2.94540000
H	-4.15573200	-2.82132900	4.42254100
H	-6.92688600	-3.27283900	1.25009600
H	-5.74027900	-4.40199200	3.21182000
H	-4.38356500	-0.41491500	3.03086700
H	-6.07195000	-0.89968000	1.17686400
C	2.73236700	2.54227300	1.26806500
C	3.49301800	1.46740400	0.81656600
C	2.91480500	0.49187400	0.00583300
C	1.54637400	0.54934000	-0.39149800
C	0.80449600	1.64532700	0.06857900
C	1.40269300	2.60270400	0.88566500
H	3.16189900	3.30497900	1.90471200
H	4.53374700	1.40534100	1.11147700
C	1.00117900	-0.51831700	-1.21769300
H	-0.23003100	1.72129800	-0.23019900
O	3.60917000	-0.57995800	-0.45797700
C	5.49404600	-1.90893600	-0.78299600
C	5.01672700	-2.65837800	-1.83300000
N	6.66077100	-2.51014300	-0.45777500
H	4.10604800	-2.53409700	-2.39877900
N	5.90478600	-3.65422200	-2.08672500
N	6.89800600	-3.55780800	-1.25619700
C	4.97085300	-0.68970600	-0.09827200
H	5.07718400	-0.77593600	0.99206600
H	5.52902200	0.20002700	-0.42131000
N	-0.22295900	-0.65647300	-1.67636700
O	-1.10528100	0.26143900	-1.41729900
H	1.67116600	-1.32853600	-1.48262500
C	7.60803700	-2.14545800	0.59281700
H	7.15029200	-2.34319100	1.56666500
H	8.45337900	-2.82613900	0.46677000
C	8.02249500	-0.69665100	0.47587000

C	7.85920500	0.17537800	1.55122500
C	8.53732500	-0.21501300	-0.73097600
C	8.20662300	1.52003700	1.42421500
H	7.45224600	-0.19538800	2.48886300
C	8.88149100	1.12642900	-0.85922300
H	8.65584500	-0.89478300	-1.57186600
C	8.71485200	1.99673500	0.21884600
H	8.07387800	2.19368100	2.26489800
H	9.27740600	1.49527500	-1.80013200
H	8.97942200	3.04447700	0.11667600
N	0.59107200	3.71118800	1.37219700
O	-0.61390000	3.68779800	1.16305800
O	1.14786400	4.61649800	1.97675000

TS1(CZ)

N	-7.61670100	2.73165700	-1.17365600
C	-6.72450700	1.58313500	-1.14219600
C	-5.90468400	1.64585500	0.16068300
O	-5.04555100	0.52962800	0.31029600
C	-7.42567700	0.24203000	-1.22640800
O	-6.86292100	-0.79809300	-1.49765000
O	-3.73884100	1.17062900	-1.75714500
P	-3.52201400	0.59315700	-0.41019900
C	-2.08490800	0.95866500	1.77889300
O	-3.28297200	-0.96136100	-0.11571600
C	-3.22160100	-1.84277400	-1.25979100
C	-2.75450100	-3.19329700	-0.77038900
H	-8.07819800	2.79405700	-2.07785900
H	-6.01247000	1.63903200	-1.97034600
H	-5.34178200	2.58518800	0.16219400
H	-6.57758000	1.65148000	1.02518500
H	-8.51267300	0.25102300	-1.00075700
H	-2.72622900	0.25971300	2.32849800
H	-1.23593400	0.41131200	1.36180800

H	-4.22490900	-1.89373300	-1.70174900
H	-2.52383600	-1.41728000	-1.98201900
H	-2.68323100	-3.88766300	-1.61224100
H	-3.44841000	-3.61272400	-0.03471900
H	-1.76827200	-3.08245400	-0.31444500
C	-5.51941700	-3.92739100	2.05641700
N	-6.30820500	-4.18808200	0.95774800
C	-5.15190100	-2.62054000	1.95881300
C	-6.42628000	-3.08659600	0.21678300
N	-5.73109700	-2.12796300	0.81378500
H	-4.53056700	-2.00791000	2.59088300
H	-6.98519400	-2.98019700	-0.69946100
H	-5.59790700	-1.16395200	0.46151100
H	-5.29554200	-4.68138700	2.79247400
H	-8.35534000	2.62635000	-0.47913800
H	-6.74236800	-5.07722700	0.73838500
O	-2.83537900	1.52570300	0.69124200
C	-1.63742300	2.10139800	2.66391100
H	-2.49998700	2.62890600	3.08027900
H	-1.03190800	1.71667000	3.48912900
H	-1.03757900	2.81234600	2.08818700
C	2.90894700	3.08248100	0.51909200
C	3.53610300	1.84562700	0.42307000
C	2.79423700	0.71089800	0.09067000
C	1.39531000	0.77305700	-0.15842700
C	0.78574300	2.02779100	-0.06093500
C	1.54509900	3.14492600	0.28035000
H	3.46755100	3.97388800	0.77398200
H	4.60195600	1.78407700	0.60668400
C	0.67522500	-0.46941300	-0.44694200
H	-0.27447300	2.10850300	-0.25429300
O	3.34973700	-0.52162200	-0.01761600
C	5.07473500	-2.08208900	-0.04309700
C	4.38755700	-3.10352700	-0.65674500

N	6.24476600	-2.65125100	0.32455000
H	3.40361900	-3.09137400	-1.10013200
N	5.16539800	-4.21681500	-0.63292900
N	6.28715900	-3.93722300	-0.04273300
C	4.74162100	-0.64684400	0.19673000
H	5.00447200	-0.34877900	1.22144300
H	5.29799400	-0.00145600	-0.49704300
N	-0.57005900	-0.62725200	-0.79557000
O	-1.28997200	0.45089400	-1.01540200
H	1.22540600	-1.39545200	-0.31891200
C	7.37288100	-2.03577000	1.01787200
H	7.07006800	-1.79276600	2.04083100
H	8.14178500	-2.81087300	1.06347900
C	7.85249400	-0.80083600	0.28952700
C	7.95908700	0.41867400	0.95636100
C	8.15482800	-0.87116600	-1.07325000
C	8.36788400	1.56151900	0.26900600
H	7.71516800	0.47759600	2.01425900
C	8.55851100	0.26879500	-1.75991700
H	8.06082900	-1.82118600	-1.59480100
C	8.66474900	1.48794400	-1.08919100
H	8.44585100	2.50810100	0.79443900
H	8.78856800	0.20864100	-2.81900100
H	8.97511400	2.37800700	-1.62740200
N	0.87708300	4.43676000	0.38399100
O	-0.33345000	4.48066800	0.21706300
O	1.55599100	5.42105800	0.63642900

IN(CZ)

N	-8.18723700	-0.00566200	-2.02256400
C	-7.12182800	-0.75324300	-1.36823000
C	-5.86069000	0.12094300	-1.29855900
O	-4.82035600	-0.61799600	-0.71876900
C	-7.45090600	-1.18485400	0.04255700

O	-7.03347000	-2.19722900	0.56398400
O	-3.24480200	-0.04108200	-2.54268200
P	-3.14689300	-0.05784500	-1.04684600
C	-2.93103700	2.49519200	-0.06032800
O	-2.67039500	-1.36171200	-0.17650600
C	-3.19562000	-2.66671900	-0.43756300
C	-2.17084900	-3.66538800	0.06123900
H	-9.02798700	-0.57502100	-2.08900700
H	-6.88240400	-1.64830100	-1.95058500
H	-5.60155400	0.42089700	-2.31928000
H	-6.07175200	1.03182600	-0.71450000
H	-8.08451100	-0.47358500	0.61552200
H	-3.54131800	3.07521100	0.63863300
H	-1.92516800	2.41348600	0.35760400
H	-4.15669600	-2.79210400	0.07212200
H	-3.37181400	-2.78344300	-1.51245600
H	-2.52165600	-4.68724200	-0.10866300
H	-2.00163800	-3.53027700	1.13374700
H	-1.21965200	-3.52676600	-0.45979300
C	-3.65908400	-0.55739900	3.94198400
N	-4.85553800	-1.22591500	4.07875400
C	-3.52258500	-0.28886300	2.61496600
C	-5.42953200	-1.36352300	2.88312400
N	-4.63516000	-0.79769900	1.98372100
H	-2.74294900	0.20778500	2.06145300
H	-6.36700400	-1.85551100	2.67338100
H	-4.80606500	-0.74973700	0.94161700
H	-3.02755200	-0.33625100	4.78609900
H	-8.43667800	0.80856800	-1.46196700
H	-5.24799400	-1.56715300	4.94814400
O	-3.55929900	1.20907700	-0.08899500
C	-2.91990700	3.16347700	-1.42263700
H	-3.93630000	3.20812600	-1.82671500
H	-2.53066000	4.18095000	-1.33435000

H	-2.29421200	2.60373400	-2.12277800
C	2.66186600	3.09272500	0.69130600
C	3.27722500	1.86237600	0.50589800
C	2.59686900	0.84229800	-0.16657900
C	1.28930100	1.03999400	-0.67068700
C	0.69428100	2.28389200	-0.49150000
C	1.38198000	3.28223800	0.19028700
H	3.16539300	3.89286000	1.21920900
H	4.27658600	1.70962600	0.89468600
C	0.64586000	-0.06406800	-1.40586300
H	-0.29000500	2.47507500	-0.89496300
O	3.11736400	-0.38743400	-0.37211100
C	4.76846700	-2.02937500	-0.34851600
C	4.16818500	-2.90014900	-1.22809600
N	5.83374500	-2.71961900	0.11779300
H	3.27865900	-2.76273900	-1.82364700
N	4.89104200	-4.04942500	-1.25186600
N	5.89766900	-3.93378300	-0.44059000
C	4.44487700	-0.63075800	0.06076100
H	4.51902100	-0.51253900	1.15001700
H	5.13564500	0.08230000	-0.40896900
N	-0.59960000	-0.33454700	-1.53908000
O	-1.45084100	0.50764600	-0.89780600
H	1.30540300	-0.77067700	-1.90177700
C	6.84028000	-2.29264600	1.08665200
H	6.36910100	-2.19898300	2.06946000
H	7.56268500	-3.11120800	1.12991000
C	7.48258500	-0.98987300	0.66891800
C	7.47707400	0.10951500	1.52621100
C	8.05514900	-0.87291900	-0.60079700
C	8.04052300	1.31916000	1.12030300
H	7.02572900	0.02196400	2.51157800
C	8.61443800	0.33375600	-1.00709500
H	8.05107700	-1.72934300	-1.27131400

C	8.60657000	1.43247600	-0.14658000
H	8.03036000	2.17174600	1.79180200
H	9.05522300	0.42017700	-1.99522900
H	9.03937600	2.37501200	-0.46685900
N	0.73036000	4.57050700	0.39153300
O	-0.42110600	4.69923700	0.00417600
O	1.36375500	5.45731800	0.94116000

TS2(CZ)

N	-8.07774400	0.17838600	-2.07317600
C	-7.04416900	-0.65192600	-1.46995700
C	-5.84665300	0.23013300	-1.08908400
O	-4.81893900	-0.57154800	-0.55836200
C	-7.48987500	-1.37455800	-0.21701500
O	-7.10423200	-2.47400700	0.11504800
O	-3.23940900	-0.06655900	-2.42867100
P	-3.02295000	-0.02587000	-0.95163700
C	-2.82068800	2.52560000	-0.01226700
O	-2.62367900	-1.33379900	-0.07799200
C	-3.15182000	-2.62739100	-0.40694900
C	-2.05730500	-3.64324200	-0.15191100
H	-8.86974700	-0.39542100	-2.35433100
H	-6.69683100	-1.39949300	-2.18994700
H	-5.49572400	0.73783000	-1.99193400
H	-6.15803100	0.99423500	-0.35868000
H	-8.18447800	-0.79638800	0.43156900
H	-3.41100900	3.10550100	0.70274000
H	-1.80155900	2.44703000	0.37192400
H	-4.03432800	-2.82101000	0.21154000
H	-3.46736500	-2.63831700	-1.45434600
H	-2.41598800	-4.65019900	-0.38336200
H	-1.74760800	-3.61808800	0.89664200
H	-1.18721900	-3.42453900	-0.77667300
C	-4.47030300	-0.35156800	4.05019800

N	-5.41624700	-1.34476100	3.94852000
C	-4.19397800	0.03194200	2.77144600
C	-5.69566600	-1.54866400	2.65413800
N	-4.96809700	-0.72232800	1.91907600
H	-3.51034000	0.77460900	2.39299200
H	-6.40411200	-2.27051600	2.27561800
H	-4.91979600	-0.66205700	0.70231600
H	-4.09148100	-0.01652100	5.00164500
H	-8.43570400	0.84309000	-1.38786700
H	-5.83896800	-1.84439600	4.72072500
O	-3.44582700	1.23193700	-0.00641900
C	-2.86198200	3.17796800	-1.38079400
H	-3.89065600	3.20200200	-1.75370800
H	-2.48694700	4.20209000	-1.31254800
H	-2.24667800	2.62536100	-2.09635300
C	2.75915300	3.08826900	0.63177100
C	3.35966200	1.84651900	0.47922500
C	2.67278200	0.82132100	-0.17939200
C	1.37185200	1.02620300	-0.69636000
C	0.79261500	2.28194200	-0.55320900
C	1.48749200	3.28544800	0.11250000
H	3.26776600	3.89253700	1.14847400
H	4.35270400	1.68898500	0.88193800
C	0.71741600	-0.08854100	-1.40668500
H	-0.18431800	2.48090900	-0.97082500
O	3.17950200	-0.41730900	-0.35797600
C	4.82515200	-2.06631600	-0.31510200
C	4.23425500	-2.93560100	-1.20244400
N	5.88178900	-2.75963800	0.16618900
H	3.35416900	-2.79549100	-1.81122900
N	4.95331400	-4.08743800	-1.21510700
N	5.94903700	-3.97442000	-0.39019200
C	4.50313300	-0.66516900	0.08616900
H	4.56879900	-0.54143300	1.17521600

H	5.20001400	0.04282500	-0.38193600
N	-0.52836200	-0.35959200	-1.51706300
O	-1.36059600	0.51190700	-0.86941200
H	1.36694400	-0.80652600	-1.89953400
C	6.87488000	-2.33677700	1.15090100
H	6.39155600	-2.25447500	2.12881100
H	7.60064400	-3.15231500	1.19524500
C	7.51577200	-1.02704700	0.75334500
C	7.49753300	0.06276500	1.62262600
C	8.09923400	-0.89333900	-0.50979700
C	8.05875800	1.27942700	1.23514100
H	7.03777700	-0.03760300	2.60286400
C	8.65604000	0.32051400	-0.89783900
H	8.10499300	-1.74210300	-1.19000200
C	8.63535000	1.40956400	-0.02544600
H	8.03873200	2.12431400	1.91613700
H	9.10487200	0.41993900	-1.88110600
H	9.06638300	2.35766400	-0.33138400
N	0.85166300	4.58688900	0.27743800
O	-0.29126600	4.72369000	-0.13174000
O	1.48925900	5.47462200	0.81988400

C2(CZ)

N	-9.11680800	-1.18723000	-0.78077000
C	-7.65935300	-1.26928400	-0.73108900
C	-7.08158200	0.14479300	-0.57866200
O	-5.67757800	0.15658300	-0.64036700
C	-7.17285700	-2.12502000	0.41870900
O	-6.34770400	-3.00719600	0.32874600
O	-3.06394000	-0.21236100	-3.08600800
P	-2.66623600	0.25739000	-1.74891500
C	-3.19712800	2.15793700	0.00700500
O	-2.90067600	-0.73617400	-0.53802700
C	-3.56477200	-2.01075000	-0.73477000

C	-2.58748000	-3.04468400	-1.24981200
H	-9.51850300	-2.11610600	-0.88953300
H	-7.28251700	-1.70281000	-1.66322000
H	-7.47736900	0.75421400	-1.39702800
H	-7.44247500	0.58011300	0.36744100
H	-7.64440700	-1.88693500	1.39715700
H	-3.33652300	1.32081300	0.69769700
H	-2.20228500	2.58931100	0.15831900
H	-3.95121600	-2.26897300	0.25155300
H	-4.41498700	-1.86754400	-1.40319300
H	-3.08622700	-4.01586700	-1.31953300
H	-1.73304200	-3.13676600	-0.57398300
H	-2.22116600	-2.76646300	-2.24151800
C	-4.69939000	0.18544900	4.18036900
N	-4.76820600	-1.17974600	4.05808300
C	-4.94795600	0.67157800	2.92629700
C	-5.04823100	-1.47051900	2.76864500
N	-5.16243300	-0.36960200	2.05158800
H	-4.99256200	1.70179400	2.60248900
H	-5.17675800	-2.47935400	2.40019200
H	-5.35024700	-0.08217700	0.26140200
H	-4.49067100	0.66795600	5.12163200
H	-9.47507800	-0.82268300	0.10180200
H	-4.63780200	-1.85289200	4.80128200
O	-3.26532300	1.66218400	-1.34999100
C	-4.28930300	3.19031300	0.16864700
H	-4.23755600	3.63220400	1.16785300
H	-4.17349800	3.98992800	-0.56764200
H	-5.26421100	2.71529200	0.03202600
C	2.99230200	3.07179200	0.39066900
C	3.58192600	1.81874600	0.33128200
C	2.89762200	0.75458400	-0.26586900
C	1.60046000	0.93408900	-0.81449300
C	1.02992000	2.20514900	-0.75686800

C	1.72751700	3.24236300	-0.15441900
H	3.50300000	3.90534900	0.85667700
H	4.56857300	1.68229700	0.75578500
C	0.96064300	-0.24836900	-1.41484600
H	0.05778900	2.39882300	-1.18186700
O	3.40626200	-0.49013400	-0.35007500
C	5.03939800	-2.14320200	-0.14240600
C	4.48887200	-3.06255900	-1.00486500
N	6.06305600	-2.81154800	0.43644600
H	3.64701000	-2.95626300	-1.67154800
N	5.19663800	-4.21743900	-0.90713400
N	6.14790800	-4.05864100	-0.03880700
C	4.71309000	-0.71756100	0.15619000
H	4.73906600	-0.52420600	1.23656300
H	5.43055800	-0.04488800	-0.33180600
N	-0.24712600	-0.47225600	-1.76693800
O	-1.08221700	0.63516100	-1.56457000
H	1.59874300	-1.11170600	-1.57600200
C	7.00824800	-2.33414100	1.44352700
H	6.47906000	-2.20025500	2.39170600
H	7.73133500	-3.14392200	1.56625200
C	7.66695000	-1.04578600	1.00697100
C	7.60772200	0.08819400	1.81604600
C	8.30724400	-0.97626800	-0.23337500
C	8.18425100	1.28501300	1.39113800
H	7.10316000	0.03800700	2.77791600
C	8.87939100	0.21781200	-0.65903400
H	8.34429700	-1.85897100	-0.86785900
C	8.81730100	1.35118200	0.15299800
H	8.13286600	2.16411800	2.02560600
H	9.37240300	0.26705200	-1.62482300
H	9.26001600	2.28376000	-0.18245800
N	1.09684800	4.55726500	-0.08620800
O	-0.03693100	4.67496400	-0.52267900

O	1.73520500	5.47149800	0.40830200
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DE

C	-4.53306600	-0.28947800	-1.43724000
C	-3.56958800	0.70989700	-1.43075100
C	-2.69495900	0.86888800	-0.35761700
C	-2.74268900	0.01891900	0.77714900
C	-3.71954600	-0.99027400	0.75176600
C	-4.57665700	-1.12670900	-0.32888000
H	-5.22007500	-0.42350800	-2.26229800
H	-3.47842400	1.40003700	-2.26330700
C	-1.90694600	0.11831900	1.96121300
H	-3.81190900	-1.67037300	1.59088400
H	-2.11305200	-0.58051100	2.77789700
O	-1.80914000	1.91378700	-0.43161300
N	-0.93992300	0.98579000	2.09761400
O	-0.28790200	0.95887600	3.21907400
C	0.37700200	2.72843200	-0.80188800
C	0.40453200	3.80829000	-1.65802300
N	1.34281100	3.01760700	0.10457100
H	-0.20626800	3.99860600	-2.52859300
N	1.36259600	4.67121500	-1.24533100
N	1.93266200	4.18004100	-0.18265500
C	-0.48772200	1.51218100	-0.80342300
H	-0.51799800	1.08875200	-1.81485600
H	-0.11007600	0.76244900	-0.10500000
C	1.83552700	2.22728000	1.23359500
H	2.60238800	2.85683700	1.69328900
H	1.03285200	2.05286100	1.95665000
C	2.42682800	0.91233400	0.77511300
C	3.32371000	0.87031000	-0.29447100
C	2.07758900	-0.26968900	1.42955000
C	3.87127400	-0.33740600	-0.71315600
H	3.59428700	1.78898500	-0.80999700

C	2.62172700	-1.48654600	1.02216200
H	1.36273000	-0.22194200	2.24928600
C	3.50986800	-1.50384200	-0.04589500
H	4.56495200	-0.37496800	-1.54592100
H	2.34933400	-2.41033600	1.52111600
N	-5.57671800	-2.19460300	-0.29703000
O	-5.58982100	-2.94726300	0.66382900
O	-6.35277300	-2.28330600	-1.23549200
Br	4.23191500	-3.16141200	-0.62859800

Cl(DE)

N	-6.87215100	-2.80668900	-2.15055900
C	-5.47396500	-2.62836500	-1.76389600
C	-5.25154800	-1.13662400	-1.52368800
O	-4.01597200	-0.83870700	-0.85526800
C	-5.14723900	-3.48516200	-0.55557200
O	-4.94116700	-3.06555900	0.56517700
O	-2.52916900	-2.80037300	-1.74436400
P	-2.60447500	-1.35603600	-1.44391200
C	-2.37153400	0.97654300	-2.65829000
O	-1.68609100	-0.83460800	-0.25906000
C	-0.73401700	-1.77312200	0.31678800
C	0.05918800	-1.04562300	1.37404000
H	-7.02341000	-3.72796800	-2.55342500
H	-4.84764200	-2.98052900	-2.58813500
H	-5.30017600	-0.60138400	-2.47643400
H	-6.03020300	-0.74763800	-0.86329500
H	-5.19185500	-4.57487400	-0.73772900
H	-3.36093200	1.30383100	-2.99039100
H	-2.22816400	1.28982800	-1.62075700
H	-1.30076700	-2.60793000	0.74200400
H	-0.08639900	-2.13280700	-0.48306000
H	0.71673100	-1.75778800	1.88167000
H	-0.60239200	-0.58887200	2.11838600

H	0.67774000	-0.26909700	0.91692400
C	-2.89248100	0.45301100	3.40349100
N	-2.79995800	-0.83270900	3.88840000
C	-3.51315200	0.36167700	2.19420200
C	-3.34074500	-1.68195500	3.01563100
N	-3.77670500	-0.97013600	1.98544400
H	-3.78924300	1.12046400	1.47897300
H	-3.41318000	-2.75279000	3.12358600
H	-4.22237800	-1.38091600	1.15640200
H	-2.50865000	1.30321700	3.94303500
H	-7.48366700	-2.72598200	-1.33988900
H	-2.38458000	-1.10275900	4.77304400
O	-2.35196500	-0.47146300	-2.73229000
C	-1.26358900	1.50354500	-3.54186800
H	-1.45182300	1.24526100	-4.58795200
H	-1.21093500	2.59352000	-3.45585100
H	-0.31411200	1.06149600	-3.22351400
C	6.03594300	-2.52333500	1.05519900
C	5.80162500	-1.26985200	0.50795600
C	4.64464600	-1.00366100	-0.22361000
C	3.64980000	-1.98980800	-0.42520400
C	3.90902300	-3.25814000	0.11810400
C	5.06920500	-3.49821000	0.83712800
H	6.93157700	-2.74669800	1.61965800
H	6.52977200	-0.47267600	0.62064500
C	2.41789700	-1.81008400	-1.17875700
H	3.18982800	-4.05809800	-0.01599000
H	1.89456700	-2.71363600	-1.50771400
O	4.53634300	0.23754500	-0.79849000
N	1.88883100	-0.64396600	-1.42508800
O	0.76324000	-0.64248300	-2.07576500
C	4.17367200	2.56123400	-0.56680600
C	5.20127500	3.47323600	-0.46236400
N	3.34051900	3.12675900	-1.47233700

H	6.09350200	3.42561700	0.14468800
N	4.93907000	4.52192800	-1.27909400
N	3.80513900	4.30570700	-1.88377900
C	3.95232800	1.22501700	0.05550800
H	4.44234500	1.20277100	1.03544300
H	2.88406800	1.01043600	0.17394100
C	2.02250400	2.66302900	-1.89454500
H	1.81167100	3.17703500	-2.83616500
H	2.07275600	1.58357300	-2.07010900
C	0.97277200	2.96474900	-0.84635400
C	0.88438900	4.22183300	-0.24238900
C	0.08097900	1.95840800	-0.48161200
C	-0.09571600	4.48104900	0.71201500
H	1.58521500	5.00671600	-0.51699800
C	-0.89675400	2.20387100	0.48035500
H	0.14690600	0.97791400	-0.96093300
C	-0.97731600	3.46162400	1.05860700
H	-0.17411300	5.45722700	1.17768900
H	-1.57331400	1.40658100	0.76834600
N	5.28486900	-4.83535600	1.39205900
O	4.42954600	-5.68528100	1.20368400
O	6.31218300	-5.03706200	2.01987000
Br	-2.33479000	3.79238200	2.35014000

TS1(DE)

N	3.47979300	-5.84473300	1.27909900
C	2.89107700	-4.65507200	0.66919000
C	3.24453300	-3.41719700	1.47934900
O	2.64100400	-2.27919100	0.88622900
C	3.32106100	-4.52501400	-0.78091500
O	3.85246300	-3.55232300	-1.27761400
O	0.48027200	-2.86531400	2.02923500
P	1.21099200	-1.68578900	1.49675800
C	1.49008200	-0.01536900	3.66481900

O	0.81637600	-0.96911600	0.11063200
C	0.66774300	-1.79066700	-1.06142100
C	-0.08913100	-0.98529700	-2.09479600
H	3.08379100	-6.69111900	0.87727200
H	1.79855200	-4.76243100	0.68400200
H	2.91485600	-3.55929700	2.51217400
H	4.32891800	-3.25527800	1.47497200
H	3.16876600	-5.43716100	-1.38965300
H	2.39678400	0.44333400	4.06706400
H	0.76003700	0.75670700	3.42856200
H	1.65839900	-2.08162600	-1.42492100
H	0.12119300	-2.70399100	-0.79633000
H	-0.24421600	-1.58762500	-2.99431500
H	0.47249300	-0.08848800	-2.37088400
H	-1.06255200	-0.68132800	-1.69947500
C	4.53679500	1.39488000	-0.48718500
N	4.84647300	1.04148700	-1.78178600
C	4.07633300	0.26657400	0.11998700
C	4.59473400	-0.25350500	-1.96624100
N	4.12589300	-0.73419900	-0.82216700
H	3.69025500	0.08562100	1.11240600
H	4.74336200	-0.80668200	-2.87995600
H	3.83727900	-1.70792900	-0.65777100
H	4.64315400	2.40725800	-0.13303700
H	4.48276800	-5.87645400	1.10387800
H	5.18724500	1.67222000	-2.49842300
O	1.93661500	-0.60809800	2.42812300
C	0.92464000	-1.03366900	4.63300500
H	1.64874200	-1.83279100	4.82056700
H	0.70153100	-0.53962400	5.58357800
H	0.00912800	-1.46386100	4.22558400
C	-5.61403800	-1.75103000	-1.68949400
C	-5.41393100	-0.58411300	-0.96602600
C	-4.28820600	-0.41459700	-0.16049000

C	-3.30268900	-1.42410900	-0.04761200
C	-3.51719800	-2.59705600	-0.78470300
C	-4.64416200	-2.73952700	-1.57907500
H	-6.48348200	-1.89582600	-2.31758900
H	-6.13614200	0.22492700	-1.00515900
C	-2.09673100	-1.37056400	0.77792000
H	-2.79613000	-3.40566400	-0.73408300
H	-1.49890900	-2.28237200	0.83708400
O	-4.20558700	0.75751900	0.54535200
N	-1.73857300	-0.30783500	1.42445900
O	-0.62552800	-0.35360600	2.12123700
C	-3.52543400	3.02006500	0.68432500
C	-4.51656400	3.97757000	0.69715600
N	-2.64115500	3.46901600	1.60840200
H	-5.42716800	4.01729500	0.11736000
N	-4.18871500	4.93605200	1.59557200
N	-3.04595900	4.62285900	2.13846300
C	-3.39165600	1.75090000	-0.08792200
H	-3.75400700	1.91296800	-1.10969000
H	-2.35123500	1.41257400	-0.11806300
C	-1.33615800	2.92168900	1.97794600
H	-1.07016100	3.42273600	2.91197700
H	-1.43657700	1.84751700	2.15643400
C	-0.30503200	3.17712100	0.90012700
C	-0.02973600	4.47197200	0.45385500
C	0.37230700	2.09541300	0.34143200
C	0.92540100	4.68922700	-0.53470200
H	-0.56182700	5.31856400	0.88159300
C	1.31609800	2.29700900	-0.66338800
H	0.17184800	1.09064500	0.70391200
C	1.58765800	3.59247000	-1.08055600
H	1.15229600	5.69265000	-0.87785400
H	1.82858500	1.44883900	-1.10519500
Br	2.90130400	3.87780900	-2.42450500

N	-4.82012800	-3.98374100	-2.32954000
O	-5.80055600	-4.08476800	-3.04912300
O	-3.97984200	-4.85907100	-2.20091100

IN(DE)

N	4.62082700	-5.34813800	2.00494100
C	3.98480100	-4.51561200	0.99361900
C	3.15289500	-3.42766800	1.68804800
O	2.48894600	-2.66634000	0.71148100
C	4.95828700	-3.82701600	0.06267200
O	4.71399200	-3.54097800	-1.09048600
O	0.32078500	-2.92424400	1.86357000
P	1.04132000	-1.78017500	1.20968800
C	1.80474300	0.28001100	2.89826800
O	0.85492100	-1.37930600	-0.37089000
C	0.93646800	-2.35963800	-1.41155600
C	0.18683200	-1.79679900	-2.60122200
H	5.15774500	-6.09028900	1.56191300
H	3.30647200	-5.12242300	0.38551400
H	2.43385600	-3.92169300	2.34840500
H	3.80764200	-2.78936200	2.30260600
H	5.93172800	-3.54875600	0.52069700
H	2.78827600	0.70981900	3.11071600
H	1.19272700	1.04150900	2.40903800
H	1.98463000	-2.56339900	-1.65222400
H	0.48733700	-3.29993700	-1.06787600
H	0.22046100	-2.49731800	-3.44016600
H	0.63796200	-0.85116600	-2.91767200
H	-0.85974100	-1.60989100	-2.33984200
C	3.97135800	1.41523300	-1.34077100
N	4.92354600	0.60646500	-1.92140100
C	3.24470900	0.61254300	-0.51587400
C	4.78558100	-0.64150300	-1.47365200
N	3.77270800	-0.65378200	-0.61634500

H	2.39796300	0.82002500	0.11826500
H	5.37744500	-1.49732000	-1.75916900
H	3.39045700	-1.49416100	-0.11341700
H	3.88402800	2.46405200	-1.57986100
H	5.28648100	-4.79569000	2.54455600
H	5.62317600	0.90210400	-2.59191200
O	2.08636100	-0.78334300	1.97880500
C	1.15729700	-0.21798300	4.17545700
H	1.77559100	-0.99496100	4.63540600
H	1.05419000	0.60696700	4.88701200
H	0.16724400	-0.62810900	3.96631800
C	-5.83617600	-1.96880200	-1.29891400
C	-5.54720000	-0.87358400	-0.49867300
C	-4.28561600	-0.71496900	0.07677000
C	-3.26466000	-1.66521700	-0.13903700
C	-3.56776900	-2.77049000	-0.93929000
C	-4.82698200	-2.90059900	-1.50443300
H	-6.81088800	-2.10351500	-1.75029000
H	-6.30096200	-0.11978600	-0.29673200
C	-1.90670600	-1.61929500	0.43091500
H	-2.81744600	-3.53170900	-1.12331900
H	-1.31996500	-2.53160500	0.33874600
O	-4.09650600	0.37260600	0.88551300
N	-1.47336000	-0.56458400	1.01233700
O	-0.22050800	-0.52060600	1.51755700
C	-3.65544500	2.69703700	1.10328800
C	-4.63999900	3.61932500	1.38386300
N	-2.63518000	3.06771800	1.91501100
H	-5.63319400	3.69977900	0.96680400
N	-4.17626100	4.48264100	2.31865300
N	-2.95777000	4.14249100	2.63095200
C	-3.62910400	1.52871900	0.17866100
H	-4.29467000	1.73188100	-0.66745500
H	-2.61872100	1.34029200	-0.19876300

C	-1.28512500	2.51089200	2.00407200
H	-0.91578000	2.79087700	2.99346300
H	-1.36176400	1.42482700	1.94101800
C	-0.39157600	3.06168500	0.91380600
C	0.01151600	4.39922200	0.95827300
C	0.02659600	2.25460100	-0.14540600
C	0.83768600	4.92731200	-0.02692300
H	-0.31814900	5.03212400	1.77831900
C	0.83452900	2.77809400	-1.15472400
H	-0.25754400	1.20502300	-0.17766800
C	1.24238000	4.10248300	-1.07252200
H	1.16847900	5.95900400	0.01702500
H	1.15377800	2.15535000	-1.98396800
N	-5.10273600	-4.06929000	-2.34180300
O	-4.20360700	-4.87371700	-2.51920900
O	-6.21924500	-4.17766600	-2.82005400
Br	2.40748300	4.79389400	-2.40130800

TS2(DE)

N	3.60044000	-5.99898100	1.16990200
C	2.95435400	-4.96798200	0.37131200
C	2.53564200	-3.81284300	1.29173200
O	1.90757000	-2.81241900	0.51813200
C	3.82535200	-4.39655900	-0.73316800
O	3.39938400	-3.97844800	-1.78670400
O	-0.30341700	-3.05841000	1.65865800
P	0.46307700	-1.83200600	1.27820700
C	1.50875400	-0.42693400	3.38040600
O	0.36072600	-1.18383400	-0.20877200
C	0.26285900	-1.99064100	-1.39355500
C	-0.54010100	-1.19803000	-2.40434600
H	3.84192500	-6.79655500	0.58612600
H	2.04846600	-5.37021100	-0.09331600
H	1.83429000	-4.19328400	2.03759000

H	3.41314600	-3.39698300	1.80972100
H	4.91099200	-4.34883500	-0.49862700
H	2.53606000	-0.18334600	3.66471700
H	0.97907200	0.49849800	3.15078700
H	1.26781200	-2.21598800	-1.76100300
H	-0.22377400	-2.94089000	-1.14795300
H	-0.61699700	-1.75481600	-3.34223600
H	-0.05492000	-0.23872200	-2.60763900
H	-1.55000400	-1.00199400	-2.03075500
C	4.83760500	0.68898500	-0.24909900
N	4.80540900	0.12056900	-1.50024900
C	4.06434600	-0.11078100	0.54015500
C	4.04370600	-0.98291400	-1.45527000
N	3.58019100	-1.14535600	-0.22639500
H	3.80983400	-0.01825100	1.58342500
H	3.86345200	-1.64306100	-2.29046500
H	2.72581200	-2.01695600	0.14466400
H	5.37521800	1.60184400	-0.05064000
H	4.47727200	-5.64723200	1.55319900
H	5.26150100	0.48486300	-2.32736900
O	1.66038300	-1.20656900	2.18005200
C	0.82686200	-1.21164700	4.48377900
H	1.36095900	-2.14878100	4.66636800
H	0.82669500	-0.62673900	5.40799700
H	-0.20644800	-1.43930000	4.21320300
C	-6.25403500	-0.62978700	-1.23861800
C	-5.68109100	0.44541800	-0.57601200
C	-4.43429500	0.32850800	0.03948600
C	-3.72325100	-0.88992200	0.00924400
C	-4.30479400	-1.96657300	-0.66607000
C	-5.54259300	-1.82190000	-1.27261600
H	-7.22040100	-0.55273600	-1.72036100
H	-6.19134400	1.40080300	-0.51889500
C	-2.41707100	-1.14644900	0.63987900

H	-3.79278200	-2.92105800	-0.71734600
H	-2.02363800	-2.15673900	0.52644400
O	-3.95398100	1.43034400	0.68955300
N	-1.80221900	-0.24663500	1.30848500
O	-0.58878800	-0.55480200	1.85959800
C	-2.86896000	3.53264500	0.58424300
C	-3.58260900	4.71070700	0.55456500
N	-1.88745600	3.77972900	1.48512900
H	-4.46083600	4.95771000	-0.02362200
N	-3.00691300	5.59105300	1.40792400
N	-1.97632400	5.01893100	1.96378600
C	-3.07437500	2.23214400	-0.11257500
H	-3.54025000	2.41809200	-1.08585600
H	-2.12747700	1.70177200	-0.26477600
C	-0.75726100	2.93112100	1.85913200
H	-0.44028300	3.27789000	2.84519800
H	-1.11813600	1.90243900	1.93982800
C	0.36495300	3.03428200	0.84904800
C	1.01965800	4.24997900	0.63557500
C	0.74442900	1.91173900	0.11633200
C	2.04771000	4.34243400	-0.29625500
H	0.72310500	5.13090500	1.19908500
C	1.77235500	1.98807300	-0.82229500
H	0.24521900	0.96219000	0.27625200
C	2.41090800	3.20557700	-1.01453800
H	2.56289600	5.28164700	-0.46378400
H	2.06620400	1.10704300	-1.38668700
Br	3.81714300	3.33302700	-2.28513800
N	-6.12057900	-2.97130800	-1.97217600
O	-7.21274800	-2.82936800	-2.49484000
O	-5.48050100	-4.00861500	-1.99620800

C2(DE)

N	1.18343000	6.28564200	0.47569900
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C	1.16339700	4.91028800	0.97463800
C	2.27664000	4.11487300	0.30581700
O	2.35506000	2.85634900	0.93298300
C	1.36028000	4.85663500	2.47577100
O	0.56266700	4.40488800	3.26600400
O	-0.31862700	2.59167500	-0.68549900
P	0.30689900	1.25742200	-0.63825000
C	2.46929600	-0.08036000	-1.20753100
O	0.45862200	0.58071100	0.78637400
C	0.08812000	1.29034400	1.99444200
C	-1.24289500	0.77692900	2.49828900
H	0.40699600	6.81138500	0.87150000
H	0.20132700	4.44942000	0.73310200
H	2.05494700	4.03286400	-0.76705600
H	3.22629100	4.66657600	0.41680200
H	2.30896900	5.31781300	2.83066300
H	2.96355700	-0.00734300	-0.23349300
H	1.78930400	-0.93718800	-1.20020700
H	0.89524500	1.10136500	2.70435400
H	0.05821700	2.35963800	1.78985700
H	-1.51188400	1.30136200	3.41998300
H	-1.19423700	-0.29445900	2.71456600
H	-2.03018300	0.95289800	1.75748900
C	6.57847100	0.90636500	-0.86256500
N	6.38984300	2.01526700	-1.64843700
C	5.58416700	0.95638000	0.07618700
C	5.31238700	2.68204000	-1.17568300
N	4.79872800	2.06627100	-0.12990300
H	5.37462200	0.25363300	0.86897400
H	4.94639600	3.59594400	-1.62132300
H	3.19385400	2.44547000	0.60877300
H	7.37832600	0.20546500	-1.04029300
H	2.03514000	6.75465400	0.78442800
H	6.95477200	2.28768000	-2.44156600

O	1.68940800	1.12809000	-1.39752400
C	3.47280400	-0.19448100	-2.32979500
H	4.13037000	-1.04519800	-2.12438300
H	2.97108200	-0.35323600	-3.28793900
H	4.08626300	0.70845800	-2.39024800
C	-6.80447600	0.30735300	-0.12333600
C	-5.99400400	-0.80891600	0.01672600
C	-4.65610200	-0.76877300	-0.37613200
C	-4.10310800	0.40675100	-0.91974700
C	-4.92811000	1.52056800	-1.08468900
C	-6.25006300	1.45525400	-0.67620000
H	-7.84526400	0.29324000	0.17517100
H	-6.38794200	-1.73637100	0.41809600
C	-2.70274400	0.54216800	-1.35063600
H	-4.54281800	2.43695900	-1.51746400
H	-2.46760400	1.32497200	-2.07359300
O	-3.92329500	-1.91630500	-0.28603700
N	-1.77775000	-0.19475900	-0.87155600
O	-0.53055900	0.12226900	-1.47309900
C	-2.87315600	-3.56610500	1.05140200
C	-3.21780200	-4.60843100	1.88166700
N	-1.96816900	-4.11669400	0.20620600
H	-3.91497800	-4.61872900	2.70627900
N	-2.51758000	-5.70886500	1.50916100
N	-1.76634800	-5.40251500	0.49236900
C	-3.31769700	-2.14627200	0.99578000
H	-4.04455100	-1.97039300	1.79524300
H	-2.47834500	-1.45136500	1.11072600
C	-1.21686700	-3.48566300	-0.87621600
H	-1.32916000	-4.11073000	-1.76451200
H	-1.69135700	-2.51928400	-1.06525300
C	0.24103500	-3.31564900	-0.51815300
C	1.23555000	-3.78360000	-1.37554100
C	0.60738400	-2.67400100	0.66735800

C	2.58290200	-3.60185800	-1.07000800
H	0.96223500	-4.29215400	-2.29568800
C	1.94608900	-2.49682700	0.99567400
H	-0.15605800	-2.29444700	1.34180100
C	2.91841500	-2.95386700	0.11163400
H	3.35662800	-3.95192800	-1.74451300
H	2.23041800	-1.97676700	1.90393600
N	-7.09592600	2.63984800	-0.84536200
O	-6.59389800	3.63271400	-1.34226900
O	-8.25533900	2.56663600	-0.47827400
Br	4.74315900	-2.59639900	0.47703200

DZ

C	2.34259600	-1.83742800	0.83681000
C	1.51732200	-0.72014100	0.73908200
C	2.01486000	0.47582600	0.22498000
C	3.36507600	0.61245100	-0.21339400
C	4.17488400	-0.52691700	-0.10739300
C	3.65383600	-1.71152700	0.40880400
H	1.97413900	-2.77482700	1.23255000
H	0.48877800	-0.80199900	1.06961500
C	3.82076100	1.89005100	-0.73415500
H	5.20010200	-0.45477700	-0.43537800
O	1.25120300	1.59600000	0.10651100
C	-0.72309500	2.82785000	0.14023500
C	-0.28872600	3.87937100	-0.63259000
N	-1.94440300	3.22184600	0.56831900
H	0.64148800	3.98908600	-1.16859300
N	-1.25262500	4.83634500	-0.63536500
N	-2.25206200	4.43357900	0.08760600
C	-0.10959400	1.50714300	0.47078700
H	-0.21260900	1.28281800	1.54210100
H	-0.60617800	0.70351500	-0.09063800
N	5.01489900	2.21072200	-1.19452600

O	5.94996800	1.31909800	-1.21748800
H	3.10308500	2.70255300	-0.75291100
C	-2.88341600	2.50660900	1.42798600
H	-2.47259900	2.45484800	2.44056000
H	-3.78222900	3.12706600	1.45347600
C	-3.16685900	1.12327500	0.88999300
C	-2.97035100	-0.00328800	1.68595600
C	-3.58627000	0.96388700	-0.43327800
C	-3.18242000	-1.28177700	1.17274900
H	-2.63650800	0.10859800	2.71404800
C	-3.79816500	-0.30395700	-0.96108100
H	-3.73579300	1.83841800	-1.06199200
C	-3.58876800	-1.41506800	-0.14860800
H	-3.02228200	-2.15928800	1.78909100
H	-4.11773100	-0.43032900	-1.98944600
N	4.52936400	-2.87440900	0.50442000
O	4.07130000	-3.90883600	0.97020800
O	5.68311700	-2.76943000	0.11601600
Br	-3.84807400	-3.14843100	-0.87025500

C1(DZ)

N	8.98041600	-1.46886000	-2.64006200
C	7.85898400	-0.73122000	-2.06110900
C	8.30006800	0.66354200	-1.66139600
O	8.42419700	1.04996500	-0.51747600
C	7.32245800	-1.54075900	-0.88414300
O	6.35212100	-0.83352000	-0.10184900
C	3.57645300	-2.44605400	-0.72995900
C	2.63056800	-3.12211100	-1.69443100
C	3.61747000	1.43986800	0.67130300
C	2.47781400	1.26014100	1.64477800
O	4.36095900	-1.49527300	-1.48976100
O	4.26253500	0.15049500	0.51893600
O	5.30993400	0.85913100	-1.77506100

P	5.02355700	-0.22754600	-0.81454700
H	6.89271800	-2.47643900	-1.25299200
H	8.13642400	-1.77368300	-0.19306200
H	9.22694400	-1.09370700	-3.55267800
H	9.80597200	-1.38859100	-2.04858600
H	7.09117500	-0.62447400	-2.83381000
H	8.60306800	1.31342600	-2.50321400
H	4.26880300	-3.15467000	-0.26202600
H	3.02755600	-1.90604100	0.04384000
H	1.96241300	-2.36594600	-2.11332100
H	3.18175000	-3.61555200	-2.49999800
H	2.03703500	-3.86911000	-1.16107000
H	1.76413100	0.54484200	1.22669500
H	2.84493700	0.89449200	2.60876700
H	1.97357400	2.21753000	1.80447900
H	3.25640400	1.77885400	-0.29831500
H	4.37365700	2.13573300	1.05242100
C	6.12192600	0.67840400	2.82123700
N	6.97567600	1.12378900	1.83986700
C	6.03520100	1.67560600	3.74313300
C	7.40470600	2.34374600	2.13441600
N	6.84214100	2.69626600	3.28853000
H	5.48276400	1.75088000	4.66486800
H	8.08178900	2.93671100	1.54032600
H	6.98926500	3.58390100	3.75516800
H	5.64513800	-0.28595200	2.76192900
H	7.24618100	0.61455900	0.99097800
C	-2.11270900	-2.03895900	1.21856900
C	-2.75724500	-0.87663800	0.80350600
C	-2.06297400	0.08521200	0.07178500
C	-0.69002600	-0.07208600	-0.27884300
C	-0.06551400	-1.25236500	0.14514900
C	-0.77819600	-2.19539700	0.88285900
H	-2.63325900	-2.79629200	1.79033400

H	-3.79974300	-0.73657300	1.06293200
C	-0.02220200	0.98629500	-1.02235800
H	0.97096700	-1.40494900	-0.11566400
O	-2.64007700	1.23792700	-0.35773900
C	-4.37724700	2.74571400	-0.70191600
C	-3.79637200	3.47841000	-1.71067400
N	-5.48716400	3.45155200	-0.38589500
H	-2.88695500	3.28030800	-2.25696400
N	-4.57186700	4.56763000	-1.95057400
N	-5.59349400	4.54505900	-1.15067700
C	-4.00085800	1.45613600	-0.04982800
H	-4.15031600	1.50735100	1.03784600
H	-4.62133600	0.63556600	-0.43695800
N	1.21470800	1.02034500	-1.46525500
O	1.98616400	-0.00640900	-1.26917300
H	-0.59806100	1.87986800	-1.23559500
C	-6.49035400	3.16017500	0.63275000
H	-6.03755400	3.27515600	1.62191000
H	-7.25459600	3.93207400	0.51500500
C	-7.06361000	1.77237700	0.46125400
C	-7.07536800	0.87552100	1.52768700
C	-7.56790700	1.37161600	-0.77864700
C	-7.59030200	-0.40985600	1.36984600
H	-6.67739700	1.17527700	2.49346000
C	-8.08114200	0.09181800	-0.95324900
H	-7.55354900	2.06279800	-1.61777400
C	-8.08712900	-0.78487900	0.12834700
H	-7.59997600	-1.10767300	2.19951600
H	-8.47214400	-0.22304600	-1.91426900
N	-0.08358400	-3.39489400	1.33468100
O	1.12514000	-3.46786200	1.16175100
O	-0.73674300	-4.27552200	1.87580400
Br	-8.79376400	-2.52876100	-0.09983200

TS1(DZ)

N	8.33150600	-3.10490900	-1.24695900
C	7.48686900	-1.92137700	-1.20351800
C	6.68263200	-1.95153900	0.11024100
O	5.87101300	-0.80165200	0.26924000
C	8.24006700	-0.60987700	-1.29554600
O	7.71873300	0.44879400	-1.57865200
O	4.48384600	-1.48242400	-1.72224100
P	4.32690300	-0.81077000	-0.41105000
C	2.87013600	-0.94026200	1.79610700
O	4.17762800	0.76710000	-0.19623600
C	4.22514800	1.59613900	-1.37926300
C	3.83459900	2.99645600	-0.96877700
H	8.78676800	-3.17970000	-2.15342900
H	6.76190700	-1.94825500	-2.02187500
H	6.08425000	-2.86830000	0.11780200
H	7.36647800	-1.98345800	0.96566500
H	9.32456700	-0.65786200	-1.06367900
H	3.54650000	-0.25507900	2.32021600
H	2.06928900	-0.36393900	1.32754600
H	5.24541600	1.55453300	-1.78127200
H	3.52606100	1.18909000	-2.11136900
H	3.84718300	3.65593900	-1.84101200
H	4.52435000	3.39993900	-0.22024900
H	2.82486000	2.97385900	-0.55266500
C	6.52511600	3.65735900	1.96174700
N	7.33789200	3.86786700	0.86982100
C	6.10090800	2.36692800	1.87650000
C	7.41533200	2.75247500	0.14439200
N	6.67143000	1.83373000	0.74547100
H	5.44723200	1.79026500	2.50966500
H	7.97784600	2.60903300	-0.76455800
H	6.49832300	0.87248500	0.40392900
H	6.32647900	4.42961500	2.68591800

H	9.07623100	-3.03479000	-0.55453300
H	7.81497400	4.73337700	0.64535800
O	3.60436000	-1.61937800	0.76191100
C	2.32704100	-1.99670800	2.73299900
H	3.14163800	-2.55619900	3.20091100
H	1.73194400	-1.52370700	3.51912500
H	1.69170500	-2.69725300	2.18330600
C	-2.34808700	-2.55278400	0.83967700
C	-2.82763700	-1.26060800	0.65808300
C	-1.97678600	-0.26045300	0.18624600
C	-0.60934500	-0.51531900	-0.11551200
C	-0.14953800	-1.82308600	0.06951400
C	-1.01752700	-2.80424300	0.54466900
H	-2.99317000	-3.34322200	1.20116700
H	-3.86578300	-1.05170100	0.88645300
C	0.23131900	0.60236300	-0.54888700
H	0.88177100	-2.04859600	-0.16070000
O	-2.38873500	1.01627800	-0.01564900
C	-3.91461500	2.77104400	-0.09495400
C	-3.17310300	3.61955200	-0.88361900
N	-4.96151600	3.52997800	0.30401400
H	-2.24983200	3.42641400	-1.40791500
N	-3.79820300	4.82466900	-0.92219500
N	-4.87871200	4.76464700	-0.20646000
C	-3.73539600	1.33483000	0.27305900
H	-3.95168600	1.16883000	1.33716200
H	-4.41490300	0.70084800	-0.31355000
N	1.48279400	0.59228300	-0.91139100
O	2.09286800	-0.56797300	-0.99682200
H	-0.22025800	1.58831800	-0.52998600
C	-6.07354100	3.16521600	1.17769700
H	-5.69897000	3.04176800	2.19801700
H	-6.74739600	4.02499800	1.16177100
C	-6.75388000	1.90407900	0.69812100

C	-6.88301700	0.80342900	1.54320200
C	-7.22131700	1.81878300	-0.61580900
C	-7.46530600	-0.37810400	1.08801300
H	-6.51724300	0.85739700	2.56514700
C	-7.80271300	0.64715500	-1.08555000
H	-7.11952600	2.67135600	-1.28276700
C	-7.91384400	-0.44176400	-0.22487100
H	-7.55729100	-1.23744800	1.74258500
H	-8.16120900	0.57624100	-2.10621800
N	-0.50619300	-4.15679300	0.73429700
O	0.67719400	-4.36880900	0.51046700
O	-1.28297300	-5.02163300	1.11119800
Br	-8.67793100	-2.05297400	-0.86731200

IN(DZ)

N	-8.99809700	0.69523400	-2.15635000
C	-8.01949000	-0.17127900	-1.51342900
C	-6.68552500	0.57900200	-1.38759100
O	-5.73508900	-0.27328700	-0.80949400
C	-8.41689500	-0.62245100	-0.12640800
O	-8.12253200	-1.69584400	0.35562200
O	-4.05747100	0.24838700	-2.55863700
P	-4.00927500	0.13147900	-1.06461400
C	-3.56472800	2.58827200	0.08034900
O	-3.68986300	-1.26279600	-0.26420400
C	-4.35045400	-2.48992100	-0.58945600
C	-3.47498100	-3.61464800	-0.07467200
H	-9.89131700	0.21536600	-2.24240500
H	-7.85210000	-1.06354600	-2.12519100
H	-6.37296400	0.88559600	-2.39109100
H	-6.82538000	1.48670600	-0.77733700
H	-8.98014400	0.12894800	0.46828600
H	-4.13200900	3.18558100	0.80077200
H	-2.58624300	2.37298200	0.51530600

H	-5.34306400	-2.51680100	-0.12834300
H	-4.48705200	-2.55769200	-1.67444600
H	-3.93838800	-4.58290900	-0.28398500
H	-3.33934800	-3.52176200	1.00722200
H	-2.49129500	-3.58437200	-0.55099700
C	-4.67069300	-0.59431600	3.87012200
N	-5.91599300	-1.17845500	3.94459300
C	-4.49161800	-0.24399800	2.56762900
C	-6.47848000	-1.18714200	2.73595700
N	-5.62873300	-0.62072300	1.88896600
H	-3.66803100	0.22969700	2.05936200
H	-7.44753300	-1.58823600	2.48019800
H	-5.77595200	-0.49133600	0.85186800
H	-4.03729900	-0.48560200	4.73463800
H	-9.16867900	1.51711900	-1.57770300
H	-6.34786300	-1.54852800	4.78287800
O	-4.32407000	1.38156200	-0.04738500
C	-3.44207500	3.33465800	-1.23526300
H	-4.43492600	3.49702200	-1.66697700
H	-2.96596300	4.30458500	-1.07054100
H	-2.84488200	2.76385000	-1.95112600
C	2.06534100	2.59057800	0.94670000
C	2.54917900	1.30988300	0.71953700
C	1.77802500	0.39712100	-0.00613400
C	0.50830200	0.75309800	-0.52137600
C	0.04302500	2.04337000	-0.29389800
C	0.82128700	2.93418900	0.43791100
H	2.64070900	3.31162100	1.51379000
H	3.51873400	1.03578500	1.11685000
C	-0.22543900	-0.24294800	-1.32399400
H	-0.90802300	2.35718100	-0.70097000
O	2.17115700	-0.87160200	-0.25588300
C	3.64749800	-2.67282500	-0.28642200
C	2.96570600	-3.44623500	-1.19655100

N	4.64538100	-3.47894800	0.14332600
H	2.09220500	-3.20042500	-1.78029400
N	3.57715000	-4.65682900	-1.27215900
N	4.59246700	-4.67005400	-0.46489100
C	3.45918200	-1.26821100	0.18227900
H	3.52564900	-1.20636300	1.27683200
H	4.22662000	-0.60923400	-0.24579600
N	-1.48718900	-0.37992100	-1.49908400
O	-2.26904300	0.51006100	-0.83456700
H	0.37235000	-0.98672500	-1.84287100
C	5.68882800	-3.19401300	1.12334800
H	5.23154500	-3.08997400	2.11145100
H	6.32491000	-4.08222600	1.13360700
C	6.46667100	-1.95185700	0.75483700
C	6.62527700	-0.91635700	1.67390800
C	7.01951400	-1.82740000	-0.52251200
C	7.33455000	0.23410300	1.33300200
H	6.19193500	-1.00092500	2.66687300
C	7.72566800	-0.68486700	-0.87880700
H	6.89223700	-2.62724400	-1.24773100
C	7.87638800	0.33412900	0.05820400
H	7.45998900	1.03882600	2.04837900
H	8.15619400	-0.58467300	-1.86868800
N	0.30836800	4.27674300	0.68254600
O	-0.82923600	4.53329700	0.31881800
O	1.03839300	5.07866500	1.24257200
Br	8.84881900	1.88883000	-0.41941600

TS2(DZ)

N	-8.79608000	0.89542900	-2.32053400
C	-7.86937600	-0.06172400	-1.73241800
C	-6.63578700	0.68774100	-1.20742800
O	-5.72404100	-0.23391500	-0.66117000
C	-8.44858600	-0.85124300	-0.57751500

O	-8.15116600	-1.99573400	-0.31375700
O	-3.99227300	0.21209100	-2.40070100
P	-3.86584600	0.12947400	-0.91460400
C	-3.44486200	2.58926100	0.16953800
O	-3.66696000	-1.26486700	-0.10917500
C	-4.31462600	-2.46870400	-0.54794700
C	-3.34511200	-3.61116600	-0.32516600
H	-9.61022100	0.41231700	-2.69397200
H	-7.53200400	-0.77258100	-2.49323100
H	-6.17562700	1.21817000	-2.04531000
H	-6.93811400	1.42795700	-0.44932900
H	-9.15643600	-0.28511200	0.06718600
H	-3.99614000	3.19304800	0.89551400
H	-2.45231200	2.38773900	0.57721500
H	-5.23907900	-2.60400100	0.02278400
H	-4.58455100	-2.37740700	-1.60418600
H	-3.79624900	-4.55654000	-0.63934000
H	-3.07969300	-3.68809200	0.73287900
H	-2.43120400	-3.44483400	-0.90168100
C	-5.80718800	-0.23381700	3.96708900
N	-6.76879000	-1.18638400	3.72299300
C	-5.38863000	0.19522600	2.74257400
C	-6.92068700	-1.32234300	2.39886900
N	-6.09449300	-0.49218100	1.78164200
H	-4.64629200	0.92811100	2.47066200
H	-7.61166700	-1.99853500	1.91744000
H	-5.92844600	-0.38006400	0.58223100
H	-5.51685600	0.04389500	4.96682000
H	-9.14404600	1.52967800	-1.60186400
H	-7.28451400	-1.70416400	4.42349000
O	-4.19849900	1.36827000	0.09038900
C	-3.37281900	3.30485100	-1.16618500
H	-4.38068700	3.45981500	-1.56347200
H	-2.88970100	4.27658200	-1.03922800

H	-2.80221100	2.71935500	-1.89246100
C	2.19319400	2.57864500	0.89988800
C	2.66959000	1.28817000	0.71807200
C	1.88752700	0.35011700	0.03650000
C	0.61333300	0.69242300	-0.47589900
C	0.15734600	1.99399900	-0.29865200
C	0.94618900	2.90912400	0.38912900
H	2.77752800	3.31778300	1.43333400
H	3.64207200	1.02617800	1.11577200
C	-0.13847100	-0.33267600	-1.22340700
H	-0.79514200	2.29761700	-0.70919400
O	2.27355200	-0.92788400	-0.16968300
C	3.75856800	-2.72574500	-0.16062100
C	3.07466000	-3.53039500	-1.04141500
N	4.76366200	-3.51349400	0.28730500
H	2.19649700	-3.30784500	-1.62744800
N	3.69139300	-4.73999300	-1.08321900
N	4.71224200	-4.72310400	-0.28282800
C	3.56905800	-1.30705700	0.26326300
H	3.65031300	-1.20765000	1.35380900
H	4.32697400	-0.65985500	-0.19787500
N	-1.40235000	-0.47097600	-1.36810800
O	-2.15842800	0.46172500	-0.71288100
H	0.44430700	-1.10110900	-1.72284300
C	5.81393600	-3.19343400	1.24958800
H	5.36585700	-3.07012500	2.23960200
H	6.46039200	-4.07376000	1.27450100
C	6.57094600	-1.95094900	0.84057300
C	6.71487500	-0.88396000	1.72553600
C	7.10772600	-1.85351500	-0.44595100
C	7.38851700	0.27344200	1.33900000
H	6.29450200	-0.94658200	2.72554200
C	7.77899600	-0.70492400	-0.84754800
H	6.99202700	-2.67915900	-1.14366600

C	7.91043900	0.34810100	0.05416900
H	7.49845500	1.10522900	2.02537300
H	8.19393100	-0.62537900	-1.84590500
N	0.43941900	4.26192100	0.58638000
O	-0.69748300	4.50919800	0.21416400
O	1.17309300	5.07941800	1.11745700
Br	8.81846000	1.92101700	-0.48852800

C2(DZ)

N	-10.13305100	-0.34777000	-0.93772800
C	-8.69765400	-0.60980200	-0.88513300
C	-7.96098200	0.69591100	-0.55307100
O	-6.56510800	0.54395700	-0.59315600
C	-8.33627100	-1.65251500	0.15092200
O	-7.59669900	-2.59243900	-0.04040000
O	-3.94262900	0.19720700	-3.03765200
P	-3.53547700	0.47087000	-1.64971400
C	-3.94762900	2.19314400	0.30881200
O	-3.89742400	-0.62264200	-0.56352900
C	-4.66530800	-1.80197100	-0.91509800
C	-3.76600700	-2.86127200	-1.51369900
H	-10.63980600	-1.20215300	-1.15925600
H	-8.35074100	-0.96703300	-1.86027800
H	-8.25900900	1.44195100	-1.29636700
H	-8.29464300	1.05610500	0.43389500
H	-8.81207100	-1.49828400	1.14396300
H	-4.21007600	1.30018600	0.88368800
H	-2.91987800	2.48654700	0.54602300
H	-5.10917500	-2.12671900	0.02651100
H	-5.47402400	-1.51073100	-1.58684600
H	-4.34788700	-3.76660200	-1.70999400
H	-2.95205800	-3.10881000	-0.82713800
H	-3.33418200	-2.51050600	-2.45469500
C	-5.71691900	-0.13654200	4.20736400

N	-5.91685600	-1.45915300	3.90077000
C	-5.88531200	0.53532100	3.02775900
C	-6.19274100	-1.54556300	2.58112900
N	-6.18016400	-0.35317400	2.01816800
H	-5.81979000	1.59860100	2.84541700
H	-6.41183000	-2.47834800	2.07927200
H	-6.29519500	0.16361400	0.27878800
H	-5.48245600	0.19190400	5.20710200
H	-10.46602600	-0.04707600	-0.02186900
H	-5.87096100	-2.23459300	4.54810100
O	-4.00348100	1.87495500	-1.10091900
C	-4.92971300	3.31397300	0.56077800
H	-4.88113600	3.62207900	1.60915000
H	-4.69407000	4.18011100	-0.06312700
H	-5.94170200	2.96990800	0.33186200
C	2.41733500	2.64794100	0.47208700
C	2.87574800	1.34372400	0.36858000
C	2.07756900	0.37204000	-0.24389700
C	0.79602800	0.69593200	-0.76099700
C	0.35627700	2.01482200	-0.65532800
C	1.16687600	2.95936100	-0.04198000
H	3.01811100	3.41297100	0.94817300
H	3.84994600	1.09575500	0.77051800
C	0.03451300	-0.39409200	-1.39402500
H	-0.60023000	2.31871200	-1.05052600
O	2.45599900	-0.91505500	-0.37225700
C	3.91762400	-2.72953700	-0.23117500
C	3.30148800	-3.55493300	-1.14252000
N	4.84800600	-3.52176000	0.34955600
H	2.49527500	-3.33774500	-1.82620000
N	3.88139800	-4.78088400	-1.06872200
N	4.81707300	-4.75419300	-0.17033500
C	3.73787700	-1.28786500	0.11024500
H	3.79421100	-1.12854400	1.19479900

H	4.51499800	-0.67781800	-0.36914900
N	-1.19968100	-0.49076700	-1.71033200
O	-1.92685800	0.66774000	-1.40570600
H	0.58722800	-1.29882600	-1.62721300
C	5.79880000	-3.18504900	1.40490100
H	5.25074600	-3.01249600	2.33600800
H	6.41690800	-4.07708100	1.53220800
C	6.62601900	-1.97488900	1.03683300
C	6.71242200	-0.88907200	1.90631000
C	7.29355800	-1.92725400	-0.18952400
C	7.45974700	0.23682900	1.56559000
H	6.19003300	-0.91343200	2.85901300
C	8.04037200	-0.81014400	-0.54502800
H	7.22412600	-2.76701100	-0.87654900
C	8.11442800	0.26138300	0.34100200
H	7.52592800	1.08210000	2.24116100
H	8.55910300	-0.76975500	-1.49618200
N	0.67469100	4.32947100	0.07222300
O	-0.45408100	4.56968900	-0.32444400
O	1.41764300	5.16366300	0.56212400
Br	9.13042300	1.78690600	-0.13820800

EE

C	4.07346300	-0.86662900	-0.97279100
C	2.81296900	-1.44670700	-0.81806200
C	1.87947100	-0.94894200	0.07773500
C	2.16995600	0.18941900	0.87027600
C	3.44127000	0.75716800	0.70316900
C	4.38028100	0.25136700	-0.19691500
H	4.77875000	-1.28574500	-1.67970600
H	2.53964600	-2.32226800	-1.40023100
C	1.27727300	0.79467800	1.85129000
H	3.71902400	1.62801800	1.29106900
H	1.68402000	1.60893900	2.46122300

O	0.67952800	-1.62618800	0.18920600
N	0.03587500	0.43726400	2.02784300
O	-0.63514200	1.07687700	2.94278000
C	-1.61643000	-1.80550400	-0.34156700
C	-1.98139600	-3.06708700	-0.76080000
N	-2.68558000	-1.39083300	0.38071400
H	-1.42194100	-3.76826900	-1.36291600
N	-3.22103100	-3.34490800	-0.29201600
N	-3.64405100	-2.31965700	0.39185200
C	-0.36442600	-1.02491600	-0.57076300
H	-0.10358100	-1.06365700	-1.63659100
H	-0.49895100	0.01636300	-0.26825100
C	-2.92307500	-0.10825100	1.04461500
H	-3.90079900	-0.22597700	1.52047900
H	-2.16560600	0.06384600	1.81577500
C	-2.94012000	1.04109700	0.06065800
C	-3.63640600	0.94204200	-1.14644800
C	-2.26155500	2.22020800	0.37393100
C	-3.65870800	2.01532600	-2.03243200
H	-4.15896000	0.01940000	-1.39091200
C	-2.29117900	3.29610700	-0.51260000
H	-1.70384100	2.26478400	1.30780100
C	-2.98706800	3.19629700	-1.71542300
H	-4.20001900	1.93184400	-2.97009500
H	-1.76021400	4.21129100	-0.26746600
H	-3.00357300	4.03327200	-2.40695400
O	5.57096900	0.91613800	-0.24432000
C	6.53820400	0.44368900	-1.16200900
H	6.16447500	0.48812900	-2.19153900
H	7.40102200	1.10193200	-1.06115500
H	6.83609000	-0.58575900	-0.93179000

C1(EE)

N	7.06698800	1.48403700	-2.42466700
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C	5.85067500	1.40193200	-1.63538700
C	5.40396800	-0.07057900	-1.62309200
O	4.25724200	-0.28962100	-0.79525600
C	5.97424000	1.94828200	-0.22125900
O	5.04068900	2.05124200	0.54657600
O	2.77879900	1.41246300	-2.10130900
P	2.78887200	0.13671100	-1.36155900
C	2.11289200	-2.39792400	-1.67246400
O	2.01488600	0.05644100	0.02037400
C	1.34868900	1.25989900	0.48793500
C	0.50278700	0.89546200	1.68262600
H	7.28785700	2.45359200	-2.63599800
H	5.05864800	1.97810000	-2.12479300
H	5.20334000	-0.38301600	-2.65237300
H	6.19348200	-0.70684900	-1.21547600
H	6.99137000	2.26528300	0.08604600
H	3.03362200	-2.97822500	-1.78268100
H	1.88638100	-2.28479300	-0.60874900
H	2.12371100	1.99055000	0.74654600
H	0.73200000	1.64470500	-0.32414300
H	0.05029000	1.80354100	2.09205000
H	1.10417100	0.42324800	2.46824000
H	-0.29550500	0.21199100	1.38126300
C	3.33479600	-1.02016400	3.92747200
N	3.59204200	0.31562400	4.14217200
C	3.60177500	-1.25327200	2.61260200
C	4.00324700	0.88389300	3.00926900
N	4.01433200	-0.05784400	2.07600800
H	3.54115600	-2.15287900	2.02165200
H	4.28362000	1.91556300	2.86631200
H	4.24096600	0.10129500	1.08875500
H	2.99422400	-1.67251700	4.71430800
H	7.85918700	1.10912000	-1.90532100
H	3.49437500	0.80193000	5.02627400

O	2.35210900	-1.09282300	-2.25203000
C	0.94399400	-3.01253700	-2.40794000
H	1.19239400	-3.17856300	-3.46007000
H	0.67897500	-3.97202500	-1.95302300
H	0.09663300	-2.32415100	-2.33599400
C	-5.02710300	3.80798400	0.47162600
C	-5.14140800	2.45414800	0.15334700
C	-4.08464600	1.73592000	-0.38690200
C	-2.83616400	2.35780000	-0.61892500
C	-2.74367500	3.72187100	-0.31464400
C	-3.80936200	4.44331300	0.22504400
H	-5.87569800	4.33692000	0.88786000
H	-6.08531700	1.93788700	0.30617700
C	-1.66496300	1.69757800	-1.19099000
H	-1.80816600	4.24675800	-0.48981400
H	-0.90181900	2.33225900	-1.65574100
O	-4.31825000	0.42430000	-0.75662600
N	-1.46747200	0.41334100	-1.12406600
O	-0.36291000	-0.04586400	-1.64504700
C	-4.61502500	-1.83929500	-0.16599600
C	-5.86563300	-2.41708800	-0.12389300
N	-3.86933300	-2.75112200	-0.83352900
H	-6.77805600	-2.03038200	0.30622600
N	-5.81245600	-3.62197900	-0.74077100
N	-4.59492600	-3.81900900	-1.16340100
C	-4.10831400	-0.51391000	0.29578500
H	-4.67185800	-0.20797800	1.18535100
H	-3.03963600	-0.55837700	0.53596300
C	-2.42989200	-2.73470700	-1.08025500
H	-2.26148400	-3.45343400	-1.88723900
H	-2.14011500	-1.73432100	-1.41615900
C	-1.65218000	-3.10541400	0.16477100
C	-2.02584900	-4.19682100	0.95283300
C	-0.54115300	-2.33915600	0.51958300

C	-1.28763100	-4.52536900	2.08696500
H	-2.89825300	-4.78610900	0.67898300
C	0.19387100	-2.67233600	1.65766800
H	-0.26180000	-1.49031500	-0.10967900
C	-0.17382600	-3.76301700	2.44194000
H	-1.58150200	-5.37570000	2.69492500
H	1.04967600	-2.06103100	1.93237900
H	0.39915700	-4.01759700	3.32873500
O	-3.56425000	5.76049900	0.47879700
C	-4.62378900	6.52170400	1.02600800
H	-4.93793600	6.12467600	1.99822500
H	-4.23685900	7.53228900	1.15492700
H	-5.48697800	6.54426300	0.35100300

TS1(EE)

N	6.67667200	2.06981000	-1.99717300
C	5.66738500	1.67654800	-1.02839100
C	4.65102700	0.76027900	-1.72165500
O	3.63163200	0.43052700	-0.78947300
C	6.21574400	0.96798900	0.19800700
O	5.61671800	0.88202700	1.24855100
O	1.82309100	1.25568200	-2.34530200
P	2.06750900	0.22155700	-1.31572400
C	1.51443600	-2.13512500	-2.61349000
O	1.45051800	0.28566700	0.16097900
C	1.68909900	1.46242500	0.96148100
C	0.76697400	1.38431600	2.15646500
H	7.31227300	2.74959800	-1.58649500
H	5.12459100	2.56286400	-0.68271700
H	4.22869700	1.29878700	-2.57324100
H	5.13334800	-0.15838100	-2.08032100
H	7.21271400	0.49750500	0.07443500
H	2.11255100	-3.04796300	-2.66122600
H	0.52927900	-2.35516400	-2.20630100

H	2.74329800	1.48298500	1.25824700
H	1.48436900	2.35428200	0.35845200
H	0.89337600	2.27058000	2.78441100
H	0.99899300	0.49819000	2.75498100
H	-0.27435700	1.32841300	1.82487500
C	2.90929000	-2.98787200	2.56336600
N	4.01889400	-2.48526300	3.20659900
C	2.73186900	-2.22366100	1.45152800
C	4.50733800	-1.45274800	2.52249400
N	3.73591200	-1.28244800	1.45543100
H	1.99203700	-2.25592800	0.66688200
H	5.36839700	-0.85513400	2.77576200
H	3.87339800	-0.56163100	0.73140200
H	2.35239100	-3.82532000	2.95042800
H	7.24465400	1.26618000	-2.26236200
H	4.41038000	-2.83828300	4.07209700
O	2.22239900	-1.32441000	-1.64910300
C	1.41498200	-1.47496900	-3.97192500
H	2.40480400	-1.17586200	-4.33088500
H	0.98891800	-2.18710200	-4.68499300
H	0.77113200	-0.59706000	-3.91144100
C	-4.03454700	4.17914300	0.84635000
C	-4.44680200	2.96143000	0.30287400
C	-3.54920600	2.07314100	-0.27108000
C	-2.16816200	2.37499900	-0.31166000
C	-1.77142700	3.60335000	0.22869000
C	-2.67683500	4.49652500	0.80460700
H	-4.76563100	4.85016900	1.28035300
H	-5.49905500	2.69099500	0.30604300
C	-1.12803000	1.52840800	-0.90241600
H	-0.72064500	3.88296200	0.21162900
H	-0.16468700	1.99808500	-1.11184400
O	-4.05604600	0.92103400	-0.83979100
N	-1.31434500	0.27330100	-1.16047200

O	-0.31361000	-0.41481900	-1.66286000
C	-4.58499500	-1.37782800	-0.67143000
C	-5.87132800	-1.69056000	-1.05652600
N	-3.85551900	-2.42444800	-1.12939000
H	-6.78097300	-1.12895300	-0.90043000
N	-5.85988600	-2.88052000	-1.70244300
N	-4.63464100	-3.32266300	-1.73442800
C	-4.03924500	-0.19109000	0.05277100
H	-4.67687500	0.02945700	0.91856000
H	-3.01661200	-0.37938900	0.38994000
C	-2.42637400	-2.69953800	-0.97374000
H	-2.26000100	-3.62146700	-1.53817800
H	-1.84107800	-1.89118300	-1.42107300
C	-2.05401500	-2.87780500	0.48166000
C	-2.82284900	-3.69724100	1.31173800
C	-0.94276100	-2.21014900	1.00085500
C	-2.48511700	-3.85484900	2.65247000
H	-3.69311100	-4.20684200	0.90265600
C	-0.61236700	-2.36623300	2.34765000
H	-0.36297100	-1.56048400	0.34372300
C	-1.37751700	-3.18662600	3.17392300
H	-3.08779300	-4.49357400	3.29100400
H	0.24167700	-1.83499300	2.75734700
H	-1.11713600	-3.29996100	4.22199700
O	-2.14002900	5.64908000	1.29528000
C	-3.02606100	6.56438300	1.91139500
H	-3.53371200	6.10857200	2.76910200
H	-2.41319800	7.39830200	2.25264300
H	-3.77609800	6.93085400	1.20120700

IN(EE)

N	6.32991700	2.25785200	-2.38381000
C	5.43373600	2.00449300	-1.26379000
C	4.24352000	1.16750600	-1.75329300

O	3.34479100	0.97927200	-0.69055300
C	6.07646800	1.25569700	-0.11852700
O	5.77805700	1.40456300	1.04757000
O	1.43809700	1.68500100	-2.08674900
P	1.66802400	0.56713700	-1.10942200
C	1.63713400	-2.03077400	-2.09170900
O	1.34106300	0.68659100	0.49575500
C	1.77734700	1.80845100	1.27103000
C	0.83685000	1.92236000	2.45356100
H	7.12873600	2.80890100	-2.07777100
H	5.04606300	2.95123000	-0.87459400
H	3.76328300	1.70924400	-2.57340000
H	4.60140100	0.19942300	-2.13920200
H	6.83647800	0.50154700	-0.41603500
H	2.39919200	-2.81576900	-2.06160300
H	0.79464900	-2.34395800	-1.47020000
H	2.81334000	1.65878400	1.59251600
H	1.75037100	2.71554500	0.65485500
H	1.13406900	2.75622000	3.09573100
H	0.85920000	1.00169400	3.04461800
H	-0.18992700	2.09046900	2.11269800
C	3.22427500	-2.71383000	2.38829900
N	4.42653800	-2.19623900	2.81703000
C	2.81595300	-1.92335600	1.35851200
C	4.74169400	-1.12917900	2.08252700
N	3.77571100	-0.95166700	1.19031200
H	1.93347600	-1.95689800	0.74087100
H	5.61708800	-0.50775300	2.19408600
H	3.72317300	-0.18372100	0.47203400
H	2.77409500	-3.57974800	2.84536800
H	6.70637000	1.37807200	-2.73560600
H	4.99179400	-2.55897300	3.57545800
O	2.28646200	-0.89914600	-1.49922600
C	1.20434800	-1.76859200	-3.52074300

H	2.05799500	-1.43929900	-4.12090300
H	0.80559000	-2.68704000	-3.96254500
H	0.42986100	-0.99963900	-3.54844700
C	-4.62953600	3.81899500	0.65449200
C	-4.77427400	2.54226900	0.11209300
C	-3.68028500	1.79858500	-0.30841300
C	-2.38028200	2.33113300	-0.18646600
C	-2.24587000	3.61442700	0.34661700
C	-3.34863100	4.35845300	0.77283100
H	-5.50829300	4.36960300	0.96770800
H	-5.76252000	2.10678700	-0.00311700
C	-1.13476800	1.66061000	-0.60097200
H	-1.25870900	4.05939700	0.44338500
H	-0.24816600	2.29044700	-0.64762400
O	-3.91595200	0.56647200	-0.88045000
N	-1.11769600	0.41483500	-0.89138600
O	0.04571200	-0.19130300	-1.24544900
C	-4.32203800	-1.75375900	-0.62901500
C	-5.56370300	-2.25647200	-0.95292500
N	-3.46729500	-2.67226400	-1.14091400
H	-6.53900300	-1.84041000	-0.74610900
N	-5.40339600	-3.42545500	-1.61774400
N	-4.12805400	-3.67270600	-1.72208700
C	-3.91076400	-0.50037800	0.06845700
H	-4.63014100	-0.28323000	0.86685000
H	-2.91190800	-0.60379000	0.50605800
C	-2.00948100	-2.72232400	-1.03715200
H	-1.68971600	-3.43326400	-1.80362400
H	-1.61296600	-1.73418500	-1.27582400
C	-1.56857400	-3.16643200	0.34176500
C	-1.99117200	-4.40109000	0.84203800
C	-0.74809700	-2.35019800	1.12298500
C	-1.59382600	-4.82019000	2.10730300
H	-2.63606700	-5.03080600	0.23313700

C	-0.35411700	-2.77130700	2.39492400
H	-0.41806300	-1.38817700	0.73315500
C	-0.77241900	-4.00434200	2.88729100
H	-1.92457600	-5.78198200	2.48695000
H	0.27913800	-2.12895200	3.00078800
H	-0.46431200	-4.32926600	3.87635500
O	-3.07316700	5.58852400	1.28021400
C	-4.16809000	6.35806500	1.74474300
H	-4.69774700	5.84254900	2.55350800
H	-3.74602900	7.28902800	2.12137400
H	-4.87055300	6.57765000	0.93296400

TS2(EE)

N	-6.33550200	2.09081800	2.30291400
C	-5.38789600	1.95487400	1.20604600
C	-4.33633600	0.90222100	1.58191900
O	-3.36853100	0.81067700	0.55826200
C	-6.01464100	1.52774900	-0.10491100
O	-5.59019800	1.83824900	-1.19629500
O	-1.52749300	1.69292600	1.97974600
P	-1.57169200	0.47147100	1.11772400
C	-1.64337300	-1.89658000	2.48500300
O	-1.24164500	0.50310900	-0.47290500
C	-1.63868700	1.60066300	-1.31191000
C	-0.62148800	1.70115200	-2.42941000
H	-7.02704100	2.80399300	2.08249600
H	-4.86871100	2.90444900	1.04175600
H	-3.85729000	1.21418300	2.51331700
H	-4.81383700	-0.07614300	1.74327100
H	-6.89070400	0.85014700	-0.00720800
H	-2.37010000	-2.71289600	2.50491400
H	-0.70286300	-2.27420300	2.08033200
H	-2.64440200	1.41401800	-1.69949900
H	-1.67277400	2.52057100	-0.71727200

H	-0.89795600	2.50706600	-3.11491300
H	-0.58163300	0.76368400	-2.99159900
H	0.37598900	1.90887800	-2.02969000
C	-3.67003800	-2.84517000	-2.23384300
N	-4.64875700	-2.07106200	-2.81114700
C	-3.21463400	-2.13032300	-1.16487900
C	-4.77098700	-0.93366500	-2.11149500
N	-3.91356600	-0.94615300	-1.10357200
H	-2.44509200	-2.36377800	-0.44516600
H	-5.45589900	-0.13289700	-2.34809800
H	-3.67624600	-0.03671600	-0.26446000
H	-3.39228900	-3.80891300	-2.62863300
H	-6.85165800	1.22068600	2.42896600
H	-5.19220400	-2.31154600	-3.63034300
O	-2.21867700	-0.94908200	1.56825700
C	-1.46330900	-1.30504800	3.86907500
H	-2.41302300	-0.90306200	4.23446300
H	-1.12388200	-2.07953800	4.56295600
H	-0.72288900	-0.50196400	3.85112500
C	4.62215100	3.80816000	-0.67912900
C	4.79344600	2.52831800	-0.15250100
C	3.71870400	1.77627600	0.30090300
C	2.41435800	2.30550000	0.23010400
C	2.25210100	3.59074800	-0.28963500
C	3.33575300	4.34309500	-0.74909600
H	5.48679200	4.36521100	-1.01920200
H	5.78720000	2.09695600	-0.07695200
C	1.18788100	1.62649700	0.68452600
H	1.25979100	4.03055800	-0.34884400
H	0.29270400	2.24565800	0.73451900
O	3.97606900	0.53980200	0.85082300
N	1.18815700	0.38979400	1.00782100
O	0.01646400	-0.19904800	1.40509300
C	4.37100500	-1.77626400	0.56228300

C	5.62486200	-2.27013800	0.85003100
N	3.53753200	-2.71005300	1.08086400
H	6.59100400	-1.84136100	0.62702300
N	5.49155400	-3.45052900	1.50085700
N	4.22177800	-3.71296500	1.63067800
C	3.92761500	-0.51893200	-0.10684100
H	4.60858700	-0.29259100	-0.93565900
H	2.90952400	-0.62104200	-0.49927800
C	2.08091200	-2.77626900	1.00085900
H	1.78736400	-3.53869900	1.72765500
H	1.67322200	-1.81223900	1.31053500
C	1.61574700	-3.13717800	-0.39436500
C	2.24045000	-4.17265900	-1.09419200
C	0.55758900	-2.44381200	-0.98439300
C	1.80773700	-4.51804900	-2.37039200
H	3.07030200	-4.70480900	-0.63423300
C	0.12516600	-2.79340500	-2.26443900
H	0.07948700	-1.62784300	-0.44583600
C	0.74707400	-3.82864000	-2.95841400
H	2.29851400	-5.32426600	-2.90695300
H	-0.69729300	-2.24857000	-2.71930300
H	0.41134800	-4.09592100	-3.95571300
O	3.03757100	5.57451200	-1.23797900
C	4.11374600	6.35705900	-1.72507200
H	4.62029400	5.85652500	-2.55763600
H	3.67491700	7.29089900	-2.07438800
H	4.83985200	6.56826300	-0.93222400

C2(EE)

N	4.08044600	4.79508300	0.69758200
C	3.48022000	3.52856400	1.11852000
C	4.19490700	2.37508000	0.42821900
O	3.72587100	1.17166100	0.99063400
C	3.57896500	3.33870700	2.61840700

O	2.63603600	3.25392500	3.37206200
O	1.28809700	2.07514100	-0.71661600
P	1.28498500	0.60131200	-0.67789700
C	2.71841900	-1.52661100	-1.20474000
O	1.11683700	-0.08657900	0.73992800
C	0.98133000	0.68530800	1.95714600
C	-0.45704900	0.61873900	2.42352700
H	3.56904700	5.57450000	1.10610600
H	2.42469200	3.51503800	0.83334600
H	3.99637100	2.43498400	-0.65077200
H	5.28244600	2.48235700	0.58380400
H	4.62005400	3.32880300	3.01175100
H	3.24875400	-1.64633100	-0.25632900
H	1.75035200	-2.03342700	-1.13704500
H	1.66877800	0.23079300	2.67271000
H	1.31368000	1.70770700	1.77495000
H	-0.56514300	1.15271600	3.37208300
H	-0.76439900	-0.42143200	2.57275600
H	-1.12406900	1.07691200	1.68561000
C	6.96921500	-2.07723100	-1.04367200
N	7.07516300	-0.93398600	-1.79523800
C	6.08255000	-1.77256500	-0.04699500
C	6.26890400	0.00162600	-1.24414100
N	5.65163000	-0.47308800	-0.18131800
H	5.72910900	-2.40698200	0.75295100
H	6.16463900	0.99726900	-1.65119100
H	4.31596400	0.46146900	0.63935400
H	7.51963000	-2.97309000	-1.28194400
H	5.03542000	4.86217100	1.04995900
H	7.65371400	-0.80926200	-2.61527200
O	2.49925500	-0.10574400	-1.40372800
C	3.52749900	-2.03965300	-2.37249300
H	3.76081000	-3.09661000	-2.21833100
H	2.96453000	-1.93636100	-3.30384500

H	4.46576900	-1.48579400	-2.46206600
C	-5.36970700	3.13477400	-0.33445400
C	-5.23926500	1.74859500	-0.27825500
C	-4.05109500	1.12040800	-0.62645400
C	-2.95735800	1.89527700	-1.04990300
C	-3.09995400	3.28030000	-1.13547200
C	-4.29164400	3.90900000	-0.76907300
H	-6.31237900	3.58916600	-0.05417200
H	-6.07999000	1.13371200	0.02840600
C	-1.65145800	1.34190300	-1.43418100
H	-2.27360300	3.89594400	-1.47849200
H	-1.01853600	1.95003100	-2.08184000
O	-3.99629500	-0.25229600	-0.62957200
N	-1.22766900	0.21945500	-0.99593300
O	0.06360600	-0.06602200	-1.53915000
C	-4.32680300	-2.24053100	0.59293500
C	-5.44260600	-2.83421900	1.13944900
N	-3.78052400	-3.22346100	-0.15974100
H	-6.18333300	-2.41074100	1.80160700
N	-5.50624800	-4.11824700	0.70817200
N	-4.49356000	-4.34518400	-0.07900200
C	-3.78633300	-0.85339700	0.65240300
H	-4.32076700	-0.29588500	1.42825900
H	-2.71320300	-0.84266800	0.88051200
C	-2.51182500	-3.20384500	-0.88907200
H	-2.65261800	-3.83679700	-1.76790600
H	-2.34149100	-2.17381000	-1.21488900
C	-1.37920200	-3.69964000	-0.01905500
C	-1.26352900	-5.05923300	0.28053100
C	-0.46146400	-2.79596200	0.51479900
C	-0.23786300	-5.50776900	1.10712500
H	-1.98285500	-5.76210300	-0.13197900
C	0.56876800	-3.24521200	1.34086900
H	-0.54459900	-1.73861400	0.27973800

C	0.68061800	-4.60081000	1.63904500
H	-0.15104600	-6.56580900	1.33467200
H	1.28097400	-2.52815900	1.74009200
H	1.48151100	-4.95388400	2.28151700
O	-4.30750500	5.26033500	-0.87749900
C	-5.50506600	5.92925700	-0.51774100
H	-5.75678500	5.74788400	0.53285300
H	-5.31363700	6.99068600	-0.66904300
H	-6.33950300	5.61338200	-1.15325000

EZ

C	2.52595000	1.87012100	-0.32473300
C	1.37106200	1.07101700	-0.34335700
C	1.45281500	-0.29819700	-0.16051500
C	2.70570100	-0.94506900	0.04674400
C	3.84143000	-0.12625200	0.05983700
C	3.75561100	1.25988500	-0.12241500
H	2.42919000	2.93936400	-0.46816500
H	0.41493700	1.55765700	-0.50340500
C	2.73336900	-2.39161600	0.22615300
H	4.80364600	-0.59210900	0.21557900
O	0.35049300	-1.12441000	-0.16740300
C	-1.93324100	-1.57978700	-0.19469600
C	-1.88212300	-2.85900800	0.30962800
N	-3.22629200	-1.42871900	-0.56150500
H	-1.03817100	-3.39540400	0.71575200
N	-3.12347500	-3.40386600	0.22593500
N	-3.93317500	-2.53453600	-0.29762200
C	-0.90171600	-0.50773800	-0.32702300
H	-0.97845400	-0.01402500	-1.30784200
H	-1.05859400	0.26514500	0.44016400
N	3.76001600	-3.18467000	0.45376200
O	4.95121300	-2.68447600	0.55178200
H	1.78211000	-2.90989000	0.16320400

C	-3.86545500	-0.26787600	-1.17483500
H	-3.48581400	-0.15266100	-2.19445500
H	-4.92742000	-0.51913300	-1.23053700
C	-3.62063900	0.98584200	-0.36702500
C	-3.05659500	2.11210100	-0.96444200
C	-3.92538200	1.00829500	0.99654900
C	-2.79810400	3.25420600	-0.20708600
H	-2.80982400	2.09403700	-2.02324900
C	-3.66459800	2.14573900	1.75346800
H	-4.35707300	0.12589800	1.46363400
C	-3.09839000	3.27070600	1.15234500
H	-2.35504700	4.12547800	-0.67908300
H	-3.90029500	2.15508000	2.81298700
H	-2.88905300	4.15604700	1.74440700
O	4.95062300	1.92794300	-0.08458800
C	4.90622900	3.32898000	-0.25692000
H	4.31645900	3.80997400	0.53283800
H	5.93740300	3.67855600	-0.20214800
H	4.48231200	3.59797800	-1.23203600

C1(EZ)

N	-8.36893500	1.33279100	-2.11141000
C	-7.13477900	0.64820300	-1.72851700
C	-7.38323700	-0.84151400	-1.58804000
O	-7.43371100	-1.42764400	-0.52700200
C	-6.63250900	1.27400800	-0.43183600
O	-5.54374200	0.55016700	0.15626600
C	-2.93179900	2.54813800	-0.09598300
C	-2.24581400	3.64431400	-0.87686600
C	-2.46592300	-1.43402600	0.36246400
C	-1.28504200	-1.22381200	1.27911700
O	-3.69714700	1.76076500	-1.04026400
O	-3.34664300	-0.29060700	0.52354400
O	-4.37237900	-0.56616500	-1.87470600

P	-4.17618700	0.29445400	-0.68952100
H	-6.33241300	2.30965700	-0.61391100
H	-7.42655400	1.26076600	0.31876300
H	-8.62242400	1.10998600	-3.07077400
H	-9.14199500	1.03328000	-1.51947300
H	-6.40605300	0.79221700	-2.53166500
H	-7.61482600	-1.36942600	-2.53218900
H	-3.62288600	2.94327600	0.65663000
H	-2.19990400	1.88913000	0.37395800
H	-1.61447700	3.18295000	-1.64070400
H	-2.97376100	4.30692800	-1.35306200
H	-1.61057500	4.23114000	-0.20693800
H	-0.75860100	-0.31589700	0.96985200
H	-1.61018100	-1.13139500	2.32026200
H	-0.60161400	-2.07445400	1.20283300
H	-2.14627000	-1.50356100	-0.67625600
H	-3.04969500	-2.31940300	0.63594700
C	-4.87985500	-1.76878500	2.74641600
N	-5.77970100	-1.80337100	1.70640200
C	-4.89215000	-3.00527900	3.31449300
C	-6.32981700	-3.00777000	1.62763800
N	-5.80173200	-3.75165900	2.59749700
H	-4.34635200	-3.41514500	4.14786400
H	-7.06448100	-3.31620500	0.90088100
H	-6.03967500	-4.72110600	2.77256000
H	-4.31116600	-0.88261200	2.97590400
H	-5.99285700	-1.02703200	1.06738900
C	2.81895000	2.70627900	1.23538800
C	3.51349500	1.57126800	0.78628900
C	2.89281500	0.63118300	-0.01833600
C	1.53369400	0.78291300	-0.41534900
C	0.86506000	1.92203700	0.04468400
C	1.49423800	2.87196900	0.85891800
H	3.33340500	3.42273500	1.86422300

H	4.54849300	1.45293500	1.08807100
C	0.92226200	-0.23679800	-1.26384400
H	-0.16409300	2.06203800	-0.25043200
O	3.52564200	-0.49945900	-0.48186000
C	5.34482100	-1.92021100	-0.78282800
C	4.84148700	-2.66161000	-1.82655800
N	6.48327400	-2.56751600	-0.44543900
H	3.93923000	-2.50462700	-2.39767900
N	5.68729100	-3.69734900	-2.06511000
N	6.68011800	-3.63415000	-1.23063700
C	4.87164200	-0.67113800	-0.11478000
H	4.97516100	-0.75185600	0.97793300
H	5.48009800	0.18611500	-0.43928800
N	-0.31595200	-0.33120000	-1.68605300
O	-1.18069100	0.58548700	-1.34687200
H	1.56342900	-1.04994100	-1.58883600
C	7.43766700	-2.23343500	0.60789000
H	6.96052600	-2.38748100	1.58032100
H	8.24658300	-2.96056700	0.50427400
C	7.93216000	-0.81172000	0.47011500
C	7.80856900	0.08642800	1.52905300
C	8.48671400	-0.38141300	-0.73829600
C	8.23689700	1.40582700	1.38481000
H	7.37023000	-0.24418800	2.46763600
C	8.91146300	0.93495800	-0.88396400
H	8.57415000	-1.08102000	-1.56655900
C	8.78597200	1.83124500	0.17825300
H	8.13510200	2.10006000	2.21294100
H	9.33861200	1.26428700	-1.82598300
H	9.11451600	2.85930800	0.06264400
O	0.71074900	3.93135500	1.23100900
C	1.31124600	4.92010200	2.04244600
H	2.16430800	5.38751600	1.53615100
H	0.54418400	5.67201000	2.22759500

H	1.64908400	4.50059900	2.99761100
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TS1(EZ)

N	-7.65937800	2.81047600	-1.16069400
C	-6.76859500	1.66110300	-1.12651500
C	-5.92380700	1.74544400	0.15906000
O	-5.06362100	0.62992100	0.31254800
C	-7.47310000	0.31982600	-1.17597600
O	-6.91463600	-0.72692200	-1.42990800
O	-3.79992700	1.21996700	-1.80173700
P	-3.56179700	0.67194200	-0.44679600
C	-2.06392700	1.07455200	1.69380400
O	-3.31497000	-0.87592100	-0.13199600
C	-3.26055800	-1.77395000	-1.26418000
C	-2.78792300	-3.11671100	-0.75934700
H	-8.13444700	2.86102100	-2.05853900
H	-6.07286200	1.70152100	-1.96926600
H	-5.35903500	2.68326300	0.13308300
H	-6.57953300	1.76754200	1.03629300
H	-8.55824200	0.33584700	-0.94235200
H	-2.69923200	0.39426900	2.27306200
H	-1.22908800	0.51252100	1.26845200
H	-4.26731500	-1.83215700	-1.69713200
H	-2.56723300	-1.35615000	-1.99465800
H	-2.72302900	-3.82262600	-1.59215900
H	-3.47470100	-3.52725200	-0.01195000
H	-1.79734400	-2.99768500	-0.31521600
C	-5.49807800	-3.80782800	2.13077900
N	-6.31134200	-4.08470000	1.05420500
C	-5.13464100	-2.50205800	2.00659700
C	-6.44801200	-2.99384500	0.30081300
N	-5.74068900	-2.02630000	0.86839000
H	-4.50018500	-1.88015600	2.61622600
H	-7.02786300	-2.90076700	-0.60379900

H	-5.61739900	-1.06838000	0.49857700
H	-5.25614300	-4.55146600	2.87170900
H	-8.38729300	2.71680100	-0.45332600
H	-6.74961100	-4.97716400	0.85773000
O	-2.83481400	1.62257000	0.60969800
C	-1.58990900	2.23407300	2.54276700
H	-2.44058700	2.78296400	2.95636400
H	-0.98114200	1.86063200	3.37108400
H	-0.98211400	2.92045500	1.94566600
C	2.85106300	3.12482500	0.54622600
C	3.48804500	1.88114900	0.42421000
C	2.77144900	0.75261500	0.06035500
C	1.37801700	0.82429400	-0.20935100
C	0.76827000	2.07638400	-0.09755400
C	1.48946300	3.21186300	0.29126300
H	3.43719000	3.98829100	0.83686900
H	4.55273200	1.82813300	0.62322500
C	0.65755200	-0.41526000	-0.52153100
H	-0.28961600	2.16021700	-0.30849700
O	3.33823800	-0.49318900	-0.06146900
C	5.08827800	-2.02431600	-0.04946600
C	4.43541000	-3.06178200	-0.67405700
N	6.26290800	-2.56870900	0.34065600
H	3.45922900	-3.07154200	-1.13432400
N	5.23645500	-4.15835900	-0.63460800
N	6.34081300	-3.85427900	-0.02381800
C	4.71922200	-0.59649400	0.18460200
H	4.96034100	-0.29728000	1.21615900
H	5.28767100	0.06054600	-0.49036600
N	-0.58213500	-0.57981500	-0.88633100
O	-1.31072300	0.49384600	-1.11301400
H	1.20878100	-1.34179100	-0.39366400
C	7.36335600	-1.92682300	1.05267700
H	7.02881200	-1.66780000	2.06181800

H	8.14012100	-2.69091500	1.13515200
C	7.84952600	-0.69959200	0.31566100
C	7.92751400	0.53180400	0.96414200
C	8.18958600	-0.79000400	-1.03685200
C	8.34607000	1.66636600	0.26908600
H	7.65348000	0.60641700	2.01367800
C	8.60303700	0.34156900	-1.73148100
H	8.11740200	-1.74942700	-1.54456000
C	8.68121800	1.57260800	-1.07893400
H	8.40189600	2.62224800	0.78039500
H	8.86250500	0.26561400	-2.78276900
H	8.99925700	2.45616800	-1.62339500
O	0.75338000	4.36050300	0.39588500
C	1.43601100	5.52456600	0.81682500
H	2.22375700	5.80284200	0.10666400
H	0.69015700	6.31827200	0.85982500
H	1.88057500	5.38718600	1.80948500

IN(EZ)

N	-8.20563300	0.67138900	-1.80994300
C	-7.17857900	-0.24056000	-1.32355500
C	-5.85693700	0.52515000	-1.16434900
O	-4.86125000	-0.36182200	-0.73392100
C	-7.50034800	-0.86680100	0.01356900
O	-7.17263400	-1.98650300	0.34469700
O	-3.27322700	0.41289000	-2.47200600
P	-3.15171900	0.13466500	-1.00247000
C	-2.73878600	2.43763100	0.43888400
O	-2.76222100	-1.33226300	-0.38325400
C	-3.39563000	-2.53157100	-0.83782900
C	-2.42748100	-3.67067300	-0.58845100
H	-9.08916600	0.17898000	-1.92133100
H	-7.02181300	-1.04602000	-2.04776500
H	-5.59810400	0.95857800	-2.13617400

H	-5.99067300	1.34961400	-0.44434800
H	-8.03824100	-0.20184300	0.72409200
H	-3.24531800	2.88131300	1.30149700
H	-1.71457400	2.19314700	0.72825000
H	-4.33744900	-2.68463800	-0.30005200
H	-3.63432400	-2.44239100	-1.90333200
H	-2.86408900	-4.61858800	-0.91570200
H	-2.19576700	-3.74549000	0.47819200
H	-1.49488500	-3.50481600	-1.13458200
C	-3.61051400	-1.15967100	3.83442500
N	-4.84886300	-1.76017700	3.89417400
C	-3.48204700	-0.67731700	2.56865000
C	-5.45504300	-1.65187600	2.71155500
N	-4.64090100	-0.99436400	1.89633100
H	-2.67989800	-0.14969300	2.07968000
H	-6.42908100	-2.03792900	2.45135300
H	-4.82670500	-0.75805600	0.88204300
H	-2.94723700	-1.13234600	4.68262600
H	-8.37224900	1.40561900	-1.12245200
H	-5.24607100	-2.22029900	4.70446800
O	-3.47761600	1.24169100	0.16982000
C	-2.76791900	3.39529100	-0.73851100
H	-3.79839600	3.67680300	-0.97653200
H	-2.20078100	4.30045400	-0.49999800
H	-2.32748000	2.92605000	-1.62298700
C	2.65535400	3.16137400	0.68628400
C	3.25118100	1.90797300	0.50460600
C	2.57789100	0.90190700	-0.17658300
C	1.28413700	1.13329000	-0.68982200
C	0.71188400	2.38746600	-0.51105400
C	1.38421000	3.40273800	0.17567700
H	3.20280800	3.92573800	1.22461300
H	4.24374600	1.74461900	0.90927200
C	0.62348400	0.06266300	-1.46381400

H	-0.26856200	2.59437500	-0.92031000
O	3.08388800	-0.35225200	-0.38765900
C	4.74901500	-1.97962100	-0.37419000
C	4.16713300	-2.84900800	-1.26765200
N	5.81844900	-2.66238900	0.09350200
H	3.28056000	-2.71528600	-1.86845100
N	4.90373500	-3.98966700	-1.29725700
N	5.90232300	-3.87053200	-0.47637000
C	4.40507900	-0.58858300	0.04499600
H	4.48241100	-0.48003300	1.13655400
H	5.09707100	0.13381200	-0.41149700
N	-0.62282400	-0.21700600	-1.56251400
O	-1.44058500	0.56259600	-0.79847700
H	1.26794800	-0.59631900	-2.04071400
C	6.80991600	-2.23288400	1.07589600
H	6.32577900	-2.14502600	2.05299500
H	7.53688900	-3.04706000	1.12622300
C	7.45082100	-0.92488900	0.67214300
C	7.43369900	0.16909100	1.53607700
C	8.03546200	-0.79811400	-0.59100700
C	7.99786500	1.38274400	1.14351200
H	6.97258000	0.07422400	2.51625800
C	8.59547700	0.41258300	-0.98419200
H	8.03998800	-1.65028400	-1.26696900
C	8.57637100	1.50572600	-0.11688900
H	7.97861100	2.23104700	1.82030900
H	9.04554000	0.50649200	-1.96747300
H	9.00992400	2.45142800	-0.42674700
O	0.71154400	4.58295400	0.28744800
C	1.36329900	5.63471000	0.97490200
H	0.67820400	6.48163400	0.95471800
H	1.57299800	5.35912000	2.01480400
H	2.30042900	5.91138400	0.47819800

TS2(EZ)

N	-8.05811700	0.92231300	-1.86214900
C	-7.07673100	-0.07615600	-1.45935500
C	-5.81740800	0.63344200	-0.94101700
O	-4.85117500	-0.32367700	-0.58320900
C	-7.55595800	-1.00458100	-0.36444200
O	-7.24265700	-2.17119000	-0.26948000
O	-3.24344900	0.38303600	-2.35185600
P	-3.02478400	0.14622900	-0.89164700
C	-2.61512100	2.45369300	0.50347200
O	-2.72706300	-1.32323200	-0.26616600
C	-3.34713100	-2.49670300	-0.81050800
C	-2.34277900	-3.62618700	-0.70944500
H	-8.89475300	0.46762000	-2.22094700
H	-6.79023100	-0.68686900	-2.32111400
H	-5.43255800	1.27552000	-1.73853000
H	-6.07193800	1.26870200	-0.07707100
H	-8.20074700	-0.52572500	0.40505900
H	-3.09936900	2.90107700	1.37608300
H	-1.58266900	2.21356100	0.76378200
H	-4.25969600	-2.71730900	-0.24721300
H	-3.63242500	-2.31236900	-1.85081300
H	-2.77176800	-4.55068000	-1.10617900
H	-2.06014600	-3.79494700	0.33353200
H	-1.44238900	-3.38057400	-1.27860600
C	-4.52823300	-0.97192300	3.99030900
N	-5.52587600	-1.87501600	3.70592200
C	-4.21707400	-0.37438100	2.80509700
C	-5.80291300	-1.82039200	2.39666400
N	-5.02269500	-0.91389700	1.82865500
H	-3.48956200	0.38602900	2.57041200
H	-6.54626500	-2.41931900	1.89102300
H	-4.96069300	-0.63899800	0.65746800
H	-4.13940800	-0.84284400	4.98681700

H	-8.35407900	1.46753700	-1.05294600
H	-5.98312700	-2.48545800	4.37141900
O	-3.35781300	1.24680900	0.26981500
C	-2.68618300	3.39607900	-0.68336700
H	-3.72495400	3.66611300	-0.89593600
H	-2.11961000	4.30741800	-0.46906300
H	-2.26508600	2.92396500	-1.57592400
C	2.76835900	3.15992600	0.60613000
C	3.35470400	1.89836600	0.45651700
C	2.67046700	0.87763000	-0.19182100
C	1.37480400	1.10435300	-0.70101900
C	0.81148800	2.36699400	-0.55541400
C	1.49518700	3.39648500	0.09753700
H	3.32399600	3.93523900	1.11987800
H	4.34871500	1.74014900	0.85949700
C	0.70148700	0.01471900	-1.43670800
H	-0.17003700	2.57110600	-0.96362800
O	3.16640000	-0.38451300	-0.37207900
C	4.82316400	-2.02148000	-0.31724500
C	4.24241200	-2.90712500	-1.19529600
N	5.88512900	-2.69994900	0.17330500
H	3.36148100	-2.78171600	-1.80608100
N	4.97213700	-4.05260800	-1.19388400
N	5.96527400	-3.92108200	-0.36841700
C	4.48612200	-0.61903500	0.06770300
H	4.56205200	-0.48396500	1.15630000
H	5.18262800	0.08800900	-0.40549400
N	-0.54504200	-0.26674800	-1.50648400
O	-1.34081300	0.54669000	-0.73960100
H	1.33391600	-0.66130100	-2.00712600
C	6.86992000	-2.25685100	1.15675000
H	6.37935000	-2.15754000	2.12953600
H	7.59753100	-3.06936500	1.22196800
C	7.51184400	-0.95308600	0.74130200

C	7.48109600	0.15326700	1.58912300
C	8.11004500	-0.84226200	-0.51692500
C	8.04456500	1.36349400	1.18519100
H	7.00962000	0.07063600	2.56549500
C	8.66934100	0.36506200	-0.92157500
H	8.12528300	-1.70400000	-1.18045900
C	8.63617700	1.47065100	-0.07056100
H	8.01485800	2.22131600	1.84950200
H	9.12965500	0.44670900	-1.90120900
H	9.06901900	2.41364900	-0.38948800
O	0.83120600	4.58321900	0.18168100
C	1.50086900	5.65351700	0.82232000
H	0.82245000	6.50492200	0.78014800
H	1.72114700	5.41364300	1.86876900
H	2.43369200	5.90328700	0.30388400

C2(EZ)

N	-9.09936200	-0.69254500	-1.13377100
C	-7.64754700	-0.82198100	-1.03752500
C	-7.06269000	0.47788100	-0.46837700
O	-5.65785200	0.46728800	-0.45742300
C	-7.23365400	-1.97547400	-0.14851500
O	-6.42999500	-2.83117800	-0.44664600
O	-3.06563900	0.73766200	-2.91170600
P	-2.65058100	0.81957600	-1.50091500
C	-3.20936800	2.14323800	0.71443900
O	-2.90427600	-0.46154000	-0.60415500
C	-3.57969400	-1.62735500	-1.13847400
C	-2.61079000	-2.50835400	-1.89625800
H	-9.50484800	-1.54580700	-1.51256400
H	-7.22524500	-0.98998800	-2.03367200
H	-7.40553100	1.30233400	-1.10113900
H	-7.46878000	0.64228900	0.54326200
H	-7.74009000	-1.99368600	0.84126900

H	-3.41851600	1.15007600	1.12250500
H	-2.20546500	2.45309600	1.02145500
H	-3.98723600	-2.13014500	-0.26060100
H	-4.41620700	-1.30085700	-1.75776200
H	-3.12511600	-3.41804000	-2.22031700
H	-1.76621100	-2.78990700	-1.26192200
H	-2.22642200	-1.98894100	-2.77794100
C	-4.84568400	-0.90427000	4.18837600
N	-4.94036600	-2.17717200	3.68450300
C	-5.04943000	-0.07785900	3.11754200
C	-5.19172600	-2.08567800	2.36037400
N	-5.26337800	-0.82462100	1.98088900
H	-5.06259500	1.00265200	3.09599900
H	-5.33236200	-2.94611200	1.71984100
H	-5.38091400	-0.03584000	0.34718200
H	-4.64953900	-0.71234900	5.23095400
H	-9.50110400	-0.57345000	-0.20391400
H	-4.84408500	-3.03589800	4.20978000
O	-3.22963900	2.07077900	-0.72920400
C	-4.26567900	3.13832400	1.13633300
H	-4.24475700	3.26373500	2.22270500
H	-4.08615400	4.11267800	0.67437100
H	-5.25050400	2.77309300	0.83384100
C	3.27932000	3.20256000	0.50031800
C	3.73852500	1.88681300	0.40413300
C	2.96559500	0.91683500	-0.22087600
C	1.70180400	1.25506500	-0.75860500
C	1.25911200	2.57282200	-0.65673300
C	2.04057800	3.54821100	-0.03193900
H	3.90540000	3.93663200	0.99317900
H	4.70698600	1.64484600	0.82654700
C	0.96681100	0.18598100	-1.45402500
H	0.30640300	2.87033600	-1.07314100
O	3.34184300	-0.38970000	-0.34737400

C	4.84594600	-2.16910300	-0.22261800
C	4.19825200	-3.02436300	-1.08366000
N	5.84310500	-2.92314600	0.29486300
H	3.33855500	-2.83970800	-1.70925900
N	4.82590600	-4.22796900	-1.04541400
N	5.82067500	-4.16054900	-0.21448900
C	4.62958100	-0.73216600	0.12139200
H	4.69809400	-0.57493100	1.20701800
H	5.39384000	-0.10365000	-0.35766700
N	-0.27371700	0.04063200	-1.72109800
O	-1.06013600	1.10577000	-1.24392000
H	1.55767700	-0.65591700	-1.80481000
C	6.85409300	-2.54577900	1.28061400
H	6.37213400	-2.42851600	2.25562700
H	7.53447100	-3.39888700	1.33480800
C	7.56596400	-1.27567900	0.87628600
C	7.57845400	-0.17123800	1.72728800
C	8.17906200	-1.18863300	-0.37647100
C	8.19595300	1.01456700	1.33045100
H	7.09560600	-0.23500500	2.69952200
C	8.79308300	-0.00556400	-0.77391400
H	8.16182300	-2.04829500	-1.04252900
C	8.80031500	1.09898300	0.07904800
H	8.19817900	1.87133700	1.99672400
H	9.26429900	0.05801100	-1.74969600
H	9.27547900	2.02326300	-0.23432800
O	1.50421300	4.79788000	0.00333900
C	2.27561900	5.81547300	0.61576200
H	1.68674300	6.72888600	0.54052700
H	2.46357700	5.58860000	1.67130200
H	3.23209200	5.95276800	0.09867900
FE			
C	-4.79088500	-0.77541100	-1.25709600

C	-3.90579800	0.30442900	-1.26057600
C	-3.00082300	0.51639800	-0.23205200
C	-2.93638200	-0.37217600	0.86976000
C	-3.82833300	-1.45349000	0.85327900
C	-4.73962500	-1.66278100	-0.18226200
H	-5.48893100	-0.90373300	-2.07505000
H	-3.91789800	1.01751000	-2.08011300
C	-2.05276800	-0.24126500	2.02214500
H	-3.82415300	-2.16209800	1.67733000
H	-2.17507700	-0.97025900	2.83081700
O	-2.20013900	1.64091900	-0.31065400
N	-1.14010500	0.68087200	2.13920800
O	-0.43527700	0.67597200	3.23586600
C	-0.10943800	2.62782400	-0.80675800
C	-0.17761700	3.70553900	-1.66358000
N	0.85606900	2.98607100	0.07474800
H	-0.82221900	3.85110900	-2.51830200
N	0.72898300	4.63369800	-1.27646400
N	1.35760500	4.18633000	-0.22699900
C	-0.88589800	1.35230000	-0.77835200
H	-0.94623100	0.94479400	-1.79571700
H	-0.40412300	0.62131400	-0.12335300
C	1.43019900	2.23340100	1.18892100
H	2.11318200	2.93766100	1.67230200
H	0.64931700	1.94578100	1.89894000
C	2.18115900	1.00916500	0.71333100
C	3.06086600	1.08464500	-0.36862500
C	2.01150900	-0.20393400	1.38250900
C	3.77883500	-0.03421400	-0.77810700
H	3.19024600	2.02739300	-0.89555200
C	2.72919400	-1.33062600	0.98526700
H	1.30394200	-0.24966600	2.20952900
C	3.60576700	-1.22966000	-0.08781900
H	4.46484800	0.02049100	-1.61611100

H	2.60521600	-2.27772100	1.49894300
O	-5.54182400	-2.75883900	-0.05199200
C	-6.47716400	-3.00041500	-1.08544000
H	-5.97593700	-3.15583800	-2.04777300
H	-7.01396400	-3.90654000	-0.80536700
H	-7.18742500	-2.17094400	-1.18043700
Br	4.59635600	-2.76059600	-0.61990200

C1(FE)

N	-6.84804300	-2.78335300	-2.14134100
C	-5.45583800	-2.59621400	-1.73624700
C	-5.20327300	-1.09264000	-1.64136700
O	-3.98995800	-0.75705200	-0.95031900
C	-5.18008300	-3.33345700	-0.43927300
O	-4.99804700	-2.80675600	0.63939500
O	-2.51897800	-2.77937900	-1.71559600
P	-2.55858200	-1.32803900	-1.44499000
C	-2.17080500	0.97659700	-2.66784600
O	-1.70180900	-0.81362100	-0.21109700
C	-0.84891700	-1.78914600	0.45329300
C	-0.05898200	-1.07449500	1.52125600
H	-7.00876200	-3.73610100	-2.45822800
H	-4.81697600	-3.04254200	-2.50281300
H	-5.19552900	-0.65621900	-2.64458800
H	-5.99885900	-0.61903200	-1.06127700
H	-5.23904000	-4.43509500	-0.51605200
H	-3.13479800	1.34618200	-3.02872000
H	-2.03980000	1.29294600	-1.62935600
H	-1.49686200	-2.56150000	0.88068400
H	-0.18865500	-2.22655700	-0.29581600
H	0.52279800	-1.80911200	2.08612000
H	-0.71976800	-0.54523000	2.21716800
H	0.63309900	-0.36064500	1.06691600
C	-3.04139800	0.77378200	3.38937000

N	-3.12978100	-0.50683700	3.88831900
C	-3.51903500	0.72027500	2.11442600
C	-3.63830800	-1.31709500	2.96052900
N	-3.87885800	-0.58478200	1.88226500
H	-3.64024400	1.49060800	1.36952400
H	-3.82246500	-2.37539800	3.05969300
H	-4.23610300	-0.97053300	1.00128700
H	-2.64750500	1.59400000	3.96673500
H	-7.47710500	-2.61457100	-1.35804100
H	-2.85347100	-0.79915200	4.81884500
O	-2.21466600	-0.47066700	-2.72901800
C	-1.01525900	1.43870200	-3.52651500
H	-1.19319100	1.18846000	-4.57635200
H	-0.89921900	2.52370200	-3.44038300
H	-0.10390900	0.93867600	-3.18356300
C	5.88559300	-3.02056300	1.22515300
C	5.74778700	-1.78038300	0.60073900
C	4.61373500	-1.44587100	-0.12554200
C	3.54130700	-2.35887000	-0.24720700
C	3.70230100	-3.60605700	0.37084500
C	4.84425400	-3.94067300	1.09969200
H	6.78689700	-3.24818600	1.78078600
H	6.54888300	-1.04862100	0.66109800
C	2.30904900	-2.12342400	-0.99576400
H	2.91088500	-4.34695500	0.29436800
H	1.71484000	-3.00188200	-1.27079300
O	4.60241300	-0.22090200	-0.76777000
N	1.86363000	-0.94057500	-1.30338100
O	0.72637700	-0.88830100	-1.94525200
C	4.39198300	2.12719000	-0.64767400
C	5.47726700	2.97473100	-0.59389600
N	3.59231300	2.69945800	-1.57842300
H	6.36888100	2.89958900	0.01139500
N	5.27910800	3.99574800	-1.46249700

N	4.12939700	3.82391600	-2.05144000
C	4.09068800	0.83696900	0.03855500
H	4.58603000	0.83271000	1.01684800
H	3.01092400	0.70063700	0.17531600
C	2.24012400	2.30727900	-1.96359800
H	2.05540000	2.77913600	-2.93245100
H	2.21004900	1.21835600	-2.07333700
C	1.23044100	2.74676500	-0.92502400
C	1.23458900	4.04606600	-0.41118400
C	0.28531200	1.82717300	-0.47371400
C	0.29637600	4.43436900	0.54114600
H	1.97618400	4.76282400	-0.75577200
C	-0.65209700	2.20284700	0.48591200
H	0.27497900	0.81532200	-0.88954500
C	-0.63920700	3.49994500	0.97567100
H	0.29139500	5.44371700	0.93770900
H	-1.37496500	1.47701300	0.84163300
O	4.84950100	-5.18718000	1.65249600
C	5.99431400	-5.56045200	2.39563700
H	6.14591900	-4.89442700	3.25292000
H	5.80874200	-6.57347400	2.75200300
H	6.89427800	-5.55270800	1.77030400
Br	-1.94682200	4.00743900	2.26426000

TS1(FE)

N	-6.20091100	2.69475200	2.09099800
C	-5.08226900	2.25009300	1.26110800
C	-4.60749100	0.88018300	1.72040900
O	-3.51165300	0.44877500	0.92664700
C	-5.48230800	2.24742600	-0.20084100
O	-5.46503600	1.27776100	-0.93301600
O	-2.02182200	2.12419000	2.05699900
P	-1.97348000	0.75256500	1.48815300
C	-1.17366700	-0.82280500	3.59042500

O	-1.28638200	0.39870600	0.08059400
C	-1.60925600	1.19738900	-1.07130100
C	-0.65976500	0.78976100	-2.17522100
H	-6.39458600	3.68150400	1.93896500
H	-4.25166100	2.95507200	1.38625500
H	-4.34287400	0.92950300	2.78140200
H	-5.40812800	0.14102800	1.59963500
H	-5.87853300	3.20983000	-0.57681400
H	-1.62659500	-1.73869600	3.97814800
H	-0.13558500	-1.01071500	3.32111300
H	-2.65378900	1.02686500	-1.35183200
H	-1.49243100	2.25726700	-0.81919200
H	-0.84260300	1.39226800	-3.06921900
H	-0.80242800	-0.26524500	-2.42979400
H	0.37415600	0.93984700	-1.85002300
C	-3.09827700	-3.05391100	-1.67839600
N	-4.00569300	-2.75000100	-2.66917500
C	-3.19631500	-2.06071500	-0.75068800
C	-4.63864000	-1.61816700	-2.36589500
N	-4.15876000	-1.19154500	-1.20611700
H	-2.67790900	-1.88724200	0.17990700
H	-5.40132800	-1.13585400	-2.95636700
H	-4.44772200	-0.32176400	-0.73905400
H	-2.45821200	-3.92082800	-1.73265100
H	-7.04984900	2.18613000	1.84932900
H	-4.17320700	-3.29680000	-3.50601600
O	-1.91445200	-0.56896000	2.37996500
C	-1.28580600	0.30357800	4.59662600
H	-2.33514200	0.52675600	4.81465400
H	-0.79720900	0.00179300	5.52818400
H	-0.79969000	1.19907600	4.20838300
C	3.40471800	4.45347700	-2.18843400
C	3.97072000	3.49139600	-1.35116700
C	3.21601200	2.79603300	-0.41739200

C	1.82914500	3.03917000	-0.29546300
C	1.27781600	4.01525100	-1.13220800
C	2.03969900	4.71474900	-2.07008100
H	4.02709700	4.97812200	-2.90295700
H	5.03440900	3.27745100	-1.40736600
C	0.92531600	2.37177000	0.64678500
H	0.21742200	4.24530300	-1.06413700
H	-0.06049700	2.81911400	0.79517400
O	3.87556100	1.90900100	0.41148600
N	1.24429600	1.28326000	1.26526500
O	0.34104900	0.73145300	2.05441800
C	4.71930500	-0.26328100	0.82155600
C	6.08487100	-0.41232600	0.93526600
N	4.23318700	-1.06302600	1.80188000
H	6.86798100	0.05295800	0.35440400
N	6.35042000	-1.27701400	1.94308700
N	5.22087900	-1.67280800	2.45842300
C	3.89107500	0.57598200	-0.09456200
H	4.34668400	0.56951600	-1.09258000
H	2.86747100	0.19292500	-0.15896300
C	2.84380900	-1.38442000	2.12386600
H	2.88564700	-1.88797200	3.09326800
H	2.26956300	-0.45948400	2.21828100
C	2.22542200	-2.27625300	1.06924500
C	2.87158000	-3.44079500	0.64895400
C	0.99717500	-1.92485700	0.50945200
C	2.29521900	-4.26149900	-0.31561000
H	3.83430500	-3.71002400	1.07763800
C	0.41851400	-2.73069800	-0.46826700
H	0.49553700	-1.01887700	0.84607500
C	1.06989800	-3.89157500	-0.86160400
H	2.78800600	-5.17155200	-0.63963000
H	-0.52314200	-2.44369800	-0.92317600
Br	0.26700400	-5.00285300	-2.17983800

O	1.36310800	5.63017800	-2.81850000
C	2.10723500	6.35808200	-3.77778400
H	2.54348100	5.69083000	-4.52987000
H	1.40263100	7.03633700	-4.25819800
H	2.90645000	6.93826400	-3.30289200

IN(FE)

N	5.72011500	-4.25596900	1.89390400
C	4.92818100	-3.56494200	0.88562600
C	3.82504400	-2.75513100	1.58142600
O	3.01464600	-2.15045400	0.60706300
C	5.72500000	-2.61030600	0.02478700
O	5.46375500	-2.35361400	-1.13164900
O	0.95322200	-2.94281600	1.71890100
P	1.38965100	-1.64103100	1.10869800
C	1.65252900	0.44416600	2.90820200
O	1.13199200	-1.25561300	-0.46668600
C	1.46516700	-2.15456700	-1.52927300
C	0.57674400	-1.79484200	-2.70303500
H	6.45357300	-4.80495700	1.45110200
H	4.44712900	-4.29422300	0.22601900
H	3.23921600	-3.44319200	2.19866000
H	4.27615200	-1.99603400	2.24067000
H	6.57086700	-2.10523300	0.53867500
H	2.50984500	1.06967500	3.17427700
H	0.88788300	1.07928600	2.45443500
H	2.52611500	-2.05633800	-1.78162500
H	1.29583800	-3.18871500	-1.20558600
H	0.79862100	-2.43694100	-3.56005900
H	0.74239600	-0.75327300	-2.99555800
H	-0.47799100	-1.91592300	-2.43544200
C	3.44574200	2.23803100	-1.30104600
N	4.59086500	1.72533400	-1.87030600
C	2.93294200	1.24602000	-0.52261200

C	4.77219200	0.46992200	-1.46053100
N	3.77590200	0.16463200	-0.63896200
H	2.04781600	1.20410900	0.09097800
H	5.57598800	-0.19059800	-1.74695700
H	3.61289200	-0.76248500	-0.17039600
H	3.09385700	3.23567100	-1.51544900
H	6.19052300	-3.57905300	2.49381200
H	5.20663500	2.21642500	-2.50742700
O	2.17707000	-0.46016100	1.92791100
C	1.12242700	-0.27400600	4.13408900
H	1.89816300	-0.91639800	4.56238900
H	0.82144600	0.45621400	4.89168700
H	0.25800300	-0.88738200	3.87227500
C	-5.23110300	-3.26737200	-1.53956200
C	-5.20979300	-2.18098800	-0.66556900
C	-4.03927000	-1.76153100	-0.04849700
C	-2.82996900	-2.44138400	-0.30219400
C	-2.86342100	-3.53596000	-1.16798900
C	-4.04161400	-3.95033500	-1.79327100
H	-6.16567900	-3.56423600	-1.99990100
H	-6.12627900	-1.64228900	-0.44316900
C	-1.52037600	-2.11843600	0.29304800
H	-1.95108400	-4.08977900	-1.37430400
H	-0.74709800	-2.87772400	0.19038000
O	-4.11557700	-0.70202500	0.83272900
N	-1.32875300	-1.00840100	0.89878900
O	-0.11475400	-0.70836100	1.42700000
C	-4.21825100	1.64705900	1.17682300
C	-5.38094400	2.30639100	1.51208300
N	-3.29566800	2.19782800	2.00272100
H	-6.37321800	2.17980000	1.10435900
N	-5.11015900	3.20287300	2.49092700
N	-3.84114700	3.13321700	2.77871600
C	-3.94357000	0.56149900	0.19066200

H	-4.65470600	0.65288800	-0.63852300
H	-2.92529900	0.63686000	-0.20645000
C	-1.85406500	1.95564300	2.05488900
H	-1.53906200	2.26063500	3.05556600
H	-1.68767300	0.88465200	1.93207400
C	-1.12546200	2.74555200	0.98886200
C	-1.03688200	4.13666600	1.09095000
C	-0.55473200	2.10187500	-0.11019400
C	-0.37624300	4.88249600	0.12096500
H	-1.48753900	4.64156800	1.94172500
C	0.09043500	2.83901000	-1.10235600
H	-0.59556100	1.01803000	-0.18893700
C	0.18224400	4.21760200	-0.96658900
H	-0.29292500	5.96021400	0.20679300
H	0.52767800	2.34223000	-1.96249500
O	-3.92826600	-5.02272000	-2.61993200
C	-5.10533100	-5.46744300	-3.27098600
H	-5.52045700	-4.68415300	-3.91508500
H	-4.81031000	-6.32111300	-3.87991500
H	-5.86410100	-5.78092100	-2.54522800
Br	1.10951700	5.20655900	-2.29455200

TS2(FE)

N	4.30677000	-5.57460400	0.99589100
C	3.54814200	-4.59405500	0.23277000
C	2.95534500	-3.55695000	1.19688500
O	2.21439800	-2.61244100	0.45599100
C	4.36414700	-3.85000400	-0.80728500
O	3.92507700	-3.45881300	-1.86601800
O	0.04454900	-3.20778000	1.54398900
P	0.63422200	-1.87049100	1.22302500
C	1.45085600	-0.39433500	3.38027700
O	0.46702300	-1.18780900	-0.24387400
C	0.51055000	-1.94781700	-1.46108700

C	-0.39130200	-1.24729600	-2.45665700
H	4.67550600	-6.29307000	0.37692700
H	2.71729700	-5.08547000	-0.28337800
H	2.29690000	-4.06869900	1.90288900
H	3.75794900	-3.05662300	1.76018600
H	5.41777200	-3.64446800	-0.51838300
H	2.43088100	-0.01743300	3.68680100
H	0.80339600	0.45417100	3.15460600
H	1.54336700	-1.99866800	-1.81804200
H	0.17348400	-2.97174500	-1.26517400
H	-0.35513000	-1.76161000	-3.42114000
H	-0.06592700	-0.21265200	-2.60235600
H	-1.42766200	-1.23793100	-2.10483400
C	4.58529700	1.31996900	-0.14354800
N	4.67918500	0.77908200	-1.40370100
C	3.92516300	0.39324700	0.60865600
C	4.09869400	-0.42963400	-1.40153700
N	3.63163600	-0.68740800	-0.19012400
H	3.62984000	0.42207600	1.64487300
H	4.04822300	-1.09316400	-2.25200700
H	2.92617400	-1.67893200	0.13151800
H	4.96782800	2.30123400	0.08623000
H	5.11366600	-5.13059300	1.43326000
H	5.09630800	1.22679100	-2.21006600
O	1.72569200	-1.12656600	2.17296700
C	0.86780000	-1.28328400	4.46117300
H	1.52419800	-2.14043400	4.63880600
H	0.77359200	-0.72021400	5.39428100
H	-0.12002100	-1.64739100	4.17020600
C	-6.10640800	-1.56405000	-1.43060700
C	-5.70937000	-0.42785900	-0.72645200
C	-4.49014000	-0.36796000	-0.06631800
C	-3.61852500	-1.47478300	-0.10286500
C	-4.02131400	-2.60619200	-0.81483400

C	-5.24963300	-2.66386400	-1.47698300
H	-7.06784900	-1.57368400	-1.92973800
H	-6.35957300	0.44035600	-0.67825100
C	-2.30461800	-1.56224200	0.55715300
H	-3.37310700	-3.47696100	-0.86031800
H	-1.77458200	-2.50747800	0.43480500
O	-4.18903500	0.78280600	0.62901600
N	-1.82360400	-0.60420200	1.25443200
O	-0.58574600	-0.77569200	1.82712300
C	-3.42431300	3.02165600	0.59140900
C	-4.29762000	4.08764100	0.58303700
N	-2.50186200	3.37748400	1.51715200
H	-5.19446800	4.22609600	-0.00307000
N	-3.86507500	5.01415700	1.47174800
N	-2.77188900	4.57710800	2.03009900
C	-3.43661100	1.72229400	-0.14071400
H	-3.91707700	1.86844100	-1.11459900
H	-2.41960900	1.34372800	-0.30187200
C	-1.27221900	2.68083400	1.89035700
H	-1.01706900	3.04278900	2.88897800
H	-1.49234800	1.61070700	1.93937700
C	-0.16262700	2.95735900	0.89931000
C	0.32693200	4.25329700	0.71892500
C	0.36681900	1.91189800	0.14607300
C	1.33800200	4.50281700	-0.20315200
H	-0.08683300	5.07434700	1.29913000
C	1.37857600	2.14575300	-0.78359300
H	-0.00465000	0.90155300	0.28150700
C	1.84995500	3.44156100	-0.94541200
H	1.72550900	5.50554400	-0.34562100
H	1.78741600	1.32515900	-1.36744900
Br	3.22324600	3.78108200	-2.21265200
O	-5.51787600	-3.82435500	-2.12881000
C	-6.76242600	-3.91930900	-2.79990000

H	-6.84805600	-3.15965600	-3.58473700
H	-6.78841500	-4.91129000	-3.24935200
H	-7.59755200	-3.81364800	-2.09857900

C2(FE)

N	1.48074700	6.25187900	0.41037300
C	1.35600000	4.88547500	0.91886100
C	2.44293300	4.01659100	0.30072400
O	2.41812400	2.76178500	0.93884900
C	1.48972600	4.83748700	2.42712800
O	0.63436700	4.44802700	3.18940100
O	-0.21504200	2.64893500	-0.77849500
P	0.32013000	1.27750600	-0.68611500
C	2.39565800	-0.21149400	-1.19536600
O	0.38915600	0.62613400	0.75696800
C	0.02797100	1.37914600	1.94032500
C	-1.32317800	0.91580400	2.43942100
H	0.72690200	6.82944200	0.77627800
H	0.37788700	4.48197600	0.64188000
H	2.25740300	3.93893900	-0.77953100
H	3.42008300	4.51001700	0.44433300
H	2.45102200	5.24228300	2.81523800
H	2.87747600	-0.17607200	-0.21296100
H	1.64842700	-1.01003500	-1.19983000
H	0.82118100	1.18960500	2.66547400
H	0.02990400	2.44317000	1.70719000
H	-1.58834400	1.46773400	3.34607100
H	-1.30813200	-0.15187300	2.67845100
H	-2.09558300	1.09686700	1.68446700
C	6.56386000	0.61513800	-0.85503700
N	6.39120300	1.72967300	-1.63666100
C	5.57314300	0.67798500	0.08691800
C	5.32669600	2.41261300	-1.15763900
N	4.80611400	1.80194000	-0.11246400

H	5.35310000	-0.02421700	0.87740700
H	4.97392100	3.33385900	-1.59899100
H	3.22441400	2.28348400	0.62488800
H	7.35188600	-0.09779600	-1.03744900
H	2.35019600	6.66846900	0.74388700
H	6.95834900	1.99568700	-2.43037800
O	1.71626200	1.05344700	-1.39862100
C	3.40527500	-0.40946100	-2.30091200
H	3.99581800	-1.30372600	-2.07686300
H	2.90759600	-0.54166700	-3.26520300
H	4.08379500	0.44556500	-2.36110800
C	-6.82112800	0.89147900	-0.30075900
C	-6.11262600	-0.29770200	-0.13908100
C	-4.77109900	-0.39280300	-0.48164600
C	-4.10926300	0.73203600	-1.00775500
C	-4.82744500	1.91323600	-1.19216700
C	-6.17328900	2.00863100	-0.83138700
H	-7.86723200	0.92644400	-0.02132700
H	-6.60903900	-1.18078100	0.25133500
C	-2.69482900	0.75808900	-1.40532800
H	-4.34227100	2.78841700	-1.61414300
H	-2.37965800	1.54775200	-2.08957000
O	-4.14393500	-1.61176500	-0.36098600
N	-1.83721800	-0.07019900	-0.94744900
O	-0.55608400	0.17661500	-1.52079500
C	-3.23337300	-3.29611300	1.03426800
C	-3.66548400	-4.28926500	1.88399400
N	-2.35467900	-3.93246900	0.22252400
H	-4.37745800	-4.22791500	2.69371300
N	-3.03887400	-5.44622700	1.55443200
N	-2.24871000	-5.22152600	0.54580800
C	-3.57471800	-1.84923800	0.92943800
H	-4.29560400	-1.60000300	1.71567200
H	-2.68615900	-1.21759700	1.04650800

C	-1.54575800	-3.38460300	-0.86291600
H	-1.68618100	-4.02575900	-1.73571000
H	-1.95029300	-2.39319900	-1.08492300
C	-0.08501300	-3.30114100	-0.48584800
C	0.89044800	-3.83880100	-1.32400300
C	0.30460500	-2.66407300	0.69471400
C	2.24272800	-3.73018600	-1.00533300
H	0.59856000	-4.34434200	-2.24016100
C	1.64762100	-2.55729100	1.03520900
H	-0.44404600	-2.23475500	1.35574300
C	2.60168400	-3.08388300	0.17011400
H	3.00234300	-4.13364500	-1.66588100
H	1.95192500	-2.03895600	1.93798100
O	-6.75790000	3.21328600	-1.03980600
C	-8.12586100	3.34508200	-0.68950500
H	-8.27894000	3.15895800	0.37902800
H	-8.39736500	4.37375200	-0.92263200
H	-8.75009200	2.66010700	-1.27358000
Br	4.43974000	-2.81892600	0.54885000

FZ

C	2.39482200	-2.22190100	0.73387500
C	1.68774000	-1.01376900	0.62290600
C	2.30813400	0.12989200	0.15280800
C	3.68117700	0.12512000	-0.23053900
C	4.36403200	-1.09046200	-0.10653100
C	3.73275800	-2.24787500	0.36653800
H	1.88130800	-3.10111600	1.10323100
H	0.64301500	-1.00371800	0.91429700
C	4.28211600	1.35931300	-0.72097100
H	5.40688000	-1.12005900	-0.38778800
O	1.66007900	1.33863200	0.02455500
C	-0.17142900	2.76778100	0.12011500
C	0.34129700	3.78698300	-0.64841000

N	-1.32389400	3.28038300	0.60902100
H	1.25511200	3.81025900	-1.22191200
N	-0.51270500	4.84194000	-0.58885800
N	-1.51923300	4.53013100	0.16858500
C	0.30685200	1.38073800	0.39916000
H	0.18387200	1.13289400	1.46479600
H	-0.28386200	0.65282400	-0.17760300
N	5.50946500	1.57966800	-1.14451300
O	6.37120900	0.61182700	-1.15709400
H	3.64326700	2.23593800	-0.74857100
C	-2.29098400	2.64889000	1.49958000
H	-1.82507300	2.49077700	2.47664800
H	-3.09483000	3.37924500	1.61918600
C	-2.79856600	1.34410700	0.93014600
C	-2.73719400	0.17302800	1.68332300
C	-3.31564600	1.29955600	-0.36689300
C	-3.19347500	-1.03428600	1.15823200
H	-2.32762700	0.19516000	2.68965900
C	-3.77213600	0.10263600	-0.90633600
H	-3.35545500	2.20756100	-0.96351600
C	-3.70690800	-1.05268600	-0.13183200
H	-3.14732900	-1.94578700	1.74337000
H	-4.17350100	0.06451800	-1.91283000
O	4.52739300	-3.36159400	0.43077900
C	3.91953700	-4.55738600	0.87212800
H	3.09035400	-4.84927200	0.21627100
H	4.69313300	-5.32500600	0.84035500
H	3.54485800	-4.46085000	1.89829900
Br	-4.33919400	-2.68849200	-0.85180700

C1(FZ)

N	9.18649100	-1.83259800	-2.01854200
C	7.99372800	-1.06301300	-1.66635800
C	8.34452400	0.40327500	-1.50042800

O	8.41037000	0.97291400	-0.43124300
C	7.40591400	-1.66729300	-0.39521400
O	6.36552700	-0.86693700	0.18222100
C	3.56678400	-2.58769200	-0.13516100
C	2.79085100	-3.61106100	-0.93034600
C	3.49584500	1.40932100	0.32557400
C	2.28778700	1.32973800	1.22738800
O	4.43080200	-1.88531400	-1.06192100
O	4.24743200	0.17935400	0.50153800
O	5.35606300	0.36505200	-1.86815300
P	5.05033100	-0.47706100	-0.69262700
H	7.02519600	-2.67056100	-0.60610100
H	8.17756400	-1.73645500	0.37500600
H	9.48616000	-1.61945200	-2.96666400
H	9.95996700	-1.59687200	-1.39877200
H	7.28336200	-1.14483900	-2.49419600
H	8.63619900	0.92354500	-2.43199700
H	4.19596400	-3.04833400	0.63437300
H	2.89664200	-1.85466400	0.31654700
H	2.23247700	-3.09168100	-1.71361000
H	3.45775800	-4.35001100	-1.38297100
H	2.07963700	-4.12233900	-0.27475200
H	1.67340400	0.47906400	0.91787300
H	2.58898500	1.21301500	2.27331700
H	1.69719800	2.24576300	1.13579500
H	3.19952900	1.50611300	-0.71751200
H	4.16497800	2.23082100	0.60444300
C	5.81566000	1.47248800	2.79290600
N	6.73255100	1.45240400	1.76750100
C	5.87266100	2.71565100	3.34308400
C	7.33531200	2.63081200	1.67995600
N	6.82485400	3.41135900	2.63022000
H	5.33232900	3.16120600	4.16150800
H	8.09433200	2.89579600	0.96113300

H	7.10159200	4.37240200	2.79494400
H	5.20555400	0.61558100	3.02693700
H	6.91586300	0.66108500	1.13825800
C	-2.15288200	-2.17408100	1.19251800
C	-2.73244200	-0.97520000	0.74629400
C	-2.02580600	-0.10267200	-0.06313400
C	-0.69120800	-0.38988100	-0.46918900
C	-0.13786800	-1.59110900	-0.01298300
C	-0.85437100	-2.47239300	0.80655900
H	-2.73278300	-2.83481200	1.82541200
H	-3.74817700	-0.75306700	1.05470900
C	0.01198800	0.56610000	-1.32035200
H	0.86978400	-1.83577600	-0.31425100
O	-2.54598500	1.08586300	-0.52270300
C	-4.21988000	2.67941000	-0.81150800
C	-3.66197800	3.36800600	-1.86344700
N	-5.28266900	3.43802800	-0.45643100
H	-2.79008100	3.12145400	-2.44964900
N	-4.40309300	4.48432500	-2.08805000
N	-5.38304800	4.52056600	-1.23817900
C	-3.86670100	1.38812400	-0.14944700
H	-3.95766300	1.47597500	0.94387400
H	-4.55573300	0.59365300	-0.47375600
N	1.25136200	0.53923200	-1.74929400
O	2.02172200	-0.45912700	-1.41657900
H	-0.54855300	1.43909100	-1.63901000
C	-6.24519700	3.20790300	0.61580500
H	-5.73718500	3.31024900	1.57931400
H	-6.97635100	4.01507500	0.52706700
C	-6.89224100	1.84776600	0.49086800
C	-6.86912900	0.95056600	1.55679400
C	-7.49257400	1.46865100	-0.71223700
C	-7.43781900	-0.31606700	1.43295600
H	-6.39711300	1.23275300	2.49422400

C	-8.06155000	0.20856200	-0.85281700
H	-7.50678300	2.16030000	-1.55098900
C	-8.02538300	-0.67117500	0.22575500
H	-7.41552600	-1.01576700	2.26084200
H	-8.52465200	-0.09020300	-1.78658400
O	-0.17886000	-3.60534000	1.17380700
C	-0.86267500	-4.51814000	2.00797100
H	-1.76683600	-4.90317600	1.52141200
H	-0.17203100	-5.34092800	2.19282500
H	-1.14049100	-4.05410500	2.96197600
Br	-8.78712300	-2.39595700	0.03232200

TS1(FZ)

N	8.10777300	-3.46985400	-1.06228200
C	7.38590200	-2.20748900	-1.08916100
C	6.53487700	-2.11108300	0.19101600
O	5.82280700	-0.88852000	0.26949100
C	8.27128400	-0.98126600	-1.19088600
O	7.86819800	0.11877800	-1.50634400
O	4.47978500	-1.42128100	-1.81232400
P	4.31776900	-0.80233600	-0.47682800
C	2.86024700	-0.95617700	1.71420400
O	4.23972600	0.77493300	-0.22501100
C	4.23959300	1.62923200	-1.39299300
C	3.88847800	3.02605800	-0.93911900
H	8.58321700	-3.62204400	-1.94843400
H	6.69274800	-2.19061500	-1.93504600
H	5.85566200	-2.96965300	0.21301200
H	7.17982900	-2.16494200	1.07500700
H	9.34029600	-1.13665900	-0.93497000
H	3.59447600	-0.32617000	2.23028100
H	2.07158200	-0.32272000	1.29950000
H	5.24098300	1.58659500	-1.83977300
H	3.50375500	1.24070500	-2.09757600

H	3.87316900	3.69995600	-1.80049300
H	4.61851600	3.40516600	-0.21715100
H	2.89688100	3.01139000	-0.48147800
C	6.83750100	3.52380300	1.87797100
N	7.76021800	3.61445300	0.85918600
C	6.24994000	2.30284900	1.75130300
C	7.74538400	2.49482600	0.13678600
N	6.83390400	1.69078700	0.66762100
H	5.46887600	1.82590800	2.32002500
H	8.35877100	2.26835200	-0.72070000
H	6.58042100	0.75014200	0.32254200
H	6.68437000	4.32124300	2.58560800
H	8.83236200	-3.44952600	-0.34557900
H	8.36473500	4.40748600	0.67861600
O	3.51018600	-1.63232200	0.62292200
C	2.30679500	-2.01651400	2.64097400
H	3.11341700	-2.63572500	3.04326600
H	1.78439700	-1.54032700	3.47556900
H	1.60005000	-2.65916900	2.10775400
C	-2.24346800	-2.49767400	0.90416500
C	-2.75869900	-1.20719100	0.71294800
C	-1.95480700	-0.19025700	0.22419200
C	-0.58931900	-0.42351300	-0.09432800
C	-0.10285000	-1.72052300	0.08747200
C	-0.91402900	-2.74447700	0.59149800
H	-2.89568200	-3.27171900	1.28993500
H	-3.79986300	-1.02852600	0.95814300
C	0.23467900	0.71142300	-0.52481700
H	0.92976600	-1.92760700	-0.16069700
O	-2.40484800	1.09209500	0.01664200
C	-4.01358000	2.77009300	-0.07138100
C	-3.32101400	3.65310600	-0.86674900
N	-5.10191400	3.47214300	0.32014800
H	-2.38643000	3.50823200	-1.38660600

N	-4.01348400	4.82053900	-0.91664300
N	-5.09010100	4.70603000	-0.20105700
C	-3.75588500	1.34921500	0.30928400
H	-3.96626300	1.18521200	1.37662500
H	-4.41327300	0.67810300	-0.26339600
N	1.46921100	0.72620400	-0.94083900
O	2.08138600	-0.42678400	-1.11258100
H	-0.21914500	1.69464900	-0.44772300
C	-6.18895400	3.04959400	1.19815900
H	-5.80055500	2.93185800	2.21404500
H	-6.90085700	3.87840000	1.19729500
C	-6.81823100	1.76436200	0.71254000
C	-6.87617700	0.64634200	1.54271900
C	-7.31172300	1.67691000	-0.59151900
C	-7.41601900	-0.55351600	1.08312800
H	-6.48917500	0.70237000	2.55676700
C	-7.85199000	0.48735400	-1.06561200
H	-7.26445500	2.54345000	-1.24632300
C	-7.89434500	-0.61748000	-0.21914900
H	-7.45405700	-1.42582100	1.72564800
H	-8.23211200	0.41492300	-2.07832100
O	-0.29517400	-3.95514700	0.74391400
C	-1.07289900	-5.01291900	1.26793700
H	-1.92104200	-5.24563000	0.61328900
H	-0.41300100	-5.87835400	1.32616100
H	-1.44864200	-4.77216500	2.26947500
Br	-8.60943400	-2.24966800	-0.86519900

IN(FZ)

N	-8.96954500	1.16929400	-2.04550400
C	-8.04072700	0.19583900	-1.48624600
C	-6.67211900	0.86250400	-1.28022000
O	-5.76359300	-0.09101500	-0.80251900
C	-8.47307200	-0.36762400	-0.15184300

O	-8.22980600	-1.49327300	0.22862800
O	-4.07068700	0.51244600	-2.50512900
P	-4.01275800	0.26100900	-1.02723200
C	-3.43924000	2.52322300	0.43415300
O	-3.76103500	-1.21899800	-0.36851000
C	-4.46691700	-2.37300700	-0.83238600
C	-3.60436700	-3.57921700	-0.51927900
H	-9.88343100	0.74421400	-2.18660000
H	-7.91115400	-0.63839500	-2.18287500
H	-6.34355800	1.26367100	-2.24471700
H	-6.77163300	1.70269000	-0.57306700
H	-9.00944200	0.34834700	0.50807100
H	-3.94218100	3.01237300	1.27388800
H	-2.46286800	2.17183600	0.77464600
H	-5.44163100	-2.44012600	-0.33717500
H	-4.64891900	-2.28605200	-1.90914800
H	-4.09927200	-4.49703300	-0.84933400
H	-3.42654400	-3.64928500	0.55803100
H	-2.63853600	-3.49705300	-1.02522000
C	-4.71806500	-0.91888900	3.80745000
N	-6.00270900	-1.41474300	3.83978900
C	-4.51530600	-0.46996100	2.53897900
C	-6.56523600	-1.27613400	2.63875600
N	-5.67743200	-0.70151100	1.83806100
H	-3.65911700	-0.01701200	2.06719500
H	-7.56066000	-1.58306500	2.35653200
H	-5.81498800	-0.46682400	0.81527500
H	-4.07831800	-0.93057500	4.67385800
H	-9.10869300	1.93558400	-1.38755600
H	-6.45928000	-1.82561100	4.64518500
O	-4.28296100	1.41266200	0.11505500
C	-3.30720000	3.48584400	-0.73159500
H	-4.29075200	3.86473400	-1.02626900
H	-2.67291700	4.33225600	-0.45000800

H	-2.85941700	2.98249600	-1.59306400
C	2.03103900	2.65490800	0.92581100
C	2.49939700	1.35282100	0.71738600
C	1.74402700	0.44229800	-0.00941100
C	0.49308800	0.82009200	-0.54330000
C	0.04794700	2.12060100	-0.33713800
C	0.80396500	3.04045500	0.39594800
H	2.64035300	3.34150300	1.50116200
H	3.45908500	1.07535100	1.13875900
C	-0.24939900	-0.16018700	-1.36081500
H	-0.89450200	2.44128200	-0.76166600
O	2.12448100	-0.85100200	-0.24785300
C	3.62445200	-2.62942200	-0.29370700
C	2.96104200	-3.40442700	-1.21632400
N	4.62836800	-3.42697400	0.13761400
H	2.08885000	-3.16403800	-1.80439800
N	3.58860900	-4.60648800	-1.29745900
N	4.59727800	-4.61396400	-0.48141800
C	3.41261400	-1.23018700	0.18246500
H	3.48965700	-1.17494600	1.27818300
H	4.17479800	-0.55979100	-0.24059400
N	-1.51269700	-0.30501500	-1.51508900
O	-2.27820100	0.55382800	-0.78290800
H	0.34410100	-0.88032000	-1.91867900
C	5.65978800	-3.13488700	1.12719500
H	5.19133500	-3.02648000	2.10964200
H	6.29809700	-4.02135600	1.14943400
C	6.43952800	-1.89286900	0.76176300
C	6.59259300	-0.85617000	1.68026800
C	7.00100400	-1.77057400	-0.51191900
C	7.30523800	0.29318800	1.34268100
H	6.15222400	-0.93895200	2.67030100
C	7.71059600	-0.62920200	-0.86507600
H	6.87752000	-2.57136300	-1.23678400

C	7.85580400	0.39092300	0.07150100
H	7.42634500	1.09890900	2.05770700
H	8.14760300	-0.53056400	-1.85228600
O	0.25241400	4.27948100	0.53128600
C	0.99480300	5.23876100	1.26099700
H	0.39997300	6.15146800	1.25615400
H	1.15520600	4.91254700	2.29507200
H	1.96487400	5.43147300	0.78856100
Br	8.83198600	1.94467300	-0.40236200

TS2(FZ)

N	-8.81833100	1.36259400	-2.08559200
C	-7.93462500	0.30720300	-1.60985500
C	-6.64513400	0.93825800	-1.06406900
O	-5.76364800	-0.07372800	-0.64449400
C	-8.52628200	-0.54038300	-0.50432500
O	-8.28641500	-1.71651000	-0.33868900
O	-4.06364300	0.46436400	-2.38488400
P	-3.89870900	0.25389300	-0.91359800
C	-3.33273700	2.52829100	0.49217600
O	-3.72444900	-1.21539900	-0.24216600
C	-4.41625200	-2.35569900	-0.77000800
C	-3.49586500	-3.55061100	-0.62786000
H	-9.67685300	0.96222100	-2.45730900
H	-7.66151800	-0.35442100	-2.43789400
H	-6.18580800	1.52403400	-1.86528000
H	-6.88279600	1.61684400	-0.22894800
H	-9.18348500	0.01002600	0.20440400
H	-3.81627900	3.02081300	1.34046000
H	-2.34708700	2.18120400	0.80799400
H	-5.34976700	-2.49852500	-0.21581500
H	-4.67369800	-2.17575300	-1.81825300
H	-3.98450000	-4.45145300	-1.00992600
H	-3.24081100	-3.71430900	0.42300300

H	-2.57191100	-3.38428700	-1.18806300
C	-5.54844600	-0.66685800	3.93856000
N	-6.64532600	-1.45181800	3.66916900
C	-5.16678600	-0.13661200	2.74210600
C	-6.91093200	-1.39414200	2.35754500
N	-6.02816100	-0.59894300	1.77360000
H	-4.35378700	0.52648900	2.49413400
H	-7.71562200	-1.91503300	1.86022200
H	-5.92982000	-0.35190800	0.59637600
H	-5.14968000	-0.56170700	4.93393900
H	-9.09528500	1.96116800	-1.30801500
H	-7.17219000	-1.98926700	4.34601900
O	-4.18209100	1.40579400	0.20916500
C	-3.24045100	3.47732500	-0.68761800
H	-4.23276700	3.85253600	-0.95525100
H	-2.59855200	4.32631800	-0.43281800
H	-2.81669400	2.96884000	-1.55847900
C	2.13460800	2.66228000	0.83150000
C	2.59416900	1.35241000	0.65750600
C	1.82611800	0.42421400	-0.03327800
C	0.57091900	0.79348600	-0.56184300
C	0.13397900	2.10195900	-0.39059300
C	0.90317700	3.03921100	0.30492000
H	2.75402700	3.36284900	1.37855000
H	3.55719900	1.08273300	1.07616600
C	-0.18640900	-0.20781600	-1.33920700
H	-0.81192500	2.41628000	-0.81247200
O	2.19680900	-0.87666400	-0.23905400
C	3.68762800	-2.66444900	-0.24329300
C	3.01858900	-3.45786600	-1.14594500
N	4.68808000	-3.45682200	0.20575300
H	2.14722000	-3.22675800	-1.73895500
N	3.63897700	-4.66513100	-1.19836300
N	4.64870500	-4.65850400	-0.38367300

C	3.48456500	-1.25226900	0.19711400
H	3.56422600	-1.16804900	1.29063900
H	4.24897300	-0.59753100	-0.24591000
N	-1.45116500	-0.35686300	-1.46439500
O	-2.19336200	0.53232300	-0.72879900
H	0.39378000	-0.94379600	-1.89028000
C	5.71961100	-3.15016100	1.19122500
H	5.25221200	-3.03546900	2.17344100
H	6.36242000	-4.03317100	1.22021500
C	6.49246300	-1.90738300	0.81468100
C	6.63430300	-0.85984100	1.72266400
C	7.05822100	-1.79439800	-0.45793100
C	7.33942300	0.29123900	1.37569500
H	6.19085400	-0.93552600	2.71191000
C	7.76063700	-0.65143200	-0.82044900
H	6.94381100	-2.60366200	-1.17482500
C	7.89440900	0.37963800	0.10572700
H	7.45186500	1.10533700	2.08262200
H	8.20104500	-0.56009300	-1.80686400
Br	8.86249300	1.93508200	-0.37914800
O	0.35937800	4.28404400	0.40985600
C	1.11835400	5.26264900	1.09590700
H	1.29324200	4.96978600	2.13751200
H	2.08171600	5.43424500	0.60217200
H	0.52800800	6.17790200	1.07044300

C2(FZ)

N	-10.08551200	0.00005700	-1.38825200
C	-8.66055900	-0.28041800	-1.23141400
C	-7.97729000	0.93942400	-0.59808200
O	-6.58214700	0.79031700	-0.52370200
C	-8.41091600	-1.49196900	-0.35900000
O	-7.68059000	-2.41629200	-0.64076200
O	-3.84007900	0.80041400	-2.81587600

P	-3.49192400	0.81672300	-1.38460700
C	-4.03166700	2.15620100	0.82724200
O	-3.93462700	-0.43987200	-0.52662000
C	-4.69913000	-1.51576400	-1.12566900
C	-3.78525400	-2.49017000	-1.83566600
H	-10.55764400	-0.79683000	-1.81024600
H	-8.21010900	-0.46563500	-2.21202500
H	-8.20875300	1.80918600	-1.22045400
H	-8.41351300	1.11673200	0.39862500
H	-8.97177100	-1.48565500	0.60125900
H	-4.38892300	1.19041800	1.19521000
H	-3.01882900	2.33157300	1.20331900
H	-5.21743700	-1.98080100	-0.28676900
H	-5.44948800	-1.08844900	-1.79231200
H	-4.37594500	-3.32470300	-2.22514200
H	-3.03236100	-2.88443000	-1.14804800
H	-3.27445500	-2.00045800	-2.66870700
C	-6.15089300	-0.75883600	4.12304500
N	-6.35437200	-2.00107400	3.57636400
C	-6.20227000	0.11068800	3.06834600
C	-6.51881600	-1.84992200	2.24392200
N	-6.43039900	-0.58009500	1.89955200
H	-6.09658700	1.18627200	3.07917400
H	-6.71577700	-2.67414000	1.57166900
H	-6.39548500	0.24916500	0.28228900
H	-5.99495400	-0.61476100	5.18007400
H	-10.51548700	0.13555600	-0.47332400
H	-6.38260800	-2.87749500	4.07992900
O	-3.96864600	2.11208800	-0.61618700
C	-4.97912200	3.27058600	1.20781800
H	-5.01350200	3.37379700	2.29620600
H	-4.64722100	4.22155800	0.78282600
H	-5.98076700	3.04029200	0.83565700
C	2.63060400	2.75485400	0.52683900

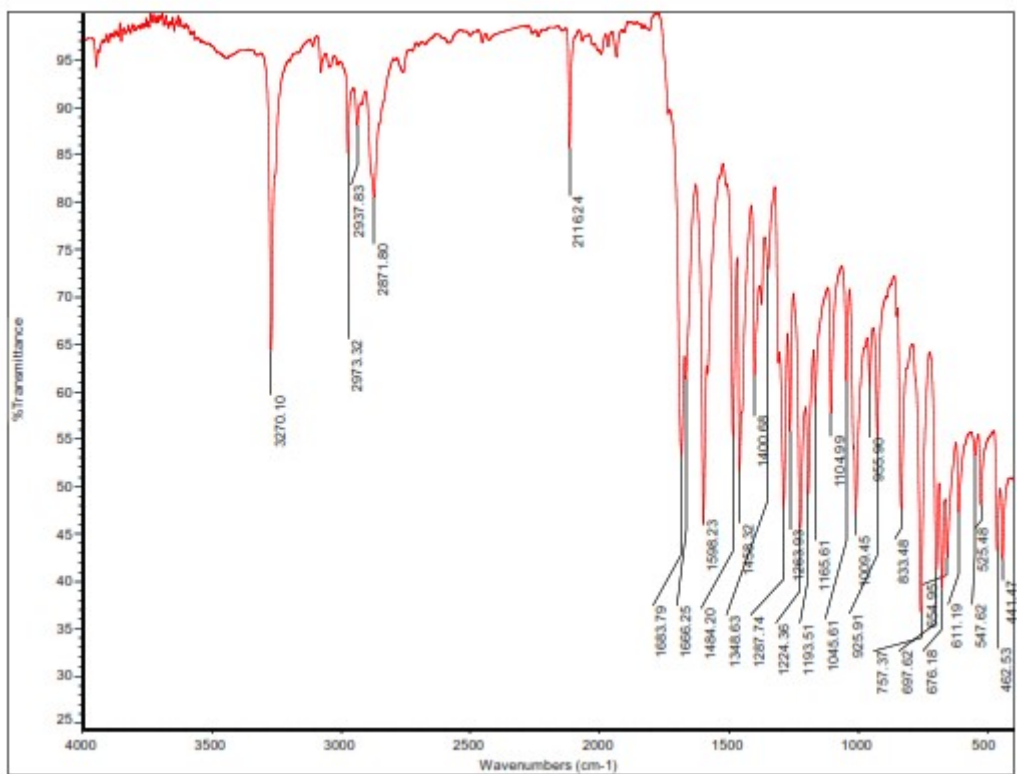
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C	0.52786400	2.23709500	-0.53499900
C	1.39473400	3.17045900	0.03936600
H	3.32219200	3.45447700	0.98075600
H	3.96883000	1.11522100	0.82197400
C	0.05694400	-0.13739000	-1.28610000
H	-0.42196000	2.58797800	-0.91407700
O	2.43934900	-0.84439900	-0.27174700
C	3.84621200	-2.70606000	-0.20744900
C	3.16223200	-3.51045600	-1.08883300
N	4.78443100	-3.52691100	0.31939300
H	2.32625900	-3.26726300	-1.72624800
N	3.71195200	-4.75192800	-1.05165800
N	4.69352600	-4.75569400	-0.20330100
C	3.72205000	-1.26107500	0.14713800
H	3.84201800	-1.11268400	1.22942700
H	4.50175300	-0.67551600	-0.36047000
N	-1.19675400	-0.20027300	-1.52283100
O	-1.89465000	0.92540600	-1.04874000
H	0.57910800	-1.02619400	-1.63007000
C	5.79050600	-3.22746600	1.33372200
H	5.29084500	-3.06635700	2.29368700
H	6.39877500	-4.13178800	1.41259900
C	6.62125300	-2.02362000	0.95336800
C	6.76892700	-0.96084200	1.84276400
C	7.23100100	-1.95770800	-0.30188700
C	7.51914100	0.16028900	1.49320900
H	6.29210200	-0.99986200	2.81863000
C	7.97908300	-0.84437300	-0.66713800
H	7.11362800	-2.77872000	-1.00481800
C	8.11402000	0.20403600	0.23903900
H	7.63369200	0.98682600	2.18526800

H	8.45130800	-0.78861300	-1.64148300
O	0.94025000	4.45187200	0.07205600
C	1.79122700	5.42754500	0.64635100
H	1.25470700	6.37337200	0.58048700
H	2.00240400	5.19939400	1.69710500
H	2.73513600	5.50352400	0.09466800
Br	9.13220900	1.72478300	-0.25162800

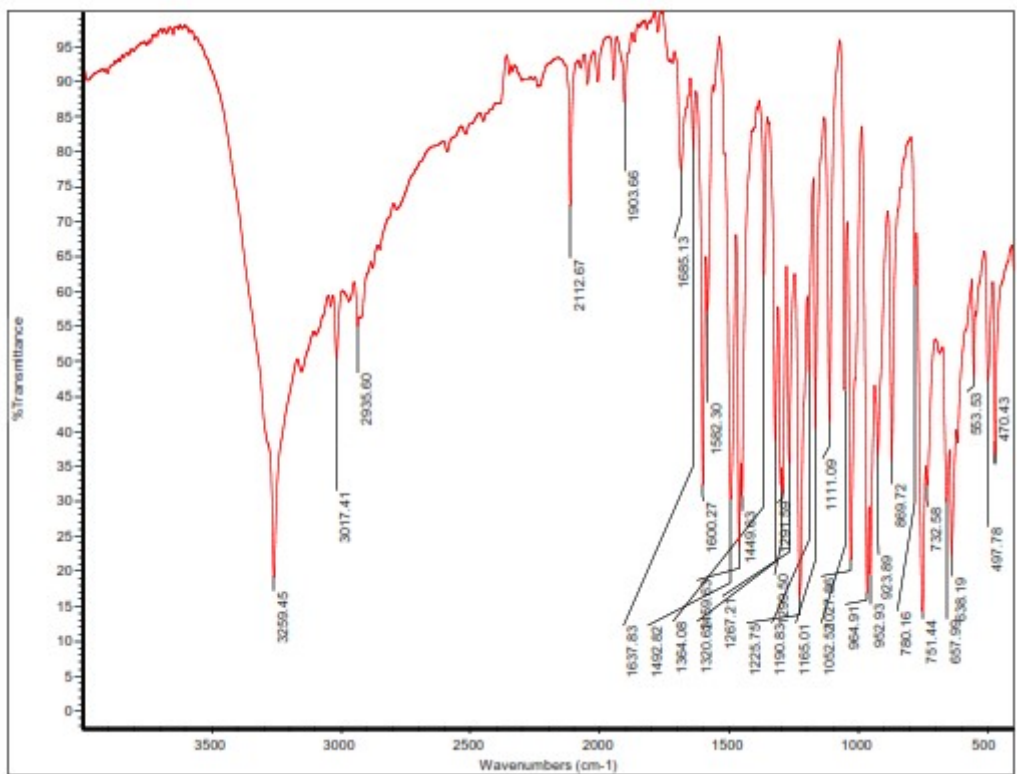
Spectra

FT-IR spectra

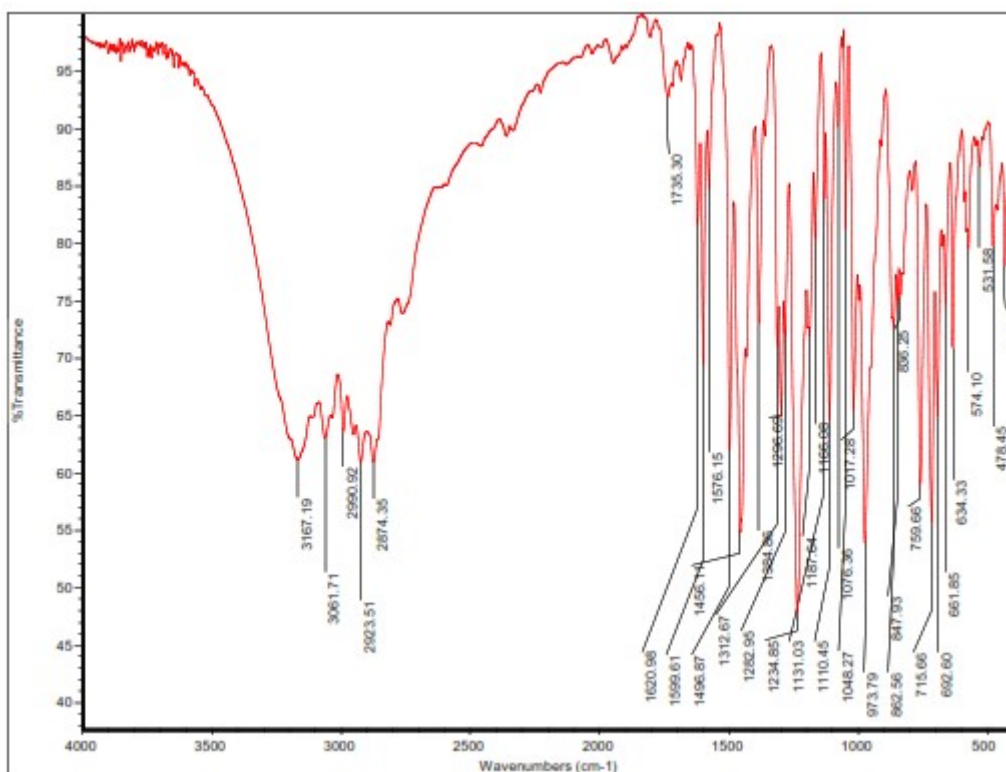
S20. O-propargylated salicylaldehyde



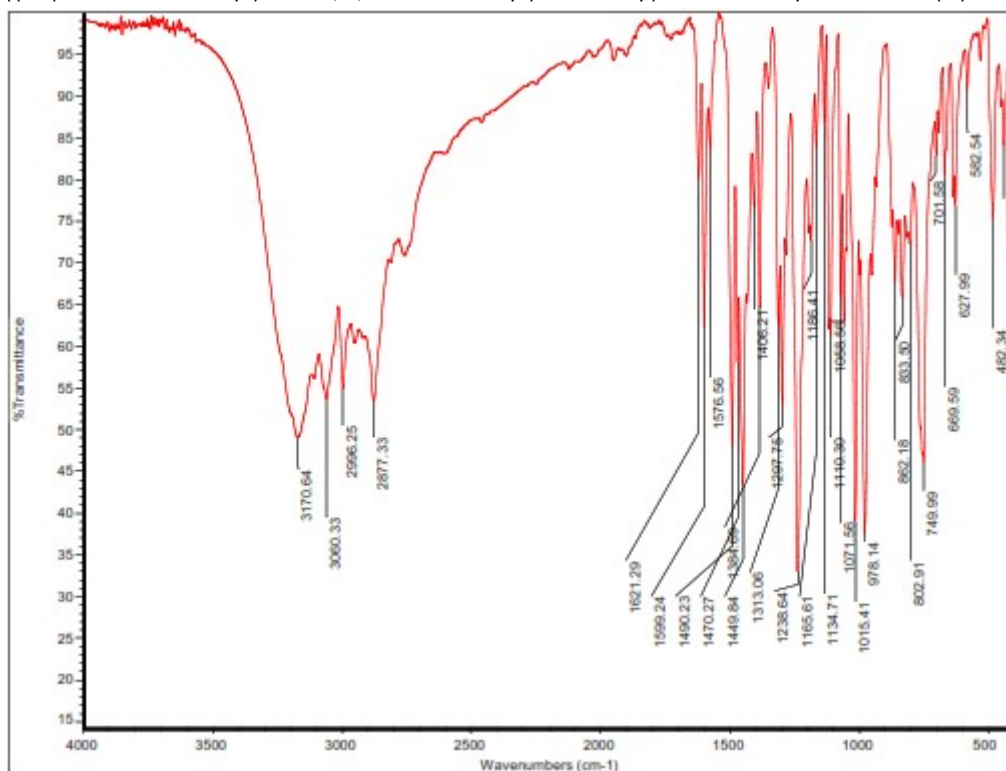
S21. O-propargylated salicylaldehyde



S22. 2-((1-benzyl-1H-1,2,3-triazol-5-yl)methoxy)benzaldehyde oxime (A)

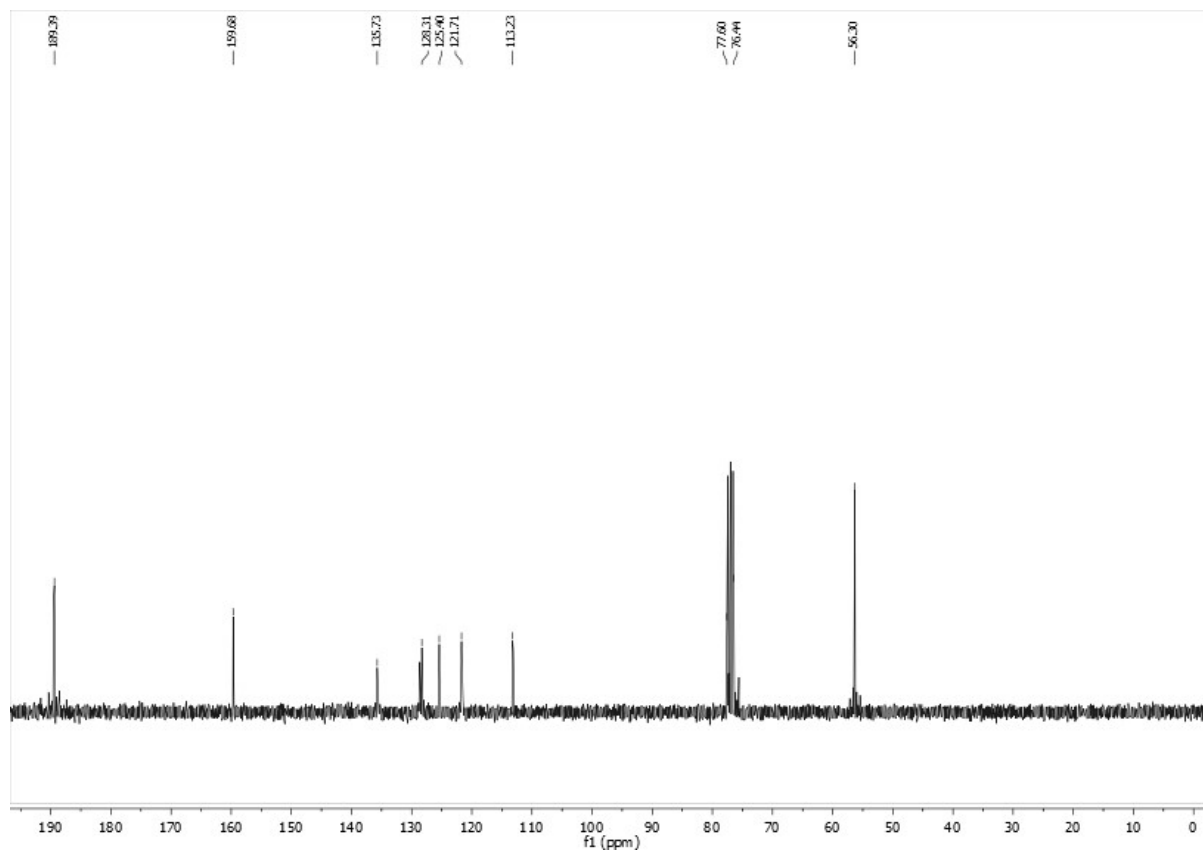
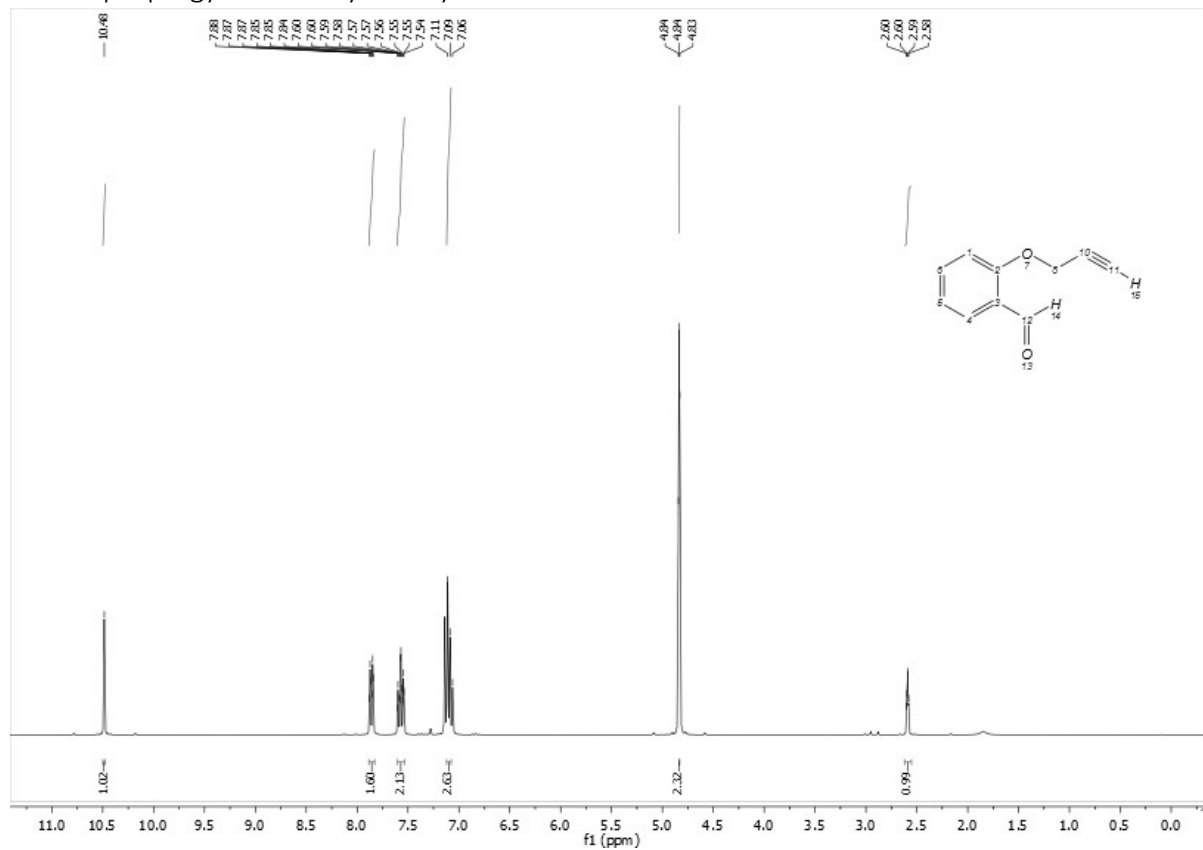


S23. 2-((1-(4-bromobenzyl)-1H-1,2,3-triazol-5-yl)methoxy)benzaldehyde oxime (B)

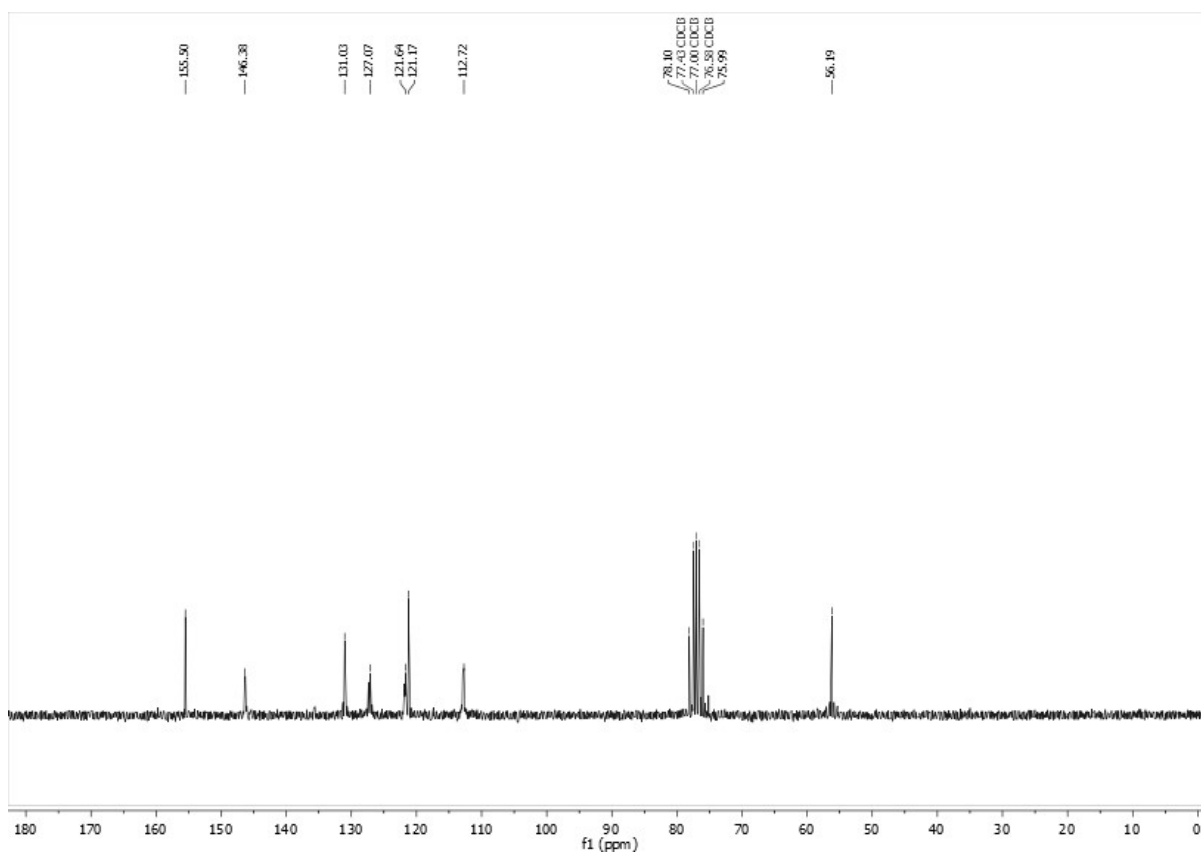
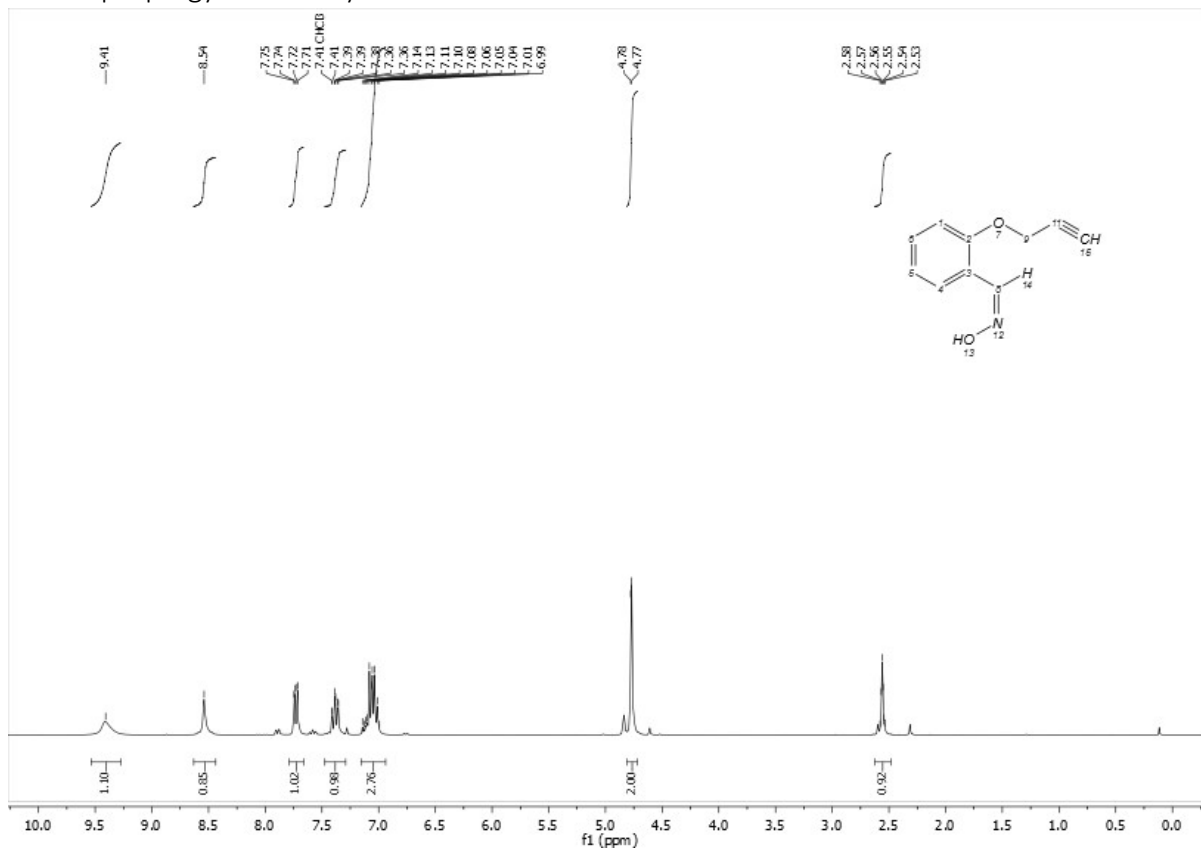


NMR spectra

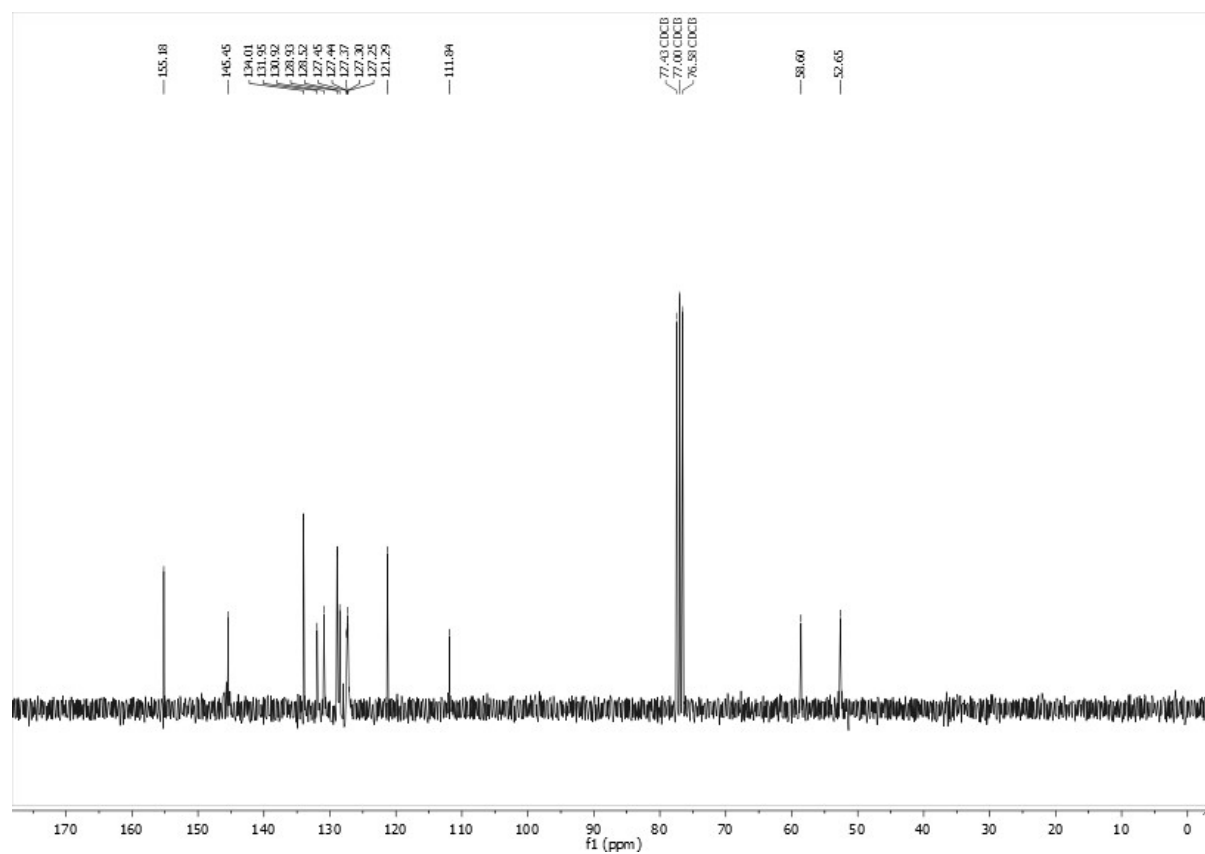
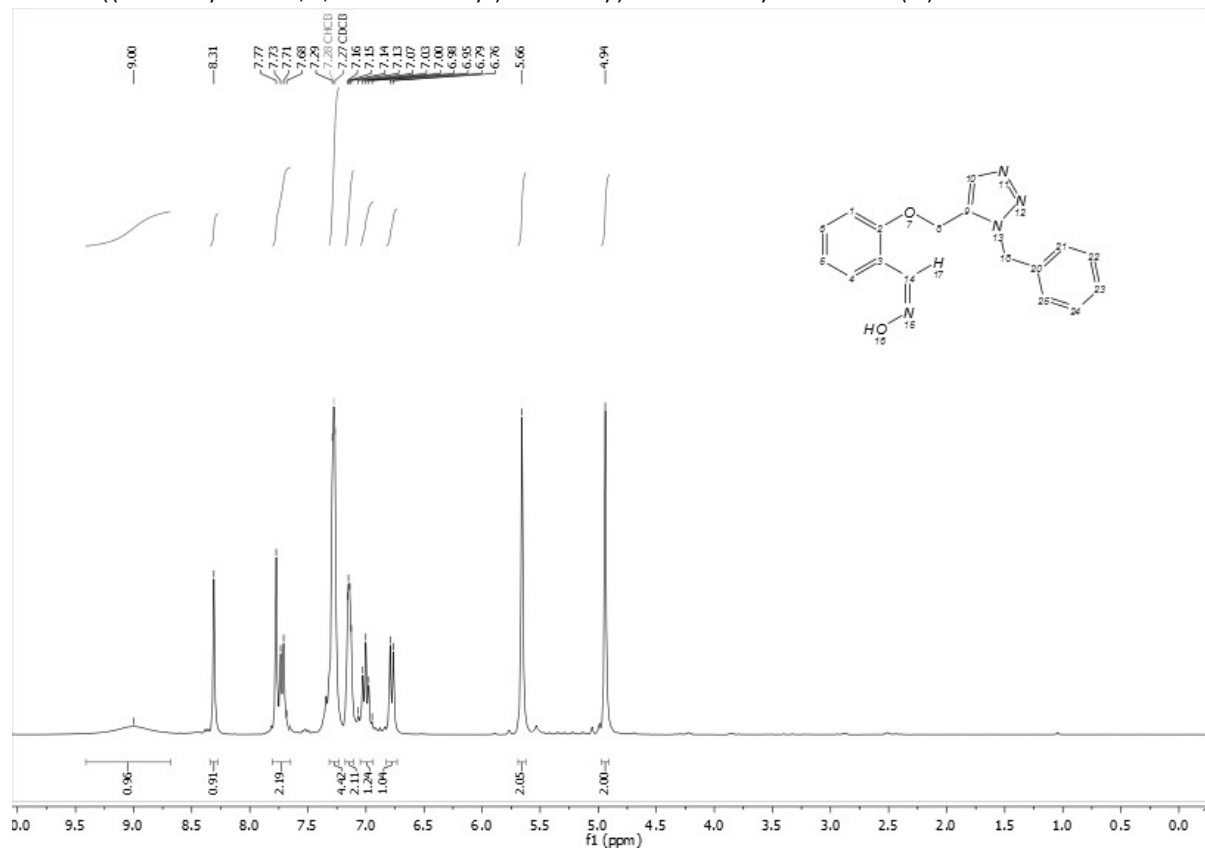
S24. O-propargylated salicylaldehyde



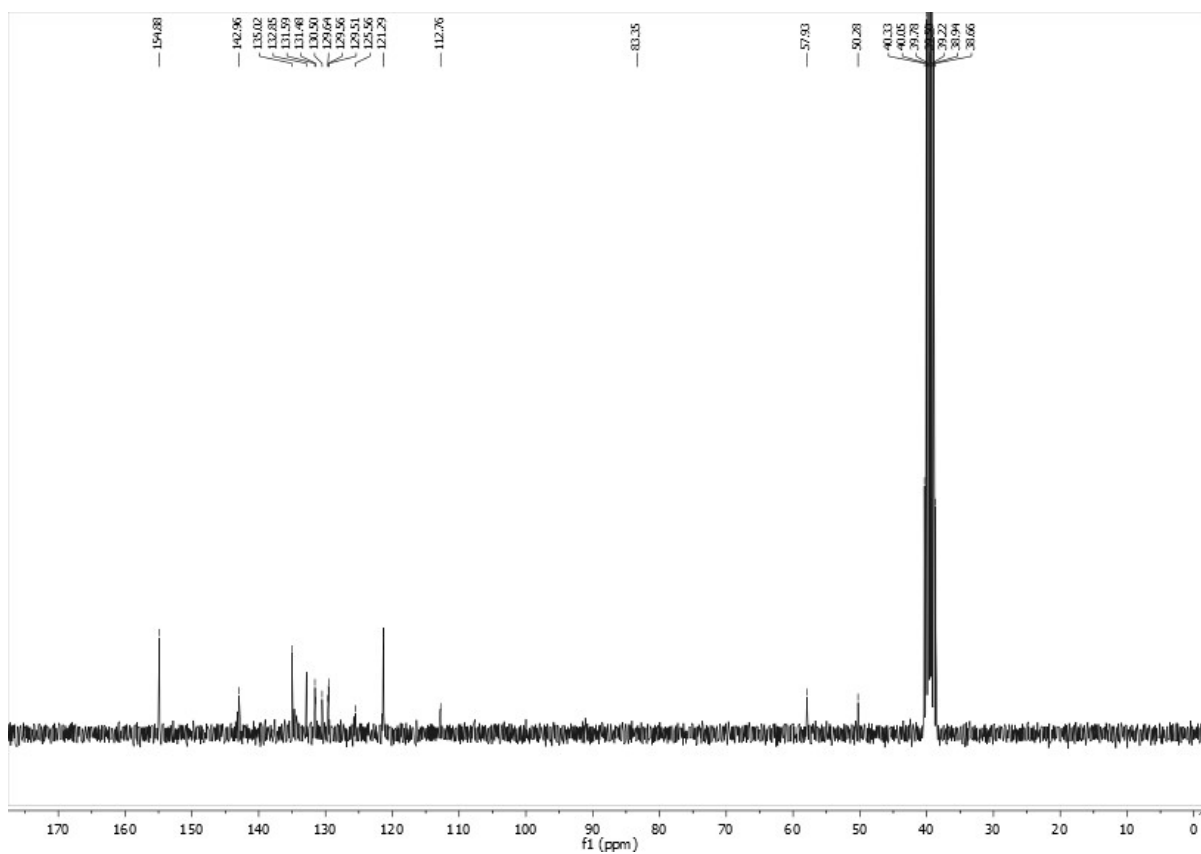
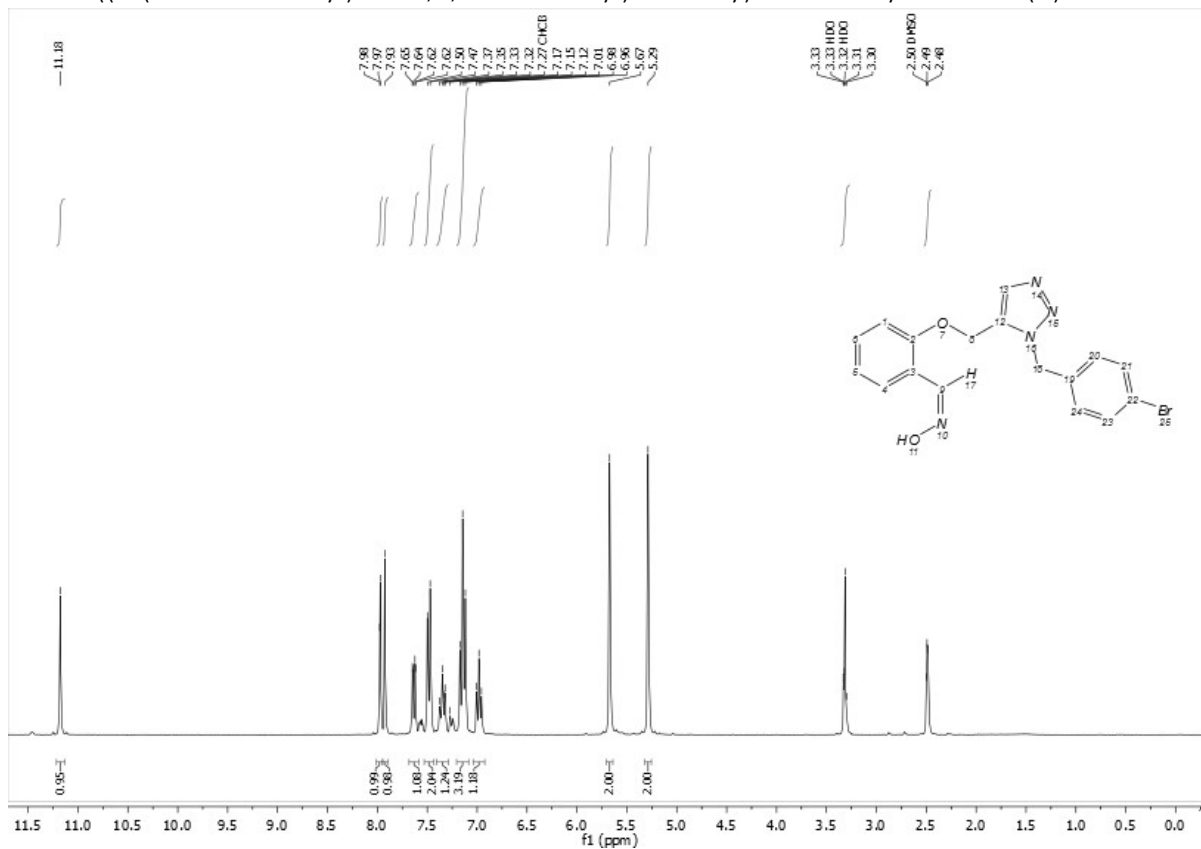
S25. O-propargylated salicyldoxime



S26. 2-((1-benzyl-1H-1,2,3-triazol-5-yl)methoxy)benzaldehyde oxime (A)

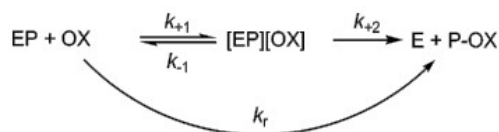


S27. 2-((1-(4-bromobenzyl)-1H-1,2,3-triazol-5-yl)methoxy)benzaldehyde oxime (B)



Determination of reactivation parameters

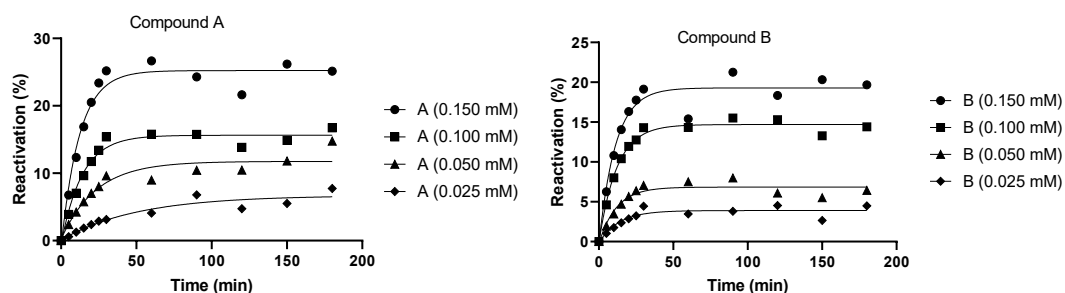
In order to determine the reactivation rate constant (k_{+2}), dissociation constant (K_{ox}) and second order reactivation rate constant (k_r) of the selected reactivators, the reactivation rate at different time intervals and at different concentrations were measured. Oxime reactivation of phosphylated cholinesterases proceeds according to following scheme.



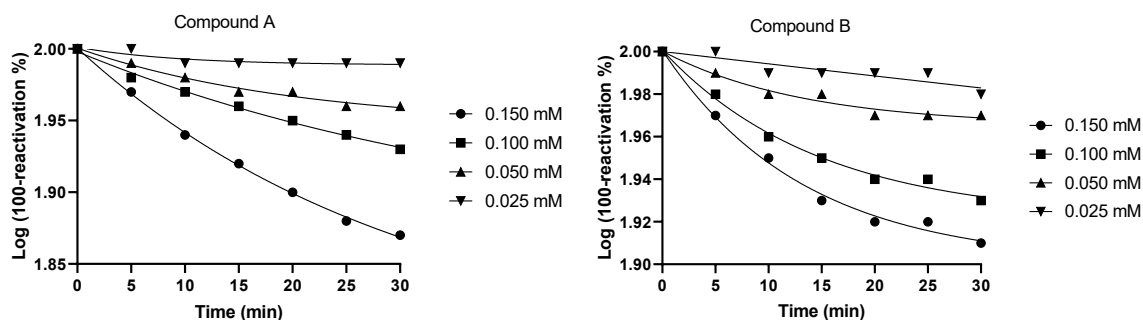
In this scheme, EP is the phosphylated enzyme, EP-OX is the reversible Michaelis-type complex between EP and the oxime (OX), E is the active enzyme and P-OX the phosphylated oxime. K_{ox} is equal to the ratio $(k_{-1} + k_{+2}) / k_{+1}$, and it typically approximates the dissociation constant of the EP-OX complex, where from it follows that: $k_r = k_{+2} / K_{ox}$.

Since k_{obs} vs $[\text{OX}]$ was linear, the slope corresponded to overall second-order rate constant of reactivation (k_r); in this case, maximum first-order rate constant (k_{+2}) and the dissociation constant of the phosphorylated enzyme-oxime complex (K_{ox}) could not be determined.

S28. Plot of reactivation vs time for compounds A and B.



S29. Plot of $\log(100 - \text{react.}\%)$ vs time for compounds A and B



S30. Plot of K_{obs} vs concentration for compounds A and B

