

SUPPORTING INFORMATION

Platination mechanism of RNase A by Arsenoplatin: Insights from theory

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Table S1 NBO charge values in |e| for every stationary point along the potential energy surface.

	APw	EAPw	TS	P
Pt	0.200	0.214	0.145	0.139
As	2.137	2.142	2.179	2.113
O_w	-0.841	-0.844	-0.906	-0.962
N_{His}	-	-0.533	-0.583	-0.514
N₁	-0.715	-0.712	-0.703	-0.707
N₂	-0.720	-0.725	-0.715	-0.709
O₁	-0.759	-0.763	-0.763	-0.774
O₂	-0.757	-0.759	-0.762	-0.767
O₃	-0.966	-0.977	-0.981	-1.024
O₄	-0.967	-0.969	-0.979	-0.972

MD simulation. We started from enzyme structure ((PDB id: 5NJ7) [1] prepared at physiological pH using PROPKA. [2] After removing water and co-crystallized ligand, the molecular dynamics simulation was carried out with only free protein. Antechamber modules of Amber16 [3] were used for generating preparatory files. MD simulation of 300 ns was performed by using FF14SB. [4] The free protein was protonated and counter ions (3Cl-) were added appropriately to make the total charge zero. The system was solvated in an orthorhombic box with a buffer of 10 Å, using TIP3P water model. The solvated structure was first minimized by applying positional harmonic restraints on all atoms (50 kcal mol⁻¹ Å²) using 5000 steps of steepest descent followed by 5000 steps of conjugate gradient (CG). In the second minimization step, the whole system was released without any restraint and then a progressive heating phase was carried out from 0 to 310 K for 50 ps, followed by 50 ps at 310 K using the Langevin thermostat in NVT ensemble. The production phase was performed for 100 ns of MDs under the following conditions: integration step of 2 fs coupling SHAKE algorithm [5],

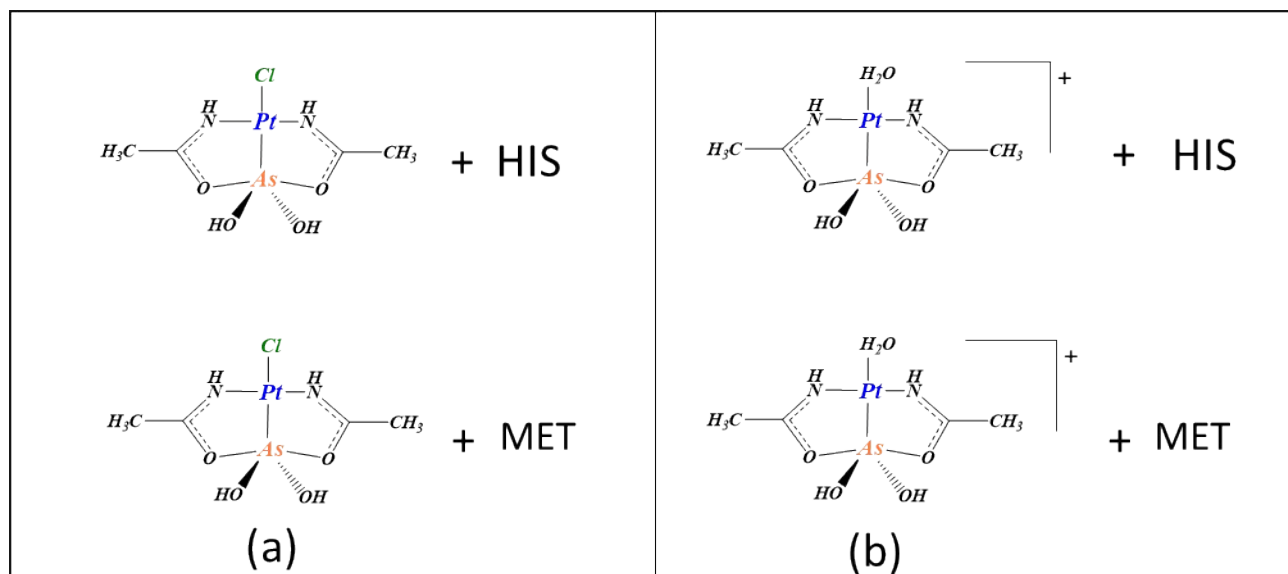
NPT ensemble at 1 bar pressure using the Berendsen barostat with a time constant $\tau_p = 2.0$ ps. The Particle mesh Ewald summation method was employed for the electrostatic potential and the long-range electrostatic interactions were calculated with 12 Å cut-off distance.

Table S2: Calculated pKa for ionizable residues of RNase A. Residues fully protonated (positively charged) or deprotonated (negatively charged) are highlighted in blue and red, respectively. Residues belonging to the catalytic triad are underlined

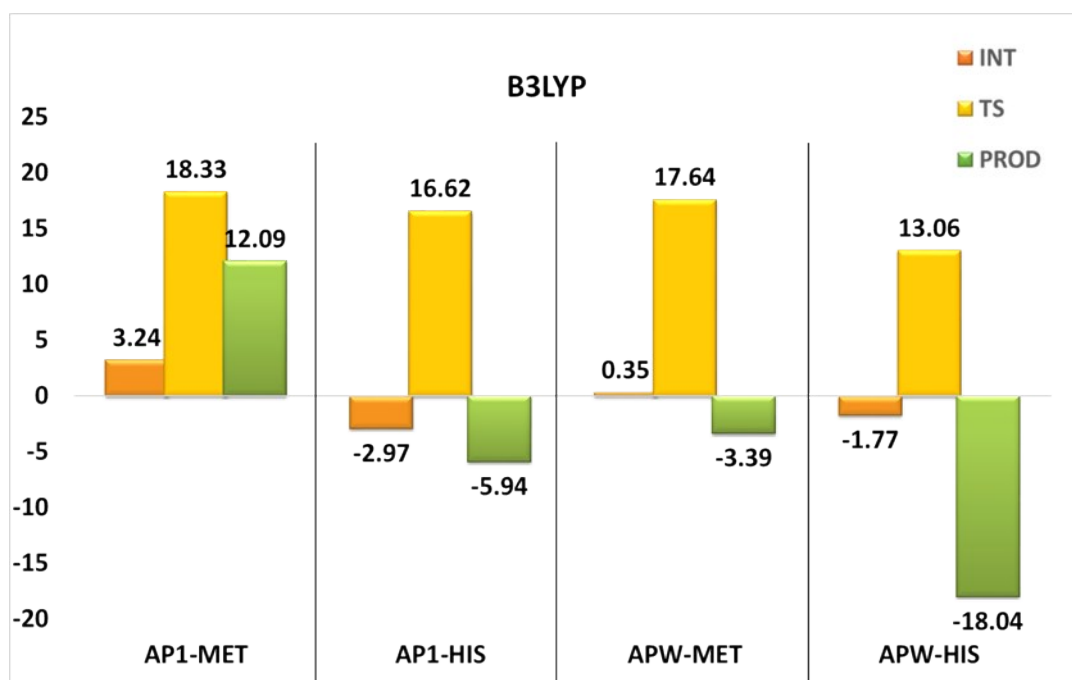
<i>Residue</i>	<i>pKa</i>	<i>Residue</i>	<i>pKa</i>
GLU2	2.87	TYR25	13.51
GLU9	4.71	TYR73	11.18
ASP14	0.12	TYR76	10.83
ASP38	4.22	TYR92	10.67
GLU49	4.04	TYR97	11.48
ASP53	4.70	TYR115	9.17
ASP83	3.88	LYS31	10.50
GLU86	4.05	LYS37	10.50
GLU111	4.57	LYS41	9.10
ASP121	2.62	LYS61	10.29
HIS12	1.37	LYS66	10.29
HIS48	5.02	LYS91	10.50
HIS105	7.19	LYS98	10.15
HIS119	5.83	LYS104	10.15
CYS26	-	LYS7	10.43
CYS40	-	ARG10	11.73
CYS58	-	ARG33	13.00
CYS65	-	ARG39	12.22
CYS72	-	ARG85	12.36
CYS84	-		
CYS95	-		
CYS110	-		

Table S3. H-bond intramolecular in apo-protein RNase A during MD simulation 100 ns.

Acceptor	Donor	Freq (%)	$\bar{d}$ (Å)
PHE-8	HIS-12	68.48	2.869
LYS-7	GLN-11	48.89	2.879
ALA-5	GLU-9	43.98	2.881
ALA-6	ARG-10	25.91	2.891
ALA-4	PHE-8	24.62	2.885
THR-3	LYS-7	18.82	2.875
THR-3	ALA-6	13.23	2.896
ALA-4	LYS-7	8.49	2.897
ALA-4	ALA-6	2.11	2.863
LYS-7	ARG-10	1.67	2.911
ALA-5	PHE-8	1.14	2.896
PHE-8	GLN-11	1.01	2.921
ALA-6	GLU-9	0.22	2.893
LYS-1	THR-3	0.19	2.861
THR-3	ALA-5	0.18	2.851
HIS-119	ASP-121	0.09	2.901
ALA-5	LYS-7	0.08	2.882
GLU-2	ALA-4	0.08	2.871
GLU-9	HIS-12	0.04	2.891
PHE-8	ARG-10	0.01	2.731



Scheme S1.



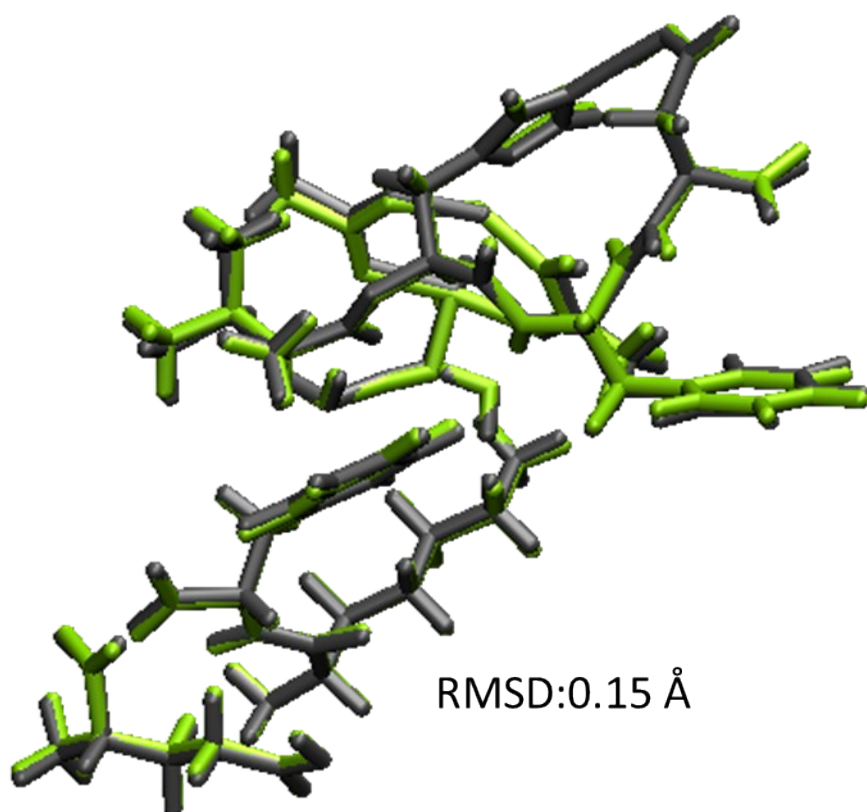
a)



b)

Figure S1

Prod_B3LYP + D3 (green)
Prod_M062X (Grey)



Overlap of the two structures
optimized in water with
B3LYP+D3 and M062X

Figure S2

References

- [1] Đ. Miodragović, A. Merlino, E. P. Swindell, A. Bogachkov, R. W. Ahn, S. Abuhadba, G. Ferraro, T. Marzo, A. P. Mazar, L. Messori and T. V. O'Halloran, *J. Am. Chem. Soc.*, **2019**, 141, 6453–6457.
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- [4] J. A. Maier, C. Martinez, K. Kasavajhala, L. Wickstrom, K. E. Hauser, C. Simemrlin. *J. Chem. Theory Comput.* **2015**, 11, 3696–3713.
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Coordinate of optimized structure

EAPw

N	11.03900000	4.88600000	101.11200000
H	10.74400000	3.99000000	101.47800000
H	11.72200000	5.28300000	101.74400000
H	10.23900000	5.50100000	101.04600000
C	11.65500000	4.69800000	99.76700000
H	10.88900000	4.40100000	99.05000000
C	12.36000000	5.97600000	99.29800000
H	11.76300000	6.83500000	99.60900000
H	13.31600000	6.03900000	99.82300000
C	12.57500000	6.10500000	97.79700000
H	12.94400000	5.16300000	97.39800000
H	11.62900000	6.33000000	97.30300000
C	13.62800000	7.17000000	97.49900000
H	14.22700000	7.38800000	98.38400000
H	14.31500000	6.78800000	96.74100000
C	13.02600000	8.47600000	96.99300000
H	12.16800000	8.74800000	97.60900000
H	13.77800000	9.26300000	97.07300000
N	12.61800000	8.34900000	95.56600000
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N	8.96443070	-6.34129943	105.60954956
H	8.74014435	-6.62636444	106.54713080
H	8.28160956	-6.43453954	104.86564394

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C	12.49729550	-9.71939673	101.32922692
H	12.04720124	-9.31927942	102.23929027
C	11.44639590	-9.66050136	100.26622627
H	11.88191677	-9.98300694	99.31981689
H	10.64848787	-10.35736879	100.53148571
C	10.83256285	-8.27965087	100.11134923
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H	11.54768513	-7.54789737	99.75485667
C	9.62296993	-8.27747086	99.19689081
O	8.62116791	-7.61902507	99.49061663
N	9.70096803	-9.02743215	98.09477631
H	8.91845155	-9.07762386	97.46192740
H	10.53527859	-9.56720858	97.91294862
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H	13.73509807	-13.51916721	101.89304083
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H	15.72996477	-12.05120028	100.96198113
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H	16.29097603	-16.28903145	98.63712064

TS

N	11.03900000	4.88600000	101.11200000
H	10.74400000	3.99000000	101.47800000
H	11.72200000	5.28300000	101.74400000
H	10.23900000	5.50100000	101.04600000
C	11.65500000	4.69800000	99.76700000
H	10.88900000	4.40100000	99.05000000
C	12.36000000	5.97600000	99.29800000
H	11.76300000	6.83500000	99.60900000
H	13.31600000	6.03900000	99.82300000
C	12.57500000	6.10500000	97.79700000
H	12.94400000	5.16300000	97.39800000
H	11.62900000	6.33000000	97.30300000

C	13.62800000	7.17000000	97.49900000
H	14.22700000	7.38800000	98.38400000
H	14.31500000	6.78800000	96.74100000
C	13.02600000	8.47600000	96.99300000
H	12.16800000	8.74800000	97.60900000
H	13.77800000	9.26300000	97.07300000
N	12.61800000	8.34900000	95.56600000
H	11.91500000	7.63000000	95.47000000
H	12.24000000	9.22800000	95.23900000
H	13.42000000	8.10800000	95.00000000
C	12.69300000	3.60400000	99.90200000
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H	7.93600000	-6.69900000	95.61300000
H	9.96100000	-5.58400000	93.77500000
H	5.10500000	-5.46300000	91.46700000
H	3.92200000	-4.29700000	92.06300000
H	6.20600000	-6.19600000	94.09100000
O	4.72000000	-2.17700000	93.50000000
H	11.45800000	-6.91700000	92.84900000
H	11.07400000	-8.81100000	91.38400000
H	10.24300000	-9.71600000	92.66100000
H	7.62611980	-9.84008203	91.78218596
H	7.01412335	-5.67752351	91.61438895
H	5.87623424	-7.99511492	91.74474392
H	14.99069524	-5.17815559	91.45235514
H	14.85747021	-4.98707543	93.20379696
H	14.44313539	-6.55160176	92.44561886
H	7.14959309	-1.26788915	90.13103211
H	6.55235334	-1.79796720	91.72140815
H	6.24572966	-2.80163915	90.27646541
H	10.05563702	-2.70071461	93.95875805
H	12.69900820	-1.92230686	90.98625049
H	7.58864171	-4.62740921	90.55229126
H	13.14400000	-5.75600000	96.87900000
H	12.87000000	-5.78800000	95.36400000
O	11.16170726	-6.41986045	89.75391380
H	10.30970726	-7.05486045	89.78591380
H	11.27270726	-6.13186045	88.83091380
H	12.12800000	-9.50400000	94.08100000
H	12.23072230	-6.77261325	91.88877485
C	13.20800000	1.52700000	99.10500000
H	13.54500000	1.06800000	98.17000000
H	6.39100000	-3.78300000	92.53000000
N	16.24900000	-7.24700000	98.15000000
H	16.16800000	-6.35600000	97.67900000
C	17.22700000	-7.38800000	99.24600000
H	17.84600000	-8.25300000	99.04500000
C	18.13100000	-6.16900000	99.36900000
H	17.54000000	-5.28500000	99.61100000
H	18.82400000	-6.35500000	100.19000000
C	18.91400000	-5.89200000	98.11500000
H	19.43600000	-6.80700000	97.82800000
H	18.26000000	-5.63300000	97.30500000
C	19.95800000	-4.80900000	98.30400000
O	20.50500000	-4.66700000	99.42700000
O	20.24900000	-4.12600000	97.30200000
C	16.53500000	-7.58800000	100.56700000

O	16.93400000	-8.49500000	101.33900000
N	15.49700000	-6.77600000	100.81700000
H	15.24300000	-6.06000000	100.15400000
C	14.65800000	-6.98700000	101.98300000
H	15.29300000	-6.86200000	102.86100000
C	13.51400000	-5.96500000	102.09100000
H	13.94600000	-4.96300000	102.06200000
H	12.85600000	-6.07300000	101.22700000
C	12.70100000	-6.10800000	103.39000000
H	12.17300000	-7.06100000	103.38900000
H	13.38200000	-6.09300000	104.24200000
C	11.67800000	-4.98300000	103.57100000
H	12.06442906	-4.23942757	104.26761296
H	11.50666826	-4.49891512	102.60847038
N	10.41552381	-5.52720689	104.05417465
H	9.70081934	-5.69551205	103.35621127
C	10.13135770	-5.82001606	105.32505521
N	10.99279931	-5.61788606	106.31265474
H	11.87069135	-5.18938166	106.09063324
H	10.74012496	-5.81476899	107.26826490
N	8.96443070	-6.34129943	105.60954956
H	8.74014435	-6.62636444	106.54713080
H	8.28160956	-6.43453954	104.86564394
C	14.04700000	-8.37600000	102.05000000
O	14.08400000	-9.02100000	103.10600000
N	13.43000000	-8.82500000	100.96700000
H	13.77381392	-8.58353087	100.05194937
C	12.49729550	-9.71939673	101.32922692
H	12.04720124	-9.31927942	102.23929027
C	11.44639590	-9.66050136	100.26622627
H	11.88191677	-9.98300694	99.31981689
H	10.64848787	-10.35736879	100.53148571
C	10.83256285	-8.27965087	100.11134923
H	10.50793898	-7.94061949	101.07868116
H	11.54768513	-7.54789737	99.75485667
C	9.62296993	-8.27747086	99.19689081
O	8.62116791	-7.61902507	99.49061663
N	9.70096803	-9.02743215	98.09477631
H	8.91845155	-9.07762386	97.46192740
H	10.53527859	-9.56720858	97.91294862
C	12.82435555	-11.20654728	101.62681888
O	12.10798088	-12.10183767	101.16722292
N	13.86884581	-11.49134748	102.40094997
H	14.42720704	-10.74822380	102.79373990
C	14.40136457	-12.84551458	102.42735542
H	13.73509807	-13.51916721	101.89304083
C	15.72665530	-12.85808303	101.66471100
C	15.94383756	-14.14061669	100.93017354
N	16.02542437	-15.34760223	101.58137897
H	16.00218146	-15.46555954	102.58478360
C	16.18503141	-16.31979841	100.70065757
H	16.35122927	-17.36219614	100.92848040
N	16.18684689	-15.78553120	99.49481792
C	16.02228230	-14.42273157	99.60673612
H	15.96852912	-13.71125968	98.79708660

C	14.58462714	-13.50156562	103.76497714
O	14.84255180	-14.67543090	103.80574690
H	16.52791155	-12.71651713	102.35958329
H	15.72996477	-12.05120028	100.96198113
O	14.27849467	-12.75268266	105.02809124
O	10.92298677	1.28042662	98.35223432
H	16.29097603	-16.28903145	98.63712064

Coordinate of optimized stucture using B3LYP functional

AP1-MET:

INT

Pt	-0.61004100	-0.72892500	-0.71975600
As	-2.16448900	0.56536500	0.46456100
Cl	0.88670800	-2.07247300	-2.03999500
O	-2.03973500	2.07124700	-0.85815600
O	-2.52198100	-0.97367200	1.78277400
O	-1.83772400	1.64970300	1.81000100
H	-0.96219900	2.08312000	1.63351100
O	-3.90862900	0.66960100	0.27733300
H	-4.31834200	-0.03037500	0.82091600
N	-0.45623900	0.86150100	-1.98375800
H	0.19573100	0.86475100	-2.76314300
N	-0.95106800	-2.19985900	0.65906500
H	-0.46353800	-3.09052600	0.62341000
C	-1.16975500	1.94787700	-1.82424400
C	-1.03386800	3.14345600	-2.72317500
H	-2.01873700	3.41868700	-3.11288600
H	-0.35082300	2.95609200	-3.55429900
H	-0.66044800	3.98668600	-2.13169700
C	-1.82601400	-2.06344300	1.62783700
C	-2.08787500	-3.15250800	2.63142000
H	-1.87035800	-2.77210200	3.63494200
H	-1.48277100	-4.04178200	2.44214700
H	-3.14879100	-3.42123000	2.60010600
N	2.95025500	-1.63949700	0.39953100
C	3.46431300	-0.22029000	0.33617800
C	4.97518400	-0.30366700	-0.05423800
O	5.53998500	0.79339400	-0.26343600
C	3.24462700	0.51158400	1.66185400
C	1.78515900	0.90821000	1.91999700
S	1.19099300	2.28478500	0.85328800
C	1.92434700	3.71495800	1.72778900
H	3.59921600	-0.11885200	2.48938200
H	3.88282600	1.39946000	1.65580100
H	1.10057300	0.07609800	1.72435600
H	1.64614200	1.20641300	2.96405600
H	1.58895400	4.61466800	1.20518500
H	1.58133700	3.74937200	2.76579500
H	3.01641400	3.67349100	1.69638200
H	2.92298100	0.28528900	-0.46754700
H	2.48447800	-1.87996600	1.27749100

H	2.30111800	-1.85717800	-0.37710400
H	3.81209800	-2.21798000	0.29216000
O	5.46410800	-1.47048200	-0.11421600

TS

Pt	0.76299700	-0.28009000	0.36331000
As	2.81610000	0.61695800	-0.30824500
Cl	-0.53666400	-1.14089100	2.48867400
O	2.15978200	2.53017700	-0.05059200
O	3.60820900	-1.21146300	-0.66289000
O	3.26955900	1.03657300	-1.97584500
H	3.03415700	1.97046500	-2.13341600
O	4.26367100	1.06495100	0.62368500
H	4.87468100	0.30367300	0.63368000
N	0.18006000	1.65091700	0.68932100
H	-0.71613000	1.87249100	1.11198200
N	1.60587600	-2.10541000	-0.00370500
H	1.09565200	-2.96746400	0.16448100
C	0.95691400	2.67514700	0.43191500
C	0.51942400	4.09374500	0.67157400
H	1.21624000	4.57217100	1.36732600
H	-0.49399100	4.14976700	1.07493600
H	0.56287400	4.64374900	-0.27427500
C	2.83881000	-2.23993200	-0.42375500
C	3.46601300	-3.58578100	-0.65918600
H	3.80555000	-3.64673800	-1.69817000
H	2.77100200	-4.40335000	-0.45595900
H	4.34529900	-3.68804600	-0.01461600
N	-5.32612000	-0.15946500	1.45897400
C	-5.21922900	0.32783700	0.02706100
C	-6.63218200	0.11105200	-0.61745200
O	-6.72657500	0.39471400	-1.83011800
C	-4.09147400	-0.37269400	-0.73211400
C	-2.70797300	-0.02533100	-0.17498700
S	-1.34269500	-0.87523300	-1.05578500
C	-1.12538900	0.22864300	-2.49664100
H	-4.24942400	-1.45881300	-0.71311700
H	-4.17755900	-0.05628000	-1.77502500
H	-2.52843700	1.05382900	-0.22810000
H	-2.58597800	-0.33776000	0.86661400
H	-0.90241500	1.24180600	-2.15345500
H	-0.27703700	-0.15804600	-3.06569100
H	-2.02124600	0.22130400	-3.12287400
H	-5.03485000	1.40453700	0.07538500
H	-4.83422100	-1.04198900	1.62456800
H	-5.00423900	0.51644100	2.15516700
H	-6.35372200	-0.33556400	1.56874200
O	-7.52627600	-0.30849200	0.17578800

PROD

Pt	0.51489100	-0.01769000	-0.09017100
As	2.83836800	-0.05691300	-0.54483800
Cl	1.12551000	-0.06272200	3.73055500
O	2.93241600	1.94790900	-0.70477000
O	2.92507500	-2.05949500	-0.41328700
O	3.63117700	-0.20640700	-2.11371900
H	3.79863700	0.68716100	-2.47011600
O	4.13273900	0.06588500	0.64533900
H	4.37005400	-0.83193500	0.94712300
N	0.67662200	2.01978800	-0.28783200
H	-0.10383800	2.65983900	-0.18385300
N	0.67222100	-2.05632000	0.01913400
H	-0.12701200	-2.65314200	0.21308000
C	1.82013700	2.61089000	-0.54696200
C	1.94065700	4.10274800	-0.68028000
H	2.66511300	4.46655700	0.05555800
H	0.98524800	4.60966200	-0.53014600
H	2.32811100	4.34225700	-1.67585700
C	1.80798400	-2.68746100	-0.15798100
C	1.91606900	-4.18427800	-0.08737900
H	2.30289400	-4.55767300	-1.04121400
H	0.95462200	-4.65656900	0.12405800
H	2.63481700	-4.45484900	0.69279500
N	-4.97662800	-1.20508200	-1.63799000
C	-4.97253700	-0.35182800	-0.38722300
C	-6.47487800	-0.10074600	-0.01605800
O	-6.67219600	0.63719800	0.97188000
C	-4.18584100	0.94467600	-0.57280200
C	-2.68350200	0.78330200	-0.82934600
S	-1.79180200	-0.08186600	0.53469600
C	-1.93915500	1.11136700	1.91203400
H	-4.60414600	1.51364600	-1.41400400
H	-4.35907100	1.55099200	0.32005900
H	-2.46693800	0.18339300	-1.71796300
H	-2.22113300	1.76263700	-0.97460100
H	-1.20138800	0.80303300	2.65787200
H	-1.72341100	2.12501000	1.56811200
H	-2.94969000	1.05561600	2.32269700
H	-4.53372100	-0.96223600	0.40584400
H	-4.66439600	-0.70813700	-2.47693700
H	-4.42519500	-2.06252400	-1.55582000
H	-5.99305400	-1.43710200	-1.75520400
O	-7.31647100	-0.69536800	-0.75172500

AP1-HIS:

INT

Pt	1.37690800	-0.05925900	-0.67362600
As	0.40512200	1.56604900	0.71112300
Cl	2.18869300	-1.90089500	-1.99863900
O	-0.65680200	2.34391700	-0.90712000
O	1.55486800	1.05185500	2.27094700
O	0.85042300	3.23234300	1.05916400

H	0.45021400	3.80240100	0.37530900
O	-1.07146800	1.34444100	1.60034300
H	-1.19315700	0.34608500	1.74970300
N	0.20153100	0.65379000	-2.18241700
H	0.16861600	0.19977200	-3.09069700
N	2.44579300	-0.61035900	0.97282600
H	3.07548300	-1.40756600	0.95965600
C	-0.59490000	1.68835400	-2.02491200
C	-1.50899100	2.16295500	-3.12080200
H	-2.54202700	1.98848600	-2.80021600
H	-1.33179700	1.63968600	-4.06323700
H	-1.37601300	3.23894300	-3.26835300
C	2.33771100	0.01902400	2.11719600
C	3.10385800	-0.39684700	3.34141500
H	3.70069300	0.44903500	3.69747200
H	3.75994900	-1.24766100	3.14564100
H	2.39392900	-0.66035200	4.13246900
N	-0.81835800	-3.09924000	-1.00299100
C	-1.50105500	-2.05092700	-0.16315300
C	-0.92506500	-2.20116200	1.27121700
O	-0.41840300	-3.31635600	1.54636600
C	-3.03705700	-2.22758000	-0.18900100
C	-3.72753100	-0.94343800	0.15437700
N	-3.73088700	0.11614300	-0.73846900
C	-4.37603200	-0.58298800	1.31218300
C	-4.37122700	1.09710000	-0.12634900
N	-4.78109800	0.72076100	1.11687200
H	-3.33979500	-2.52586200	-1.20131300
H	-3.34054100	-3.02988500	0.49184200
H	-4.56489200	-1.11518300	2.23233500
H	-5.29263700	1.29299200	1.77638500
H	-4.56439000	2.08193800	-0.52920600
H	-1.24867700	-1.08550900	-0.59770000
H	0.10920900	-2.77310500	-1.32794200
H	-1.35919000	-3.38253300	-1.82433600
H	-0.65016700	-3.91140500	-0.38742900
O	-1.06456900	-1.21833800	2.05385900

TS

Pt	-0.42309900	-0.01057600	-0.45920400
As	-2.52768700	0.52670300	0.41191800
Cl	0.85420300	0.03909500	-2.75078800
O	-3.28124900	-1.30338800	-0.04010900
O	-1.93621900	2.38554800	0.96960300
O	-3.95713100	1.28325000	-0.32671500
H	-4.53647400	0.57817900	-0.67330300
O	-3.04952200	0.22035100	2.08574600
H	-2.86433500	1.01623600	2.61928000
N	-1.22298400	-1.83828700	-0.88574400
H	-0.67065800	-2.56086100	-1.33792300
N	0.09689900	1.91193700	0.03005600
H	0.99682200	2.30862400	-0.21997800
C	-2.46675100	-2.14528900	-0.61685800

C	-3.05239300	-3.48971900	-0.94938900
H	-3.39994300	-3.96693200	-0.02722900
H	-2.32902200	-4.14142800	-1.44407000
H	-3.92127700	-3.35056500	-1.60083600
C	-0.72300100	2.73346300	0.63715100
C	-0.33074400	4.13936400	0.99874100
H	-1.03366100	4.83952300	0.53610700
H	0.68570300	4.37786600	0.67823100
H	-0.40468400	4.26146000	2.08448600
N	3.78061800	0.82317900	-1.74948700
C	3.62390000	0.33821900	-0.33197600
C	4.93774300	0.62049100	0.44595700
O	5.97070900	0.77249000	-0.26434000
C	3.26670300	-1.16730900	-0.35813800
C	2.43841900	-1.57012000	0.81671300
N	1.14105200	-1.10862300	0.97498000
C	2.75072900	-2.38761500	1.87488500
C	0.68168600	-1.63415100	2.10310900
N	1.62760600	-2.41518500	2.67688500
H	2.69377100	-1.37798000	-1.26795600
H	4.18213000	-1.76666500	-0.39979500
H	3.65181500	-2.92704300	2.12385600
H	1.52602400	-2.92844300	3.54355600
H	-0.30522100	-1.48376100	2.51465400
H	2.79915700	0.90671100	0.09753600
H	3.95716700	1.83092300	-1.77563500
H	2.91646500	0.62306400	-2.29555600
H	4.59663700	0.37814300	-2.18248200
O	4.83259200	0.63261500	1.69669800

PROD

Pt	-0.43394000	0.36373800	-0.57268500
As	-2.34567500	-0.80655600	0.10395500
Cl	1.30561200	0.52632300	4.28281700
O	-3.27628900	0.89186900	0.70464000
O	-1.58481000	-2.57291400	-0.43908700
O	-2.65756700	-1.50704500	1.69194300
H	-3.10454400	-0.83929700	2.24663000
O	-3.78100100	-1.13640800	-0.86520500
H	-3.66861400	-2.00054900	-1.30548100
N	-1.42355600	2.05737400	0.01704200
H	-1.01384300	2.98391000	-0.06042900
N	0.33048900	-1.46330300	-1.06156300
H	1.32409900	-1.56676200	-1.32189200
C	-2.62534700	2.01315500	0.54222900
C	-3.35190700	3.24806300	0.99688000
H	-4.29106100	3.33489900	0.44059500
H	-2.75836700	4.15282800	0.85005700
H	-3.60190700	3.14558500	2.05788200
C	-0.35119100	-2.56449600	-0.89174600
C	0.22606700	-3.91643400	-1.20200700
H	0.16329800	-4.54874600	-0.31046000
H	1.26574300	-3.84269900	-1.52742400

H	-0.37062100	-4.39052400	-1.98882500
N	3.23058000	-0.95113100	2.33034700
C	2.76277500	-0.59584100	0.94762300
C	3.71628200	-1.24164400	-0.09276800
O	4.91668000	-1.35861600	0.26254200
C	2.73425900	0.94718100	0.84533000
C	2.49702100	1.47436600	-0.53265400
N	1.28441300	1.36496900	-1.20457800
C	3.36774800	2.14633200	-1.35146400
C	1.42387500	1.94888700	-2.39282100
N	2.67566000	2.43238400	-2.50909800
H	1.96243500	1.31931800	1.52881900
H	3.69769800	1.33891800	1.19082100
H	4.39663300	2.43692400	-1.20696400
H	3.03811600	2.93156700	-3.31228100
H	0.66050800	2.03091100	-3.15047100
H	1.75818000	-1.00292000	0.85299300
H	3.13653000	-1.95612900	2.50168400
H	2.66769900	-0.44558300	3.06662800
H	4.22948300	-0.73090000	2.41908500
O	3.19387900	-1.55350200	-1.19940800

APW-HIS

INT

Pt	-1.78636500	-0.11481500	0.82893200
As	-0.81491600	-0.64657100	-1.22601000
O	0.08637300	-2.25710000	-0.49369600
O	-1.79835100	0.87077500	-2.14778200
O	0.65960000	0.02887100	-1.84139400
H	1.49503500	-0.52044300	-1.66112300
O	-1.48945600	-1.72318700	-2.45223900
H	-2.02925600	-1.18856300	-3.06573000
N	-0.77471700	-1.73410500	1.55909100
H	-0.80972400	-2.01370200	2.53521900
N	-2.72147100	1.41884800	-0.13140400
H	-3.34102700	2.06126100	0.35413700
C	-0.04810500	-2.49804000	0.78288100
C	0.68312800	-3.70837000	1.29152600
H	0.33481300	-4.59414500	0.75015400
H	0.52985400	-3.85607900	2.36234200
H	1.75323300	-3.59523800	1.08977500
C	-2.57159700	1.62499500	-1.41658400
C	-3.27461400	2.73951100	-2.14107700
H	-2.52948200	3.40658300	-2.58715800
H	-3.92176100	3.31457700	-1.47574000
H	-3.87373600	2.31929100	-2.95543800
O	-2.69179400	0.49619600	2.74368900
H	-2.01084000	0.72562000	3.40202800
H	-3.22196500	-0.21806500	3.14214600
N	5.15809300	-0.26444400	1.02975000
C	3.95805500	-0.01732000	0.13789800
C	3.87520600	-1.24774400	-0.81882200

O	2.92841500	-1.25584700	-1.65126400
C	4.06380800	1.31925600	-0.60085000
C	4.04161200	2.57140500	0.29163300
S	2.54207800	2.79470700	1.32858900
C	1.29314500	3.21296400	0.05700300
H	4.98642700	1.33637500	-1.19909100
H	3.23641900	1.35489900	-1.31468500
H	4.87577900	2.57598800	1.00196900
H	4.16296400	3.45979300	-0.33722300
H	0.37703600	3.47334700	0.59399000
H	1.61907500	4.07727600	-0.52979000
H	1.08794800	2.36478900	-0.60021700
H	3.07791100	-0.01511200	0.78621600
H	5.92722700	0.39203800	0.86945300
H	4.93736700	-0.25086500	2.02839600
H	5.48201000	-1.21838100	0.74777900
O	4.76183100	-2.12672400	-0.66942800

TS

Pt	-1.32237600	-0.26656400	-0.76697600
As	-1.46184100	0.99187100	1.18194500
O	-0.77063100	2.64516500	0.27319300
O	-2.13158900	-0.55732900	2.25609900
O	-0.14004500	1.11248800	2.34865200
H	0.41187100	1.88414800	2.11848600
O	-2.76771800	1.99207600	1.82096300
H	-3.32050400	1.44827900	2.41467300
N	-0.68538600	1.44809700	-1.67237900
H	-0.47221300	1.48272700	-2.66557100
N	-2.01996500	-1.82323900	0.35449600
H	-2.18771400	-2.74506000	-0.03833100
C	-0.51989400	2.56359800	-1.00756900
C	-0.02827000	3.82858800	-1.65049100
H	0.15489700	3.70088300	-2.71915900
H	0.89800900	4.14133000	-1.15755000
H	-0.77000900	4.61929200	-1.49842000
C	-2.29806200	-1.69155000	1.62699400
C	-2.82321900	-2.82182000	2.46440500
H	-2.12461800	-3.01143100	3.28579800
H	-2.95550400	-3.73562200	1.88162200
H	-3.78185700	-2.52671500	2.90303600
N	4.43541700	1.55664400	0.07365100
C	4.37940000	0.13129200	0.58608400
C	5.86769100	-0.31697800	0.79654500
O	6.03663000	-1.50831500	1.13082000
C	3.59096800	-0.78395500	-0.35005400
C	2.10365300	-0.42772000	-0.40586300
S	1.12092800	-1.56506500	-1.46408100
C	1.02262000	-3.03143500	-0.37880400
H	4.02966600	-0.75821100	-1.35590500
H	3.72728500	-1.79916200	0.03118300
H	1.65995700	-0.43049800	0.59522400
H	1.93223500	0.56389400	-0.83678200

H	0.37226300	-3.75557800	-0.87613500
H	2.00984100	-3.47728100	-0.23633400
H	0.58580800	-2.75296900	0.58316400
H	3.90303600	0.17227600	1.56971300
H	4.22630300	1.63284300	-0.92580100
H	3.82739500	2.20751300	0.57536900
H	5.44240200	1.81336100	0.21129400
O	6.73121600	0.59462500	0.62880400
O	-1.91282400	-1.17475700	-2.84323800
H	-1.48692100	-2.03206800	-3.02118400
H	-2.87049200	-1.34292600	-2.89333500

PROD

Pt	-0.48467100	0.06919800	0.05362200
As	-2.79386500	0.25638200	-0.42440800
O	-2.94934900	-1.71553000	-0.84126400
O	-2.83489100	2.20166600	-0.02674400
O	-3.66206900	0.61641000	-1.90688100
H	-3.86841200	-0.21996100	-2.36755100
O	-4.01805500	-0.03134700	0.82830000
H	-4.25776500	0.81828700	1.24714500
N	-0.71976300	-1.92778100	-0.34719800
H	0.03350900	-2.60538900	-0.29185600
N	-0.58350900	2.08409600	0.40450600
H	0.23094200	2.62977000	0.67270200
C	-1.87231100	-2.43842900	-0.72052900
C	-2.03848800	-3.89850100	-1.02964200
H	-2.79343300	-4.31859500	-0.35717000
H	-1.10434300	-4.45288000	-0.91948200
H	-2.40781900	-4.00534900	-2.05463300
C	-1.70106800	2.76243300	0.31301700
C	-1.77737600	4.23717900	0.58289900
H	-2.13526400	4.74503100	-0.31870200
H	-0.81039700	4.65140800	0.87452000
H	-2.50700800	4.41730200	1.37889500
N	4.93407900	1.22967000	-1.47694400
C	4.96955900	0.32472800	-0.26342800
C	6.48411800	0.08847600	0.06837400
O	6.71717500	-0.70380900	1.00492900
C	4.19770000	-0.97539800	-0.48142100
C	2.68731500	-0.82732300	-0.69969100
S	1.81925800	-0.01290800	0.71061400
C	1.90317500	-1.29792300	2.00741600
H	4.60385300	-1.50659800	-1.35254000
H	4.40201000	-1.61296100	0.38245400
H	2.44330300	-0.20167000	-1.56300400
H	2.23430500	-1.80763600	-0.86660800
H	1.29797400	-0.93729200	2.84086600
H	1.50661400	-2.24633700	1.64086600
H	2.94093000	-1.41131400	2.32726900
H	4.53935600	0.89640000	0.56263000
H	4.64688800	0.75365800	-2.33693700
H	4.34243100	2.05594000	-1.36046000

H	5.93886200	1.51172800	-1.58256700
O	7.29711700	0.75227800	-0.63973300
O	-2.55949800	-1.80111300	2.67536400
H	-3.15234900	-1.23010600	2.15025500
H	-1.68525000	-1.67670500	2.27076000

APW-HIS:

INT

Pt	1.17431400	-0.76901900	-0.71653100
As	0.87055400	0.20524700	1.37810300
O	0.15802600	-1.49040500	2.15148000
O	1.82838200	1.90661500	0.78657200
O	-0.51311000	1.12194600	1.86560600
H	-1.35136700	0.61229400	1.60086000
O	1.98347100	0.20150200	2.73810600
H	2.56464500	0.98197400	2.66020700
N	0.18009100	-2.38569600	0.05044300
H	-0.09870000	-3.18526000	-0.51135500
N	2.14058800	0.94002200	-1.25853300
H	2.53132500	1.06395500	-2.18848400
C	-0.14320000	-2.44723500	1.32040600
C	-0.90508300	-3.59986200	1.90641200
H	-0.41526300	-3.93225700	2.82609100
H	-0.98613700	-4.43618300	1.20877100
H	-1.90982900	-3.24576600	2.16228500
C	2.28867600	1.94570900	-0.43075900
C	3.00846200	3.20736600	-0.81761700
H	2.34703800	4.06470100	-0.65877400
H	3.33611100	3.19053500	-1.85911700
H	3.87838600	3.33552500	-0.16497300
O	1.57543200	-1.63377500	-2.70418700
H	0.76069300	-1.78583500	-3.21688400
H	2.01751500	-2.50018400	-2.64042700
N	-3.03090000	-1.38262600	-2.13106400
C	-2.60997000	-0.36324400	-1.09539500
C	-3.02738800	-0.95788700	0.27966300
O	-3.81855100	-1.93477400	0.24351300
C	-3.29310400	0.99439000	-1.37562500
C	-2.61868400	2.12552100	-0.66517800
N	-1.37189600	2.57447700	-1.06774600
C	-3.05402600	2.85493300	0.41640600
C	-1.06316100	3.55610200	-0.23916100
N	-2.05204100	3.76672400	0.67130800
H	-3.24400200	1.18703600	-2.45528400
H	-4.35215100	0.94122100	-1.09992400
H	-3.95182100	2.79921900	1.01346700
H	-2.04300400	4.45316000	1.41459800
H	-0.15366400	4.13905700	-0.25155500
H	-1.52691000	-0.25168800	-1.15991200
H	-2.25097700	-1.96747600	-2.44187500
H	-3.46449600	-0.97266700	-2.96296500
H	-3.71312700	-1.99411300	-1.63476300

O	-2.57053700	-0.39260900	1.30969400
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TS

Pt	0.64350700	-0.25287700	-0.79975600
As	2.06323100	0.80075600	0.69669000
O	1.35398400	2.62355800	0.23820300
O	2.90102700	-0.90784600	1.28526300
O	3.69908600	1.40723400	0.43815300
H	3.64566300	2.34386600	0.16717900
O	1.65516900	1.17636400	2.37336900
H	1.95772600	0.44464000	2.94454900
N	-0.04165800	1.61346400	-1.26215100
H	-0.70999000	1.76750200	-2.01232300
N	1.54589700	-1.98887000	-0.20560000
H	1.28258300	-2.89516400	-0.58126000
C	0.44738600	2.69044800	-0.69995600
C	0.00048600	4.07547000	-1.07052500
H	-0.42537600	4.56044800	-0.18563400
H	-0.74256600	4.06574200	-1.87042000
H	0.86990300	4.66127800	-1.38538700
C	2.47387100	-2.00683500	0.71554000
C	3.11910300	-3.27374600	1.19806500
H	4.20156400	-3.20405600	1.05064300
H	2.73566600	-4.15206100	0.67491200
H	2.93464300	-3.38063500	2.27207400
N	-3.08646900	2.38827500	1.14317700
C	-3.09398900	1.03320700	0.47253300
C	-4.59755300	0.64553600	0.30923600
O	-5.37527300	1.18537800	1.15133500
C	-2.32350800	0.04291900	1.36789000
C	-2.23968900	-1.32955200	0.78310900
N	-1.53201200	-1.60057100	-0.37792500
C	-2.80215200	-2.49145800	1.25312100
C	-1.66661900	-2.90290900	-0.59802400
N	-2.42904500	-3.47730000	0.36395100
H	-1.30837000	0.42942500	1.52452800
H	-2.81153800	-0.01107100	2.34775400
H	-3.42280700	-2.69344400	2.11286700
H	-2.68005800	-4.45674500	0.41621800
H	-1.23509500	-3.46384100	-1.41499400
H	-2.60580700	1.12848100	-0.49586300
H	-3.95704000	2.40236700	1.71179100
H	-3.15219100	3.15224300	0.46488300
H	-2.26661800	2.56116400	1.73232800
O	-4.86688600	-0.16478200	-0.60347100
O	-0.22519700	-0.88931700	-2.88888200
H	0.27636400	-1.58219800	-3.35296500
H	-1.10312800	-1.26661700	-2.69851300

PROD

Pt	0.32787500	-0.56497700	-0.48057300
As	2.20089900	0.79197100	-0.13686200
O	3.23293500	-0.68614300	0.75960400
O	1.32962000	2.38308700	-0.99331300
O	2.29583500	1.73322300	1.37162300
H	2.96361000	1.32227300	1.95501300
O	3.66992200	1.13359700	-1.03410300
H	3.52231900	1.92178300	-1.59169400
N	1.41411700	-2.04484000	0.42470000
H	1.04311500	-2.97814700	0.57776000
N	-0.53822200	1.08416300	-1.31621000
H	-1.54596300	1.10037700	-1.52298900
C	2.62724200	-1.83964800	0.87877900
C	3.42186800	-2.91080500	1.57040900
H	4.36479200	-3.05939900	1.03440000
H	2.87900300	-3.85705200	1.62069000
H	3.66463400	-2.57624100	2.58444600
C	0.08749300	2.23018800	-1.38855800
C	-0.57324100	3.46776300	-1.92521400
H	-0.52392700	4.25763600	-1.16866200
H	-1.61502200	3.28218000	-2.19412900
H	-0.02388400	3.81561500	-2.80656700
N	-2.62475300	1.62107300	2.47539800
C	-2.53505100	0.85676500	1.18117200
C	-3.69248600	1.26566400	0.23755800
O	-3.44618800	1.14340700	-0.99466000
C	-2.50952600	-0.65206000	1.51312700
C	-2.51649000	-1.54691700	0.31398700
N	-1.44686800	-1.65949700	-0.56786800
C	-3.50478600	-2.39094200	-0.12228100
C	-1.78359300	-2.53799300	-1.50867700
N	-3.02545800	-2.99840700	-1.26381700
H	-1.61665800	-0.85406000	2.11715400
H	-3.38779100	-0.89933800	2.12039300
H	-4.48529900	-2.60184800	0.27508600
H	-3.51495000	-3.68619600	-1.82336000
H	-1.16577400	-2.84337900	-2.33846300
H	-1.58653000	1.15928900	0.74666500
H	-2.77850100	2.61679800	2.29323200
H	-1.72209700	1.51964300	2.98713400
H	-3.41264300	1.30863100	3.05010900
O	-4.74918700	1.66061000	0.79238700
O	0.04594100	1.18293200	3.19273400
H	0.41726600	1.46663500	4.04388200
H	0.70906900	1.44269100	2.51960200

Coordinate of optimized stucture using M062X functional

AP1-MET:

INT

Pt	0.85326000	0.20084800	-0.66502400
As	2.60222600	-0.36023900	0.71043300
Cl	-1.03082300	0.80825800	-2.10319400
O	2.05810500	-2.23531000	0.84506000

O	3.32597400	1.46377000	0.72182200
O	2.61328700	-0.26994300	2.45214200
H	2.33916800	-1.12972300	2.82062700
O	4.17096600	-0.94138300	0.22064600
H	4.77750100	-0.18445400	0.12402900
N	0.32150600	-1.75855400	-0.54829400
H	-0.51878000	-2.12841200	-0.99336000
N	1.59780300	2.09463400	-0.61746000
H	1.16204800	2.87090200	-1.10678800
C	0.98504600	-2.59556800	0.19072900
C	0.57617700	-4.02637700	0.35841100
H	1.39112400	-4.67348800	0.02357100
H	-0.32909100	-4.25183400	-0.20728900
H	0.40428300	-4.22302200	1.41998600
C	2.67822400	2.37648900	0.04979500
C	3.26619100	3.75260700	0.10809600
H	3.30148300	4.07714000	1.15131900
H	2.68483300	4.46451000	-0.47797100
H	4.29167000	3.71658600	-0.26832700
N	-2.67750400	1.86914300	0.49437400
C	-3.92076600	1.02897800	0.45322600
C	-5.11004800	1.93474500	0.88774300
O	-6.19608700	1.35150600	1.06323700
C	-3.76610600	-0.23080700	1.29025300
C	-2.67698900	-1.16950200	0.77290000
S	-3.06596500	-1.94537300	-0.83303200
C	-4.09257200	-3.32469500	-0.24771400
H	-3.54023700	0.04694100	2.32919600
H	-4.73785700	-0.73220200	1.30460500
H	-1.72937500	-0.63627800	0.63768700
H	-2.48370500	-1.97103100	1.49332400
H	-4.40362400	-3.89102300	-1.12758200
H	-3.51630500	-3.97669900	0.41315100
H	-4.98310200	-2.96142600	0.27008600
H	-4.07238300	0.76022200	-0.59863100
H	-2.14722400	1.74471500	1.36253300
H	-2.04538200	1.68277200	-0.30248200
H	-3.01442800	2.85010400	0.48069700
O	-4.84805600	3.16151700	0.98222700

TS

Pt	-0.79917500	0.23675900	0.30600600
As	-2.83548300	-0.60545700	-0.30933600
Cl	0.61420800	0.99388300	2.49899300
O	-2.23079400	-2.47199200	-0.20017400
O	-3.64997000	1.16984300	-0.49766700
O	-3.38027700	-0.91881000	-1.94175300
H	-3.17618100	-1.84241000	-2.17602700
O	-4.17090800	-1.07613000	0.71747900
H	-4.76951800	-0.31584300	0.83251700
N	-0.20413200	-1.70332600	0.48289300
H	0.70755700	-1.97016700	0.84198000
N	-1.65117100	2.07138000	0.09795400

H	-1.14484600	2.93217800	0.28278500
C	-1.01384200	-2.68551500	0.21580000
C	-0.62688000	-4.12496600	0.36422600
H	-1.31530900	-4.60484100	1.06450800
H	0.39683700	-4.23427600	0.72271100
H	-0.73143900	-4.62099600	-0.60420100
C	-2.89645700	2.20527200	-0.24913800
C	-3.56519500	3.53838700	-0.38680900
H	-3.97289400	3.62842900	-1.39670800
H	-2.87236400	4.35806600	-0.19584200
H	-4.39867200	3.59073500	0.31869800
N	5.34786800	-0.16029700	1.48636100
C	5.26185700	-0.39607800	0.00378100
C	6.68322000	-0.10479100	-0.57593600
O	6.76702300	-0.09506800	-1.81581300
C	4.16366000	0.44081200	-0.63706500
C	2.76844100	0.03210900	-0.17038800
S	1.45690200	1.07922100	-0.86955300
C	1.33204600	0.37709800	-2.53814600
H	4.33800700	1.50352200	-0.42582900
H	4.26423300	0.30852700	-1.71775500
H	2.56069000	-1.00975500	-0.44089900
H	2.64319400	0.13773400	0.91258700
H	0.50496800	0.88567900	-3.03686900
H	2.25137100	0.55111500	-3.10072200
H	1.11822100	-0.69269700	-2.47936800
H	5.06202000	-1.46310900	-0.13231400
H	4.96543100	0.74924100	1.76469100
H	4.89475500	-0.88047000	2.05350100
H	6.37250900	-0.13969200	1.67955600
O	7.58579600	0.05842000	0.28470300

PROD

Pt	0.60832200	0.08611200	0.02264500
As	2.83538400	-0.38772700	-0.43918700
Cl	-0.12535100	0.82450500	3.65557000
O	3.26740600	1.47058000	-0.87200100
O	2.62252000	-2.30068200	-0.05104500
O	3.48803800	-0.87120600	-1.98188200
H	3.80664300	-0.08384700	-2.46022500
O	4.17014100	-0.33956100	0.68092000
H	4.30479300	-1.22510900	1.06550500
N	1.10519100	2.02406300	-0.40531500
H	0.45743700	2.80382300	-0.35961500
N	0.42385900	-1.91040300	0.39671300
H	-0.44353300	-2.34487300	0.69776000
C	2.31237500	2.35192600	-0.76967800
C	2.70628400	3.75912800	-1.09756900
H	3.50028300	4.07115600	-0.41403700
H	1.86344100	4.44572900	-1.01819000
H	3.10754000	3.78554000	-2.11386200
C	1.44224600	-2.71757900	0.30926700
C	1.34497100	-4.18027600	0.61628800

H	1.65341900	-4.74771600	-0.26529000
H	0.33325100	-4.46791800	0.90266000
H	2.03783700	-4.41608900	1.42819400
N	-4.69282600	-1.79496300	-0.93618700
C	-4.80178600	-0.40082500	-0.38612900
C	-6.32499500	-0.05642700	-0.34242800
O	-6.60051500	1.11983300	-0.05173600
C	-3.99224100	0.60042700	-1.19647900
C	-2.48076500	0.37441300	-1.19990300
S	-1.74584400	0.42413700	0.47401400
C	-1.99869400	2.16660700	0.90423400
H	-4.33705400	0.59485700	-2.23862000
H	-4.23135100	1.59286300	-0.80428600
H	-2.20433200	-0.60489600	-1.60346700
H	-1.98650100	1.13295800	-1.81275800
H	-1.31698800	2.37754500	1.73043300
H	-1.79697900	2.80555700	0.04176000
H	-3.02908600	2.30574100	1.23626600
H	-4.44664600	-0.44492300	0.64774000
H	-4.43084700	-1.81401300	-1.92647200
H	-4.04492700	-2.39996000	-0.42589600
H	-5.66507900	-2.16750700	-0.86588200
O	-7.09528700	-1.02130000	-0.58123400

AP1-HIS:

INT

Pt	0.85340500	0.60695100	0.74172600
As	1.66456100	-0.99860500	-0.69388400
Cl	0.18147500	2.29270500	2.38075000
O	0.98115300	-2.48107900	0.36058500
O	2.45030000	0.34890600	-1.91164700
O	3.29316000	-1.60508600	-0.47554600
H	3.26505400	-2.41012700	0.07206100
O	1.07096400	-1.82455000	-2.10701700
H	1.32613000	-1.31729900	-2.89895100
N	0.11887700	-0.95772900	1.82001500
H	-0.43705900	-0.83837900	2.66186000
N	1.69112400	1.97411300	-0.51269300
H	1.65268700	2.97441000	-0.34181000
C	0.27216100	-2.18390600	1.41723000
C	-0.37070400	-3.35112800	2.09870100
H	-1.13630600	-3.75062800	1.42416500
H	-0.83542900	-3.06446800	3.04252000
H	0.37243500	-4.13312600	2.26919700
C	2.32480600	1.60458000	-1.58807000
C	2.95494600	2.58017300	-2.53500700
H	4.01991700	2.35048200	-2.62304300
H	2.82818300	3.60979000	-2.19978900
H	2.50191100	2.45741000	-3.52225900
N	-2.50634300	2.56175700	0.54735500
C	-2.70470000	1.32524300	-0.27350600
C	-3.79495000	1.65604000	-1.33291100

O	-3.95676700	2.88477000	-1.55479300
C	-2.98473500	0.13870100	0.64561900
C	-2.74621600	-1.17737200	-0.02785700
N	-1.64468000	-1.38742700	-0.82607700
C	-3.49515600	-2.32454000	0.04895800
C	-1.73014800	-2.63706000	-1.23352400
N	-2.83094600	-3.24531300	-0.72787000
H	-2.31313900	0.22142500	1.51258800
H	-4.01289100	0.18357000	1.02250200
H	-4.41644600	-2.55696500	0.56131000
H	-3.11491800	-4.20115200	-0.89880700
H	-1.01476500	-3.13932300	-1.86923200
H	-1.75838400	1.15714700	-0.79890600
H	-1.58918500	2.58296300	1.02554100
H	-3.23119000	2.65187300	1.26636800
H	-2.62237600	3.36444200	-0.08872100
O	-4.36549600	0.68847800	-1.87017100

TS

Pt	-0.46368400	-0.04919300	-0.34395200
As	-2.54728100	0.57523800	0.35354000
Cl	0.97758500	-0.09384200	-2.62527300
O	-3.34856000	-1.16072500	-0.09304200
O	-1.97235800	2.37306500	0.88586600
O	-3.80824500	1.35632500	-0.57054000
H	-4.38658600	0.67704000	-0.96252900
O	-3.21602700	0.35413400	1.95500500
H	-3.04243000	1.15099500	2.48831400
N	-1.29556100	-1.84836400	-0.77599700
H	-0.75456800	-2.61413500	-1.16623300
N	0.11158900	1.85095100	0.14489300
H	1.04336900	2.21878500	-0.01878900
C	-2.55981600	-2.07643300	-0.58438900
C	-3.21051000	-3.38695500	-0.90494100
H	-3.66514600	-3.78832500	0.00432300
H	-2.49445600	-4.10534300	-1.30447700
H	-4.00679100	-3.21852100	-1.63453700
C	-0.73034800	2.69825400	0.65736600
C	-0.35623400	4.10185200	1.02321200
H	-0.98703200	4.79408200	0.45960900
H	0.69348900	4.30814600	0.81375800
H	-0.55462400	4.25543500	2.08702500
N	3.93348200	0.69091600	-1.88563200
C	3.67437900	0.27364300	-0.47377600
C	4.77970200	0.90943600	0.41619200
O	5.36358500	1.89854800	-0.09589000
C	3.52717200	-1.24608200	-0.39636800
C	2.64306400	-1.67660600	0.72941000
N	1.33013500	-1.26211200	0.83981600
C	2.93695500	-2.51993300	1.76750600
C	0.84903900	-1.84397600	1.92488200
N	1.78707300	-2.61331800	2.51264000
H	3.08501100	-1.59783500	-1.33655600

H	4.51055500	-1.71420900	-0.28720200
H	3.84461900	-3.03823900	2.03568400
H	1.66268700	-3.15839100	3.35624200
H	-0.15668400	-1.73683900	2.30594900
H	2.71797100	0.73378900	-0.20701700
H	4.29492900	1.65451400	-1.86130500
H	3.06027500	0.61300700	-2.43914800
H	4.65590600	0.11253600	-2.32504100
O	4.94420000	0.40081900	1.54089300

PROD

Pt	-0.53795300	0.03187200	-0.60285800
As	-2.42545100	-0.44437900	0.63292700
Cl	2.74939800	2.90272500	3.27213700
O	-3.20863900	1.33956300	0.32278900
O	-1.83761200	-2.26096100	1.05330700
O	-2.65700400	-0.20809000	2.34421400
H	-3.03415200	0.67694000	2.50080700
O	-3.91689800	-1.09640400	0.00875000
H	-3.89734000	-2.06823900	0.07999400
N	-1.39006900	1.85669000	-0.95039300
H	-0.95752200	2.57998500	-1.51668800
N	0.08641100	-1.83047600	-0.09844000
H	1.03795300	-2.15473200	-0.32714700
C	-2.54066200	2.17115800	-0.42732200
C	-3.19078300	3.50449800	-0.63918100
H	-4.17349400	3.35131200	-1.09244300
H	-2.58905300	4.15166700	-1.27755800
H	-3.33980600	3.98283400	0.33234700
C	-0.64880200	-2.61290900	0.62979300
C	-0.19850400	-3.97996400	1.04569800
H	-0.21892400	-4.04657900	2.13656300
H	0.80680400	-4.19254600	0.68010400
H	-0.89830400	-4.72131900	0.65060700
N	3.49993500	0.07542100	2.20260700
C	2.80140100	-0.26144300	0.92768900
C	3.57033600	-1.43010200	0.25869300
O	4.80331900	-1.44332700	0.46980700
C	2.81917000	1.00027500	0.04447100
C	2.44750900	0.74495300	-1.37874700
N	1.17402100	0.39706100	-1.78406200
C	3.24601300	0.79623000	-2.48835800
C	1.20295800	0.23827500	-3.09799300
N	2.44288300	0.47343200	-3.55433000
H	2.15004600	1.74929800	0.48412000
H	3.83227300	1.41920100	0.05608200
H	4.29298400	1.03058000	-2.60217600
H	2.72692000	0.43161200	-4.52564700
H	0.36475300	-0.03385700	-3.72139300
H	1.77866600	-0.55171700	1.17367300
H	3.28755300	-0.60332200	2.93905600
H	3.24875800	1.03268600	2.56115200
H	4.51192900	0.01404400	2.01923300

O	2.89012400	-2.21157700	-0.44847000
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APW-MET:

INT

Pt	-0.76869800	0.00489800	-1.04841500
As	-0.95625900	1.24268400	0.86869100
O	0.48072300	2.46169100	0.36155700
O	-2.51728900	0.20872400	1.48608300
O	-0.16126200	0.79515700	2.32756900
H	0.84338700	0.90796800	2.28017300
O	-1.90196400	2.67426400	1.14950100
H	-2.78296700	2.41668000	1.47764100
N	0.72040100	1.31361300	-1.58204200
H	1.16548600	1.32081900	-2.49562200
N	-2.33207000	-1.08887500	-0.36488600
H	-2.71416700	-1.88063700	-0.87475700
C	1.01793100	2.32701100	-0.81632800
C	1.96533000	3.41176400	-1.22342700
H	1.40900600	4.35183900	-1.27950400
H	2.42619300	3.20201100	-2.18926700
H	2.73823000	3.50371800	-0.45798700
C	-2.92353500	-0.78743400	0.75413800
C	-4.09256500	-1.55335300	1.29062400
H	-3.82254200	-1.96735700	2.26620800
H	-4.39061400	-2.35996600	0.62055400
H	-4.92990400	-0.86634000	1.43696500
O	-0.57732800	-1.42331400	-2.74566100
H	-0.00822900	-2.14494300	-2.41543600
H	-0.15419900	-1.08978400	-3.55438500
N	3.37332600	-0.70065900	-0.85404700
C	2.60576400	-0.61217200	0.43298100
C	2.98247500	0.73473400	1.10067000
O	2.44604300	0.95269000	2.21869300
C	2.84957100	-1.82278200	1.32051000
C	2.51222600	-3.16677400	0.66938700
S	0.84050300	-3.28703800	-0.04845400
C	-0.14713800	-2.87519900	1.41790600
H	3.89802600	-1.84478000	1.64531800
H	2.24985000	-1.67556400	2.22366900
H	3.19619600	-3.40500300	-0.15192900
H	2.62572800	-3.96065700	1.41335900
H	-1.18103800	-3.14265300	1.19427700
H	0.19515600	-3.46613500	2.27190400
H	-0.09800100	-1.80860000	1.65856700
H	1.54945500	-0.56974800	0.14623800
H	4.22882700	-1.25992800	-0.76529300
H	2.82336300	-1.08627800	-1.62776800
H	3.67920000	0.26458600	-1.07559500
O	3.75214900	1.47571500	0.46045300

TS

Pt	-1.18145900	-0.39034200	-0.69420500
As	-1.73154600	0.89951100	1.10480000
O	-1.44708800	2.57388900	0.13041900
O	-2.04851800	-0.64079400	2.26422900
O	-0.60411800	1.45427200	2.31512800
H	-0.27141400	2.33598800	2.06640200
O	-3.29271500	1.53087000	1.55158200
H	-3.73001700	0.91345100	2.16622700
N	-0.92087100	1.34970300	-1.70714800
H	-0.65663600	1.37780400	-2.68790600
N	-1.53412800	-1.99333900	0.51330500
H	-1.46381300	-2.95729200	0.20055500
C	-1.09724500	2.49798800	-1.12395600
C	-0.91498300	3.80874000	-1.82412900
H	-0.64116500	3.67241400	-2.87034900
H	-0.13448100	4.37700400	-1.31155700
H	-1.84543600	4.37800000	-1.75772300
C	-1.90196000	-1.83008700	1.74976700
C	-2.18467800	-2.97116900	2.67645400
H	-1.52325100	-2.89416400	3.54314500
H	-2.03779200	-3.93433400	2.18767600
H	-3.21538600	-2.89170400	3.03154400
N	4.30540000	1.84946400	0.42449900
C	4.43616900	0.37400200	0.68219700
C	5.96777200	0.07451800	0.76700300
O	6.28016100	-1.12731700	0.80956900
C	3.71345600	-0.45982300	-0.36616600
C	2.19957500	-0.27296700	-0.32829200
S	1.32085800	-1.31601500	-1.53976900
C	1.50704400	-2.93970000	-0.75177700
H	4.10149900	-0.22529300	-1.36561500
H	3.97754000	-1.49981200	-0.15632500
H	1.79667100	-0.49642400	0.66641900
H	1.90561100	0.75222300	-0.57981000
H	0.89956100	-3.64860900	-1.31840500
H	2.54762000	-3.26690500	-0.78156400
H	1.15420000	-2.89799900	0.28176800
H	4.00945500	0.19390600	1.67330000
H	4.13052300	2.06672700	-0.56146300
H	3.58441700	2.31126400	0.98336600
H	5.24703000	2.22940500	0.66383800
O	6.70610500	1.09193500	0.81134300
O	-1.70105400	-1.43621900	-2.80783500
H	-1.45947400	-2.37294900	-2.89000800
H	-2.66007700	-1.40654600	-2.95432600

PROD

Pt	-0.60598000	-0.02160600	0.08127700
As	-2.90081100	-0.03908900	-0.31849400
O	-3.01133900	-1.99264600	-0.27536800
O	-3.00894200	1.91766800	-0.41000300

O	-3.67011900	-0.05751100	-1.88216600
H	-3.84274400	-0.97874200	-2.15037400
O	-4.16867700	-0.02974800	0.87622400
H	-4.44668800	0.88804300	1.05142200
N	-0.77089000	-2.06228700	0.14345600
H	0.00047800	-2.69830900	0.31780300
N	-0.76699700	2.00859200	-0.02060200
H	0.02597100	2.63214300	0.10257900
C	-1.91466500	-2.65778400	-0.04796000
C	-2.06624600	-4.14756000	-0.02454400
H	-2.78779400	-4.41648900	0.75114200
H	-1.11753900	-4.64956200	0.16527300
H	-2.46876300	-4.47540100	-0.98645300
C	-1.90942600	2.59502700	-0.24335700
C	-2.05360300	4.08322900	-0.32461100
H	-2.45437900	4.34321800	-1.30790500
H	-1.10193500	4.59140900	-0.16982400
H	-2.77396900	4.41061700	0.42942600
N	4.86391300	1.11261600	-1.65108100
C	4.87498100	0.24288700	-0.42617800
C	6.37442600	-0.05367000	-0.10072200
O	6.57099500	-0.84485100	0.83666200
C	4.05995900	-1.02913100	-0.61284100
C	2.55933200	-0.83089800	-0.83156100
S	1.76998200	0.14972000	0.49203500
C	2.09330900	-0.87886700	1.94947400
H	4.45142900	-1.59530900	-1.46790100
H	4.23896200	-1.65106200	0.26851900
H	2.33791900	-0.28192200	-1.75217900
H	2.06353800	-1.80244000	-0.90335500
H	1.47136400	-0.46706400	2.74449200
H	1.83641500	-1.92173900	1.75566600
H	3.14717400	-0.79473400	2.22204500
H	4.47718100	0.84942300	0.39270700
H	4.56206100	0.62121300	-2.49785500
H	4.29388500	1.95686000	-1.55670800
H	5.86924100	1.37253900	-1.77366600
O	7.20579200	0.56356800	-0.81435500
O	0.31347600	1.66911200	2.80484900
H	-0.60521100	1.60829700	2.49952400
H	0.25679900	1.88215900	3.74839200

APW-HIS:

INT

Pt	0.87232300	0.58235800	-0.26563800
As	2.54102400	-0.96144900	-0.00786300
O	1.33043600	-2.46710900	-0.00864700
O	3.94933500	0.41000500	0.02830500
O	3.19060600	-1.50901200	1.51418300
H	2.71265000	-2.31044700	1.79634300
O	3.42039700	-1.76467000	-1.27922200
H	4.22039900	-1.25027600	-1.49283000

N	-0.39751600	-1.01395100	-0.35115500
H	-1.41576300	-0.94069800	-0.48052100
N	2.33287100	1.99802700	-0.16095200
H	2.14306500	2.99469000	-0.20848800
C	0.05318500	-2.21914000	-0.19041400
C	-0.82877200	-3.42922600	-0.18444700
H	-0.46979200	-4.13414700	-0.93905600
H	-1.86570600	-3.15753200	-0.38166700
H	-0.74610200	-3.91604600	0.79178200
C	3.58363500	1.66041400	-0.04547700
C	4.69825700	2.65888500	0.01382300
H	5.23232000	2.53586000	0.95957600
H	4.32953100	3.68128400	-0.06885300
H	5.40053300	2.45447100	-0.79836500
O	-0.67763200	2.10842800	-0.39913300
H	-1.42952000	1.77096300	0.21406300
H	-1.02496200	2.16972700	-1.30345000
N	-5.44785300	1.19640800	-1.92230900
C	-4.34896100	0.74273000	-1.00827900
C	-4.33026900	-0.80719500	-1.07571000
O	-5.43233400	-1.33706000	-1.34616500
C	-4.66352800	1.24211900	0.40914500
C	-3.67752700	0.74065900	1.41312700
N	-2.33384800	1.02898100	1.32293600
C	-3.89449300	-0.05804500	2.50383300
C	-1.74929700	0.41444700	2.33463200
N	-2.65869900	-0.25147700	3.07317200
H	-4.66854800	2.33923700	0.40363700
H	-5.66656400	0.90492100	0.69508300
H	-4.79442500	-0.49358300	2.90982000
H	-2.46261500	-0.79361600	3.90520200
H	-0.69022800	0.42310200	2.55378900
H	-3.40940500	1.15656800	-1.37435800
H	-5.13636600	1.26213000	-2.89627200
H	-5.85274700	2.10111800	-1.66216900
H	-6.17219200	0.45744700	-1.87955300
O	-3.23663900	-1.35696400	-0.82403500

TS

Pt	0.56935800	-0.00771200	-0.39576500
As	2.71300400	0.41390300	0.25836600
O	2.32172700	2.23262600	0.82221100
O	3.33943600	-1.36507800	-0.23243100
O	3.98849900	1.03022300	-0.75470600
H	4.02073800	2.00187500	-0.68281100
O	3.37752300	0.17344000	1.84978300
H	3.77642300	-0.71427000	1.90558400
N	0.16523300	1.90358100	0.19246300
H	-0.73664800	2.35486100	0.07800800
N	1.24497400	-1.84264200	-0.96521800
H	0.66599000	-2.54466400	-1.41772400
C	1.10357800	2.67064600	0.66347900
C	0.87860600	4.09816100	1.05260800

H	1.16257300	4.22864900	2.09978000
H	-0.16071100	4.39577400	0.91347800
H	1.52757100	4.73448200	0.44533300
C	2.48588200	-2.18491700	-0.77831000
C	3.03376900	-3.52389900	-1.16117900
H	3.84763000	-3.38138500	-1.87657300
H	2.26780700	-4.16415700	-1.59842300
H	3.44801600	-4.00211900	-0.26981500
N	-3.83782900	1.34207200	-1.52663300
C	-4.15263400	0.28396500	-0.51614400
C	-5.69903400	0.26398300	-0.32370500
O	-6.10647900	-0.29998600	0.70830100
C	-3.33584000	0.47846400	0.77098200
C	-2.65495700	-0.76999000	1.23206800
N	-1.55239500	-1.27839600	0.56863800
C	-2.96402800	-1.58375900	2.28846900
C	-1.20530000	-2.37402100	1.22328200
N	-2.03151400	-2.59280800	2.26447300
H	-2.56607300	1.24087700	0.60742600
H	-3.99579700	0.84752000	1.55963400
H	-3.74497000	-1.53259500	3.03151600
H	-1.97062000	-3.36469900	2.91660000
H	-0.36894100	-3.01703400	0.98819000
H	-3.89246400	-0.66383000	-0.99826600
H	-2.92590700	1.16578200	-1.97233200
H	-3.82464300	2.27738900	-1.10778900
H	-4.60603400	1.33879700	-2.21467600
O	-6.35251900	0.78557300	-1.26039400
O	-1.31898500	-0.05740000	-1.90143200
H	-1.03880800	-0.23543000	-2.81534000
H	-1.67733400	-0.89267100	-1.54420900

PROD

Pt	0.32405100	-0.63839100	-0.39871700
As	2.18730300	0.68143500	-0.09941400
O	3.12815600	-0.68644100	0.94726600
O	1.42524100	2.19632300	-1.06764500
O	2.30064100	1.76599100	1.27866800
H	2.72016400	1.30730700	2.03017300
O	3.65371400	0.86110400	-1.01102800
H	3.55166700	1.58957000	-1.65106300
N	1.36486100	-2.08937000	0.59043600
H	1.00542600	-3.02393600	0.75958700
N	-0.49207400	0.98354700	-1.30736900
H	-1.49888200	1.02541000	-1.50422900
C	2.54478500	-1.84749400	1.08416200
C	3.33185300	-2.86705500	1.84866300
H	4.29879200	-3.00848700	1.35944300
H	2.80729600	-3.82065900	1.90980900
H	3.51773600	-2.48520500	2.85610700
C	0.17062200	2.09234300	-1.43156100
C	-0.43991000	3.33521800	-1.99899200
H	-0.35713400	4.13544200	-1.25904300

H	-1.48761200	3.17797000	-2.25813500
H	0.11938800	3.63651500	-2.88882400
N	-2.47487100	1.51749100	2.54931400
C	-2.41265200	0.74357500	1.27083700
C	-3.51395300	1.30527500	0.33246700
O	-4.46086800	1.89607600	0.90149500
C	-2.58083000	-0.75529600	1.56076500
C	-2.57435200	-1.61169800	0.33477900
N	-1.48755100	-1.72090400	-0.51332500
C	-3.56793900	-2.41877500	-0.14598300
C	-1.81936300	-2.56094800	-1.48072700
N	-3.07159000	-3.00202200	-1.28588800
H	-1.76650100	-1.07270800	2.22532900
H	-3.52613600	-0.92059100	2.08994700
H	-4.56281800	-2.61896500	0.22006200
H	-3.55872000	-3.66236100	-1.87949700
H	-1.19018500	-2.85732700	-2.30628600
H	-1.43329700	0.94419000	0.84200900
H	-3.42286500	1.92935600	2.59667200
H	-1.76251200	2.26889200	2.50978300
H	-2.30343400	0.95354600	3.38640300
O	-3.34551100	1.09421100	-0.89051900
O	-0.29145000	2.98521000	1.55422600
H	-0.21287200	3.95061000	1.57274600
H	0.62515300	2.64670500	1.59125800