

Electronic Supplementary Information for

Surface Single-Cluster Catalyst for N₂-to-NH₃ Thermal Conversion

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Computational Details

The calculations were performed using periodic density functional theory (DFT) with the Vienna Ab-initio Simulation Package (VASP version 5.2).¹ The (011) surface of cobalt monoxide was represented by a periodic slab model constructed using bulk cell dimensions: $a = b = c = 4.2667 \text{ \AA}$. Since CoO is antiferromagnetic and has atomic moment on cobalt atoms, the primitive cubic unit cell of CoO was used to build the surface slab, which was previously proved to be the most energetically stable configuration for CoO.² The repeated slabs were separated from their neighboring images by a 12 $\text{\AA}$ -width vacuum in the direction perpendicular to the surface. Considering the usually very large relaxations of the CoO surfaces, a slab containing five layers of 60 atoms was chosen. The three top-layer slabs of the surface were allowed to relax while the other layers beneath the surface were frozen during the geometry optimization. This model was previously shown to generate reasonable results.³

The atomic core and valence electrons were represented by the projector-augmented wave (PAW) method⁴ and plane-wave basis functions with a kinetic energy cut-off of 400 eV. Inasmuch as Rh has non-negligible relativistic effects, the mass-velocity and Darwin scalar-relativistic effects were included through the PAW potentials. The generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional⁵ was used in the calculations. A Monkhorst-Pack grid of size of $2 \times 2 \times 1$ was used to sample the surface Brillouin zone. The ground-state atomic geometries were obtained by minimizing the forces on the atoms to $<0.02 \text{ eV/\AA}$. Because of the strong 3d-electron correlation effects for Co, the calculations were carried out with the DFT+U method.⁶ The parameters were set at $U = 4 \text{ eV}$ and $J = 1 \text{ eV}$.⁷ The transition states were obtained by relaxing the force $<0.02 \text{ eV/\AA}$ by using the dimer method.⁸

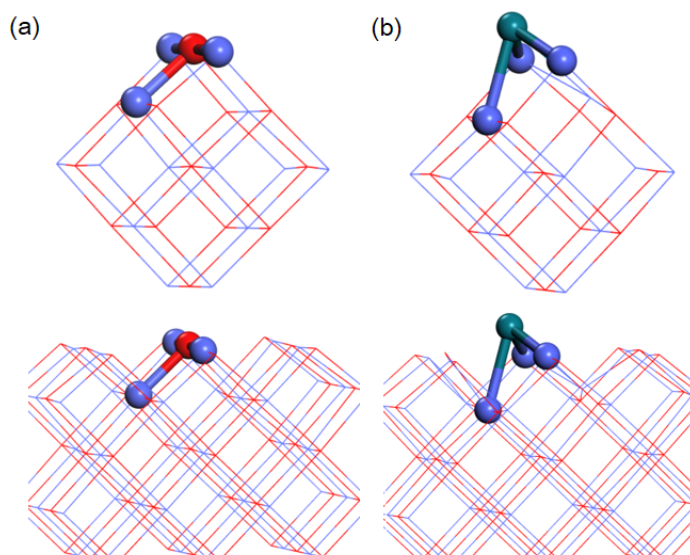


Figure S1. The schematic illustration of the surface single-cluster catalyst (SCC) with singly dispersed bimetallic site: (a) stoichiometric CoO lattice, (b) surface single cluster Rh_1Co_3 formed by doping the oxygen vacancy with a Rh atom.

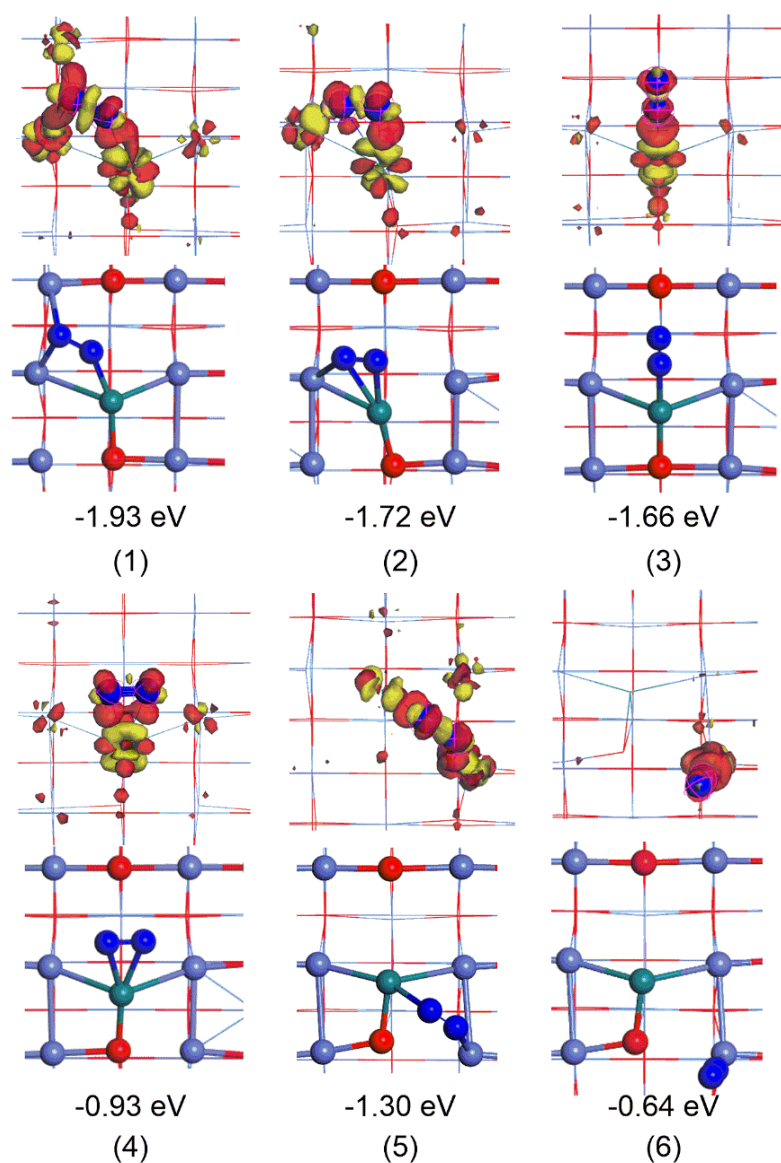


Figure S2. The optimized dinitrogen adsorption structures (top view), adsorption energies, and the computed electron density difference maps of dinitrogen and surface (a decrease in electron density is shown in yellow and the increase in red).

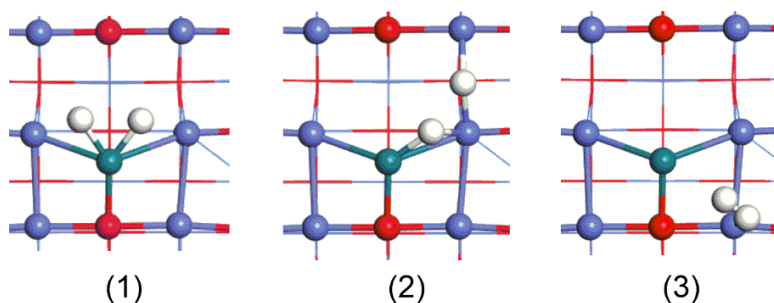


Figure S3. Three different patterns of H_2 adsorption on the Rh_1Co_3 cluster: (1) dissociative adsorption on Rh, (2) dissociative adsorption on Rh-Co, (3) molecular adsorption on Co.

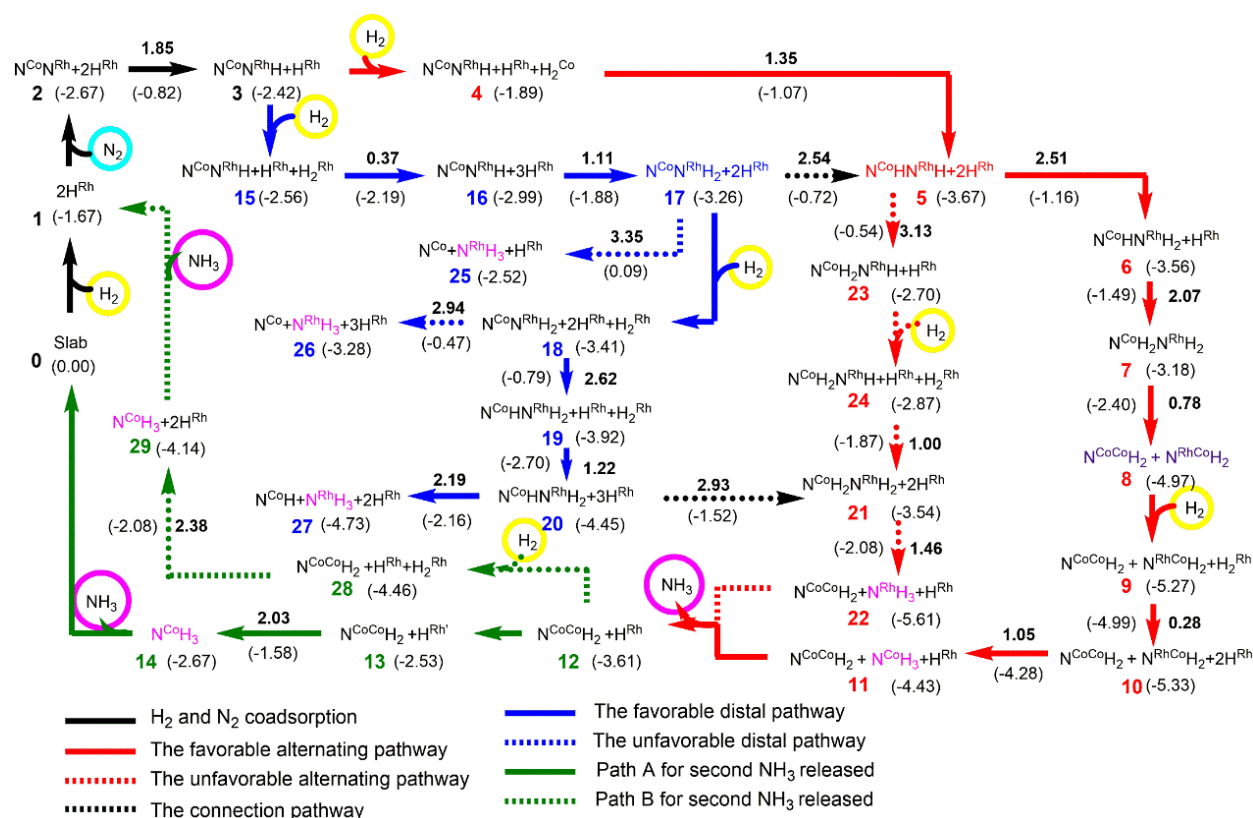


Figure S4. The reaction network of dinitrogen thermal conversion to ammonia on a singly dispersed Rh_1Co_3 cluster bimetallic site anchored on $\text{CoO}(011)$.

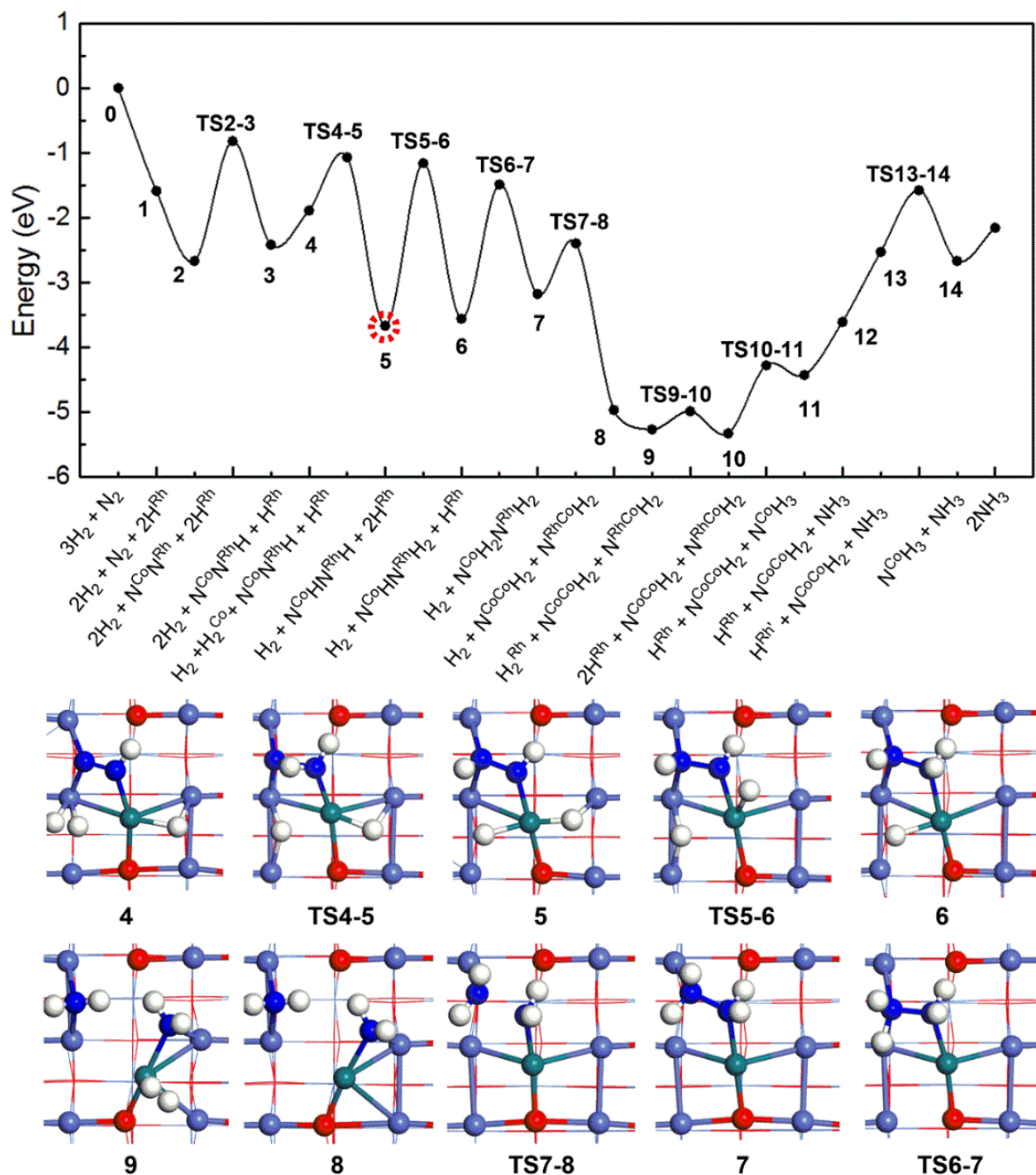


Figure S5. The energy profile and structures of the surface species for the alternating hydrogenation of N_2 on a singly dispersed Rh_1Co_3 bimetallic site anchored on $CoO(011)$ (The dash cycle denotes the crossing of the pathways).

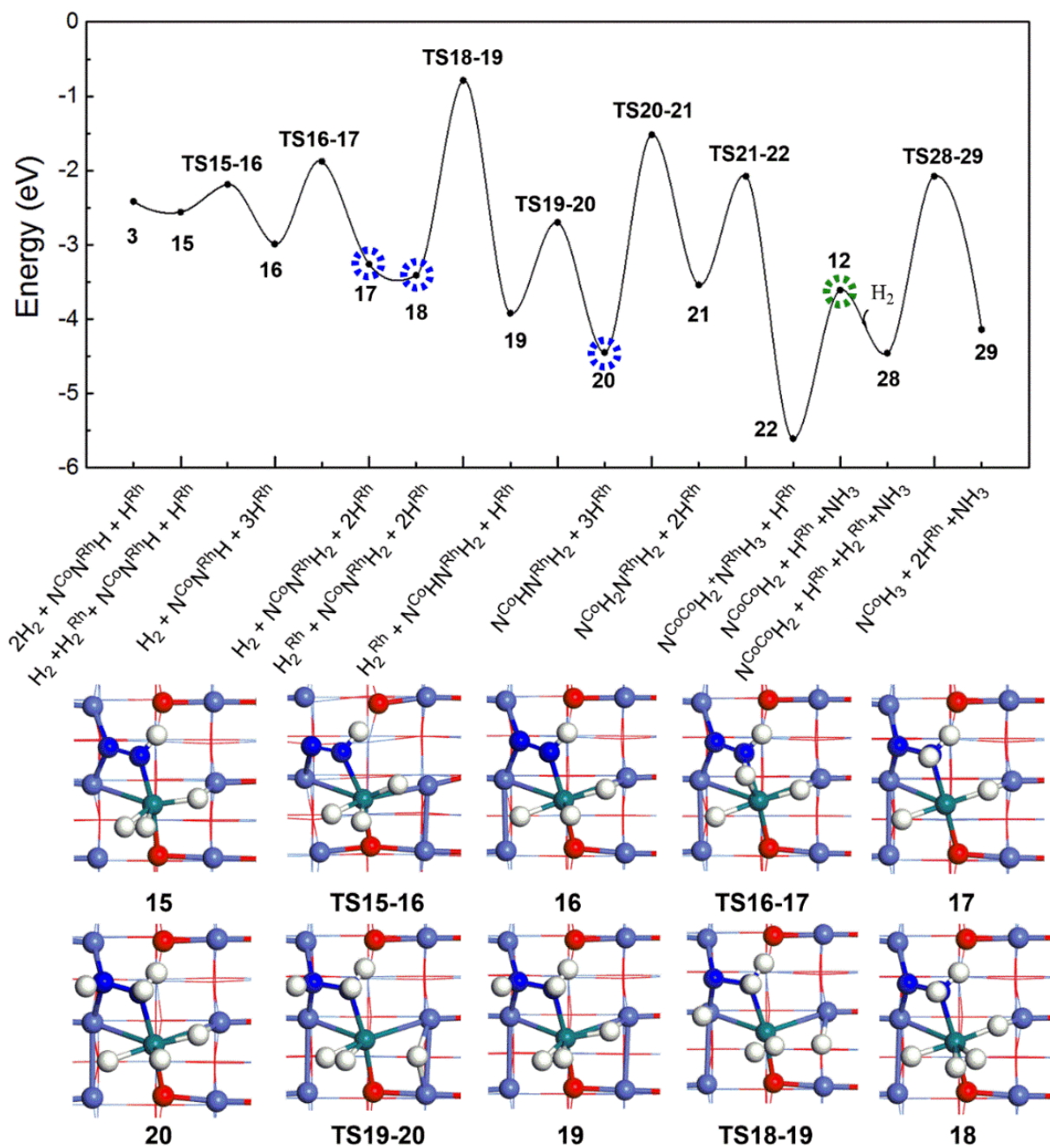


Figure S6. The energy profile and structures of the surface species for the distal hydrogenation of N₂ on a singly dispersed Rh₁Co₃ bimetallic site anchored on CoO(011) (The dash cycle denotes the crossing of the pathways).

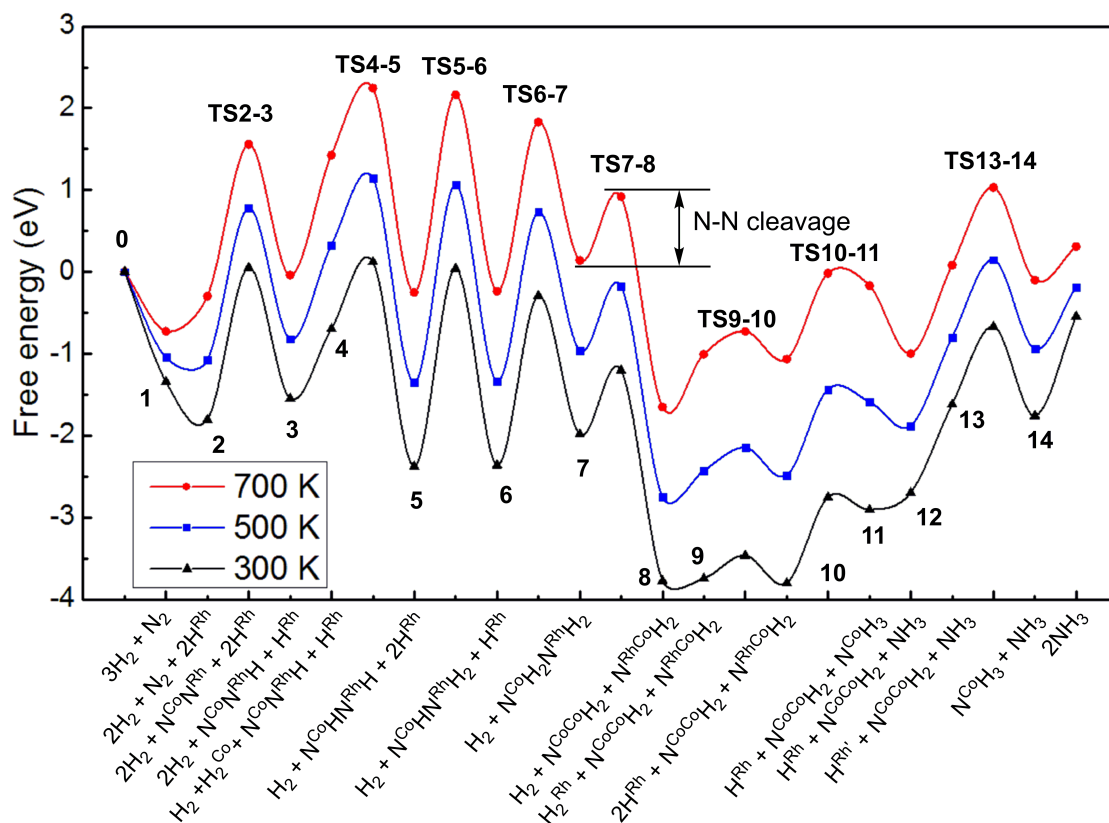


Figure S7. Gibbs free energy diagrams of alternating hydrogenation of N_2 at different temperatures for a fixed reactant pressure of $P = 1$ bar. ($H_2:N_2$ ratio is fixed at 3, and conversion of NH_3 is 10%. Free energies are calculated using ideal gas and harmonic vibrational approximations.)

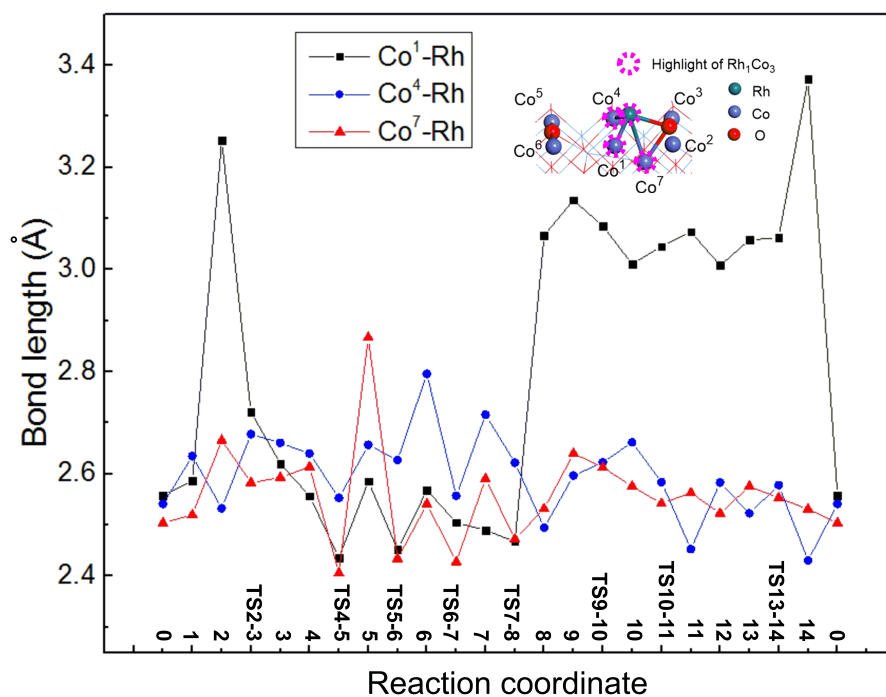


Figure S8. The variation of Rh-Co distances of Rh_1Co_3 on $CoO(011)$ surface along the N_2 -to- NH_3 thermal conversion reaction coordinate.

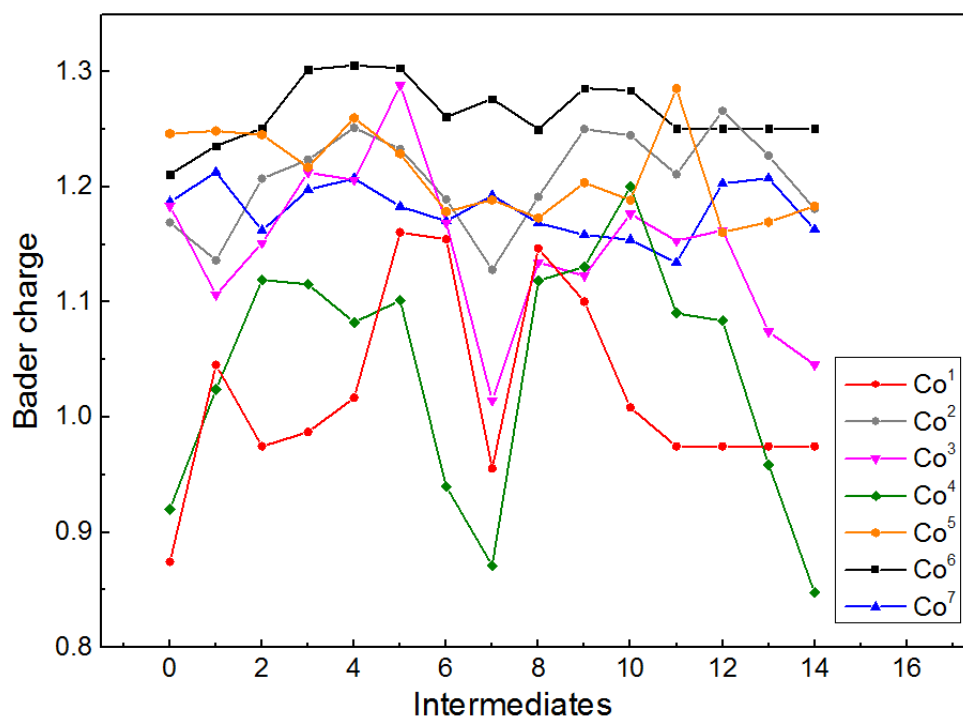


Figure S9. Calculated Bader charges on the selected Co atoms along the alternating pathway.

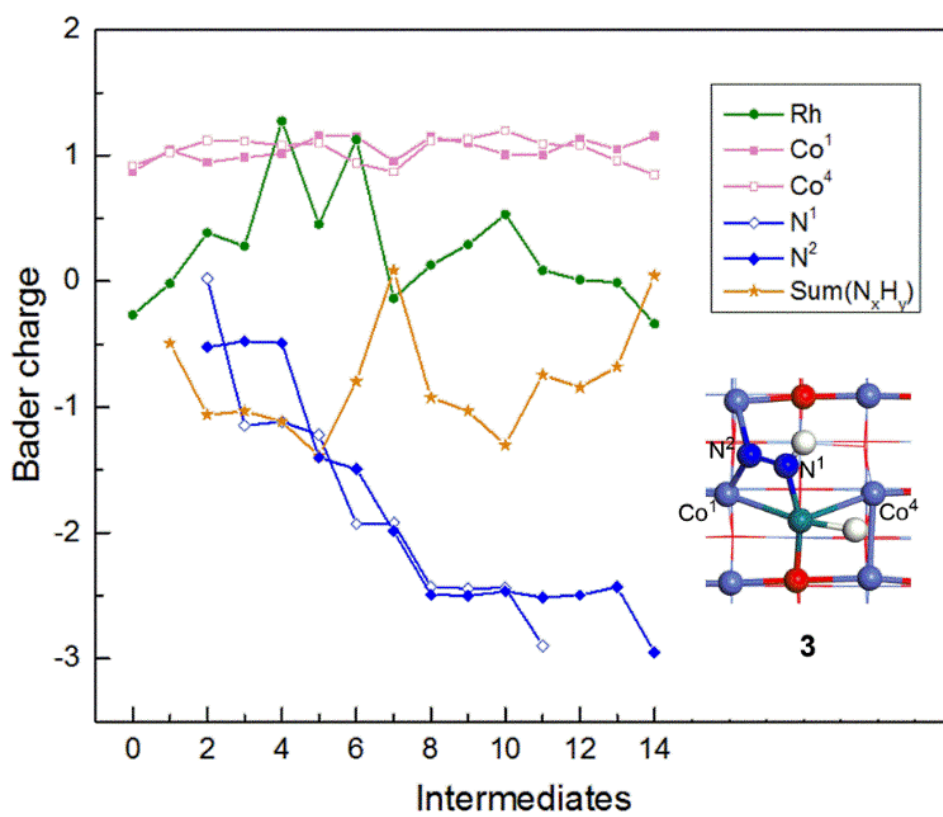


Figure S10. Calculated Bader charges on the selected moieties along the alternating pathway.

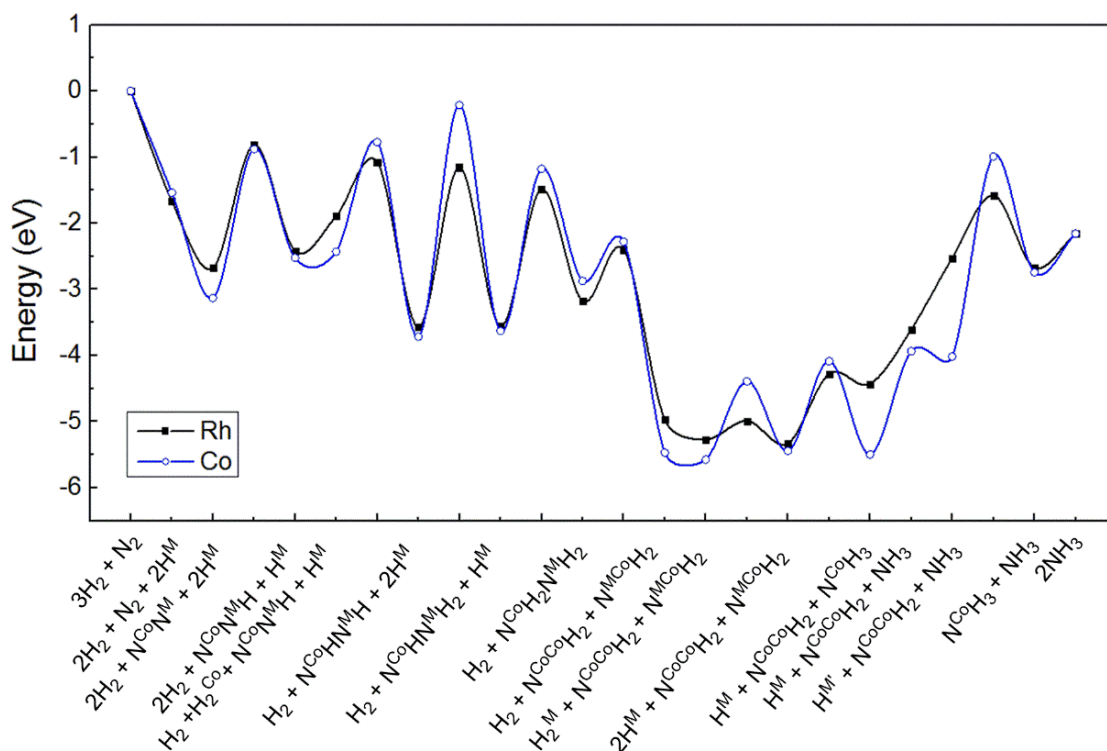


Figure S11. Energy profile for the alternating hydrogenation of N_2 on a singly dispersed Co_4 site in comparison to the $RhCo_3$ site.

Table S1. N_2 adsorption and N_2/H_2 coadsorption energies, structural parameters and Bader charge on the selected atoms of optimized adsorption configurations and calculated frequencies of N_2 adsorption.

Entry	Configuration	E_{ads}/eV	$d(N-N)/\text{\AA}$	$d(Rh-N)/\text{\AA}$	Frequency (N_{2ad})/ cm^{-1}	Charge (N_2)	Charge (Rh)
(1)	$\mu_2 - \eta_{Co1}^1, \eta_{Co6}^1, \eta_{Rh}^1 - N_2$	-1.93	1.201	1.880	1667.4 cm^{-1}	-0.769	0.102
(2)	$\mu_1 - \eta_{Co1}^1, \eta_{Rh}^2 - N_2$	-1.72	1.174	2.080	1899.7 cm^{-1}	-0.517	0.079
(3)	$\eta_{Rh}^1 - N_2$	-1.66	1.141	1.876	2174.5 cm^{-1}	-0.378	0.069
(4)	$\eta_{Rh}^2 - N_2$	-0.93	1.167	2.116	1965.8 cm^{-1}	-0.433	0.070
(5)	$\mu_1 - \eta_{Co3}^1, \eta_{Rh}^1 - N_2$	-1.30	1.163	2.154	1955.5 cm^{-1}	-0.502	0.024
(6)	$\eta_{Co3}^1 - N_2$	-0.64	1.133	NA	2230.1 cm^{-1}	-0.256	-0.170
(i)	$\mu_1 - \eta_{Co1}^1, \eta_{Rh}^1 - N_2H_2$	-2.67	1.169	2.101	NA	-0.531	0.386
(ii)	$\eta_{Rh}^1 - N_2H_2$	-1.82	1.130	2.068	NA	-1.988	0.734

Table S2. The key energetic and structural parameters of three H₂ adsorption patterns.

Entry	Configuration	E _{ads} /eV	d(H-H)/Å	d(M-H)/Å
(1)	η_{Rh}^2 -H ₂	-1.67	1.818	1.619/1.625
(2)	η_{Co4}^2 -H ₂	-0.70	1.835	1.788/1.708
(3)	η_{Co3}^2 -H ₂	-0.26	0.861	1.837/1.852

Geometrical Coordinates (in fractional coordinate) of the Optimized Structures and Energies (in eV) of Selected Intermediates (see Fig. S4 for the Numbering of the Species; 1 Hartree = 27.2114 eV)

0

E= -347.07986

O	0.1288100000000014	0.0883899999999969	0.2498199999999997
O	0.1352604910537067	0.0928363385117024	0.4288254355013947
O	0.3757697550858197	0.2520543966735502	0.3374331416589840
O	0.3788100000000014	0.2550499999999971	0.1661700000000010
O	0.3894249871078586	0.2884101934493515	0.5092777261759807
O	0.1288100000000014	0.4217200000000005	0.2498199999999997
O	0.1263395418169253	0.4228971255921863	0.4155716971438608
O	0.6288100000000014	0.0883899999999969	0.2498199999999997
O	0.6231951501517088	0.0922208510579310	0.4262626347572365
O	0.8800897100770300	0.2528405695248779	0.3355084974279379
O	0.8788100000000014	0.2550499999999971	0.1661700000000010
O	0.8753773080207594	0.2596804526178076	0.4997460797131765
O	0.6288100000000014	0.4217200000000005	0.2498199999999997
O	0.6304952943804167	0.4227379103819615	0.4126659398755947
O	0.3754072995429070	0.5899751664832564	0.3355865050446170
O	0.3788100000000014	0.5883899999999969	0.1661700000000010
O	0.1288100000000014	0.7550499999999971	0.2498199999999997
O	0.1374143589637171	0.7552795189589432	0.4198975870819197
O	0.3794377360583994	0.9283117708638429	0.3340272382679572
O	0.3788100000000014	0.9217200000000005	0.1661700000000010
O	0.3837556048291404	0.9190624679720401	0.5026097913687195
O	0.8800637730700416	0.5920895710791640	0.3343824577013592
O	0.8788100000000014	0.5883899999999969	0.1661700000000010
O	0.8776678347654254	0.5884065841303254	0.4959080897039314
O	0.6288100000000014	0.7550499999999971	0.2498199999999997
O	0.6169891596237917	0.7489218415135852	0.4208529056752042
O	0.8766992364764619	0.9227895617127047	0.3384111317558123
O	0.8788100000000014	0.9217200000000005	0.1661700000000010
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Co	0.3783689965820187	0.0850669552305803	0.4257810942556617
Co	0.3788100000000014	0.0883899999999969	0.2498199999999997
Co	0.1288100000000014	0.2550499999999971	0.1661700000000010
Co	0.1121867327363475	0.2731317115974292	0.4973315310375455
Co	0.1272955271774663	0.2521092219331393	0.3339988277013290
Co	0.3804175804850658	0.4235038119898604	0.4136430172044783
Co	0.3788100000000014	0.4217200000000005	0.2498199999999997
Co	0.8784511806284172	0.0892668388523177	0.4270610339062273

Co	0.8788100000000014	0.0883899999999969	0.2498199999999997
Co	0.6288100000000014	0.2550499999999971	0.1661700000000010
Co	0.6280929577646219	0.2714472062764699	0.4981175575074701
Co	0.6291820379540098	0.2510718284701241	0.3338203117840095
Co	0.8754712298964975	0.4211108942718340	0.4189783724103364
Co	0.8788100000000014	0.4217200000000005	0.2498199999999997
Co	0.1288100000000014	0.5883899999999969	0.1661700000000010
Co	0.1108057794874782	0.5853219263867828	0.4975210042255611
Co	0.1298232423698664	0.5890892791545639	0.3333324369469395
Co	0.3762585030605621	0.7316523480821999	0.4423064937854235
Co	0.3788100000000014	0.7550499999999971	0.2498199999999997
Co	0.1288100000000014	0.9217200000000005	0.1661700000000010
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Co	0.1332019620941693	0.9205536683514950	0.3357475290531013
Co	0.6288100000000014	0.5883899999999969	0.1661700000000010
Co	0.6454130697454232	0.5839815906433898	0.5009644530013944
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Co	0.8765009265018122	0.7559227568428781	0.4221282234372126
Co	0.8788100000000014	0.7550499999999971	0.2498199999999997
Co	0.6288100000000014	0.9217200000000005	0.1661700000000010
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Co	0.6228392201123825	0.9189569218516098	0.3361886062302517
Rh	0.3775969281149187	0.5020340826648919	0.5467993733108756

1

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O	0.3788100000000014	0.2550499999999971	0.1661700000000010
O	0.3733549867173364	0.2725577956969117	0.5038485511439464
O	0.1288100000000014	0.4217200000000005	0.2498199999999997
O	0.1258568740922841	0.4240050917454875	0.4128970562555801
O	0.6288100000000014	0.0883899999999969	0.2498199999999997
O	0.6239220275065512	0.0978755681155840	0.4282667160464280
O	0.8774029777999992	0.2522496568485836	0.3347232322992743
O	0.8788100000000014	0.2550499999999971	0.1661700000000010
O	0.8803785007728842	0.2644288076510425	0.4994577694396664
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O	0.8785098870139020	0.5926150807118464	0.4971046485728607
O	0.6288100000000014	0.7550499999999971	0.2498199999999997
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Co	0.1288100000000014	0.2550499999999971	0.1661700000000010
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Co	0.1272627073181767	0.2516600534777397	0.3334990976422431
Co	0.3776109563178230	0.4232967625589789	0.4126462638186579
Co	0.3788100000000014	0.4217200000000005	0.2498199999999997
Co	0.8790237916741521	0.0936508460333926	0.4276309177909573
Co	0.8788100000000014	0.0883899999999969	0.2498199999999997
Co	0.6288100000000014	0.2550499999999971	0.1661700000000010
Co	0.6232412009026094	0.2767945179349663	0.5008861388804244
Co	0.6299788804316133	0.2523249765698983	0.3343754134704929
Co	0.8757275454915283	0.4217519780079985	0.4200439956457390
Co	0.8788100000000014	0.4217200000000005	0.2498199999999997
Co	0.1288100000000014	0.5883899999999969	0.1661700000000010
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Co	0.1277353331758263	0.5902695808905775	0.3333395659311189
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Co	0.1288100000000014	0.9217200000000005	0.1661700000000010
Co	0.1285267462249251	0.9188800845928247	0.4998431679834682
Co	0.1309247466429894	0.9228333698935827	0.3363378977415584
Co	0.6288100000000014	0.5883899999999969	0.1661700000000010
Co	0.6507703771201538	0.5835747150599138	0.5000117006056702
Co	0.6308281083450137	0.5912216429985653	0.3332203520067135
Co	0.8792400489512644	0.7603558961871413	0.4232930160805923
Co	0.8788100000000014	0.7550499999999971	0.2498199999999997
Co	0.6288100000000014	0.9217200000000005	0.1661700000000010
Co	0.6328451127717408	0.9243601611498101	0.4969697348500390
Co	0.6269919486217023	0.9207022624678161	0.3362907756252927
Rh	0.3773325972353532	0.4886671207020395	0.5484646234095292
H	0.4883412479485809	0.6248953919125010	0.5746672495381394
H	0.2753548530703697	0.6291275119360703	0.5759821553015605

2

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O	0.3789100050000016	0.2519800070000002	0.1704400030000031
O	0.3387659728848653	0.2708842767385937	0.5040894203699161
O	0.1285700050000003	0.4216499919999990	0.2459899930000020
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O	0.6220897538351668	0.0960322170013175	0.4318393721819398
O	0.8781126653634933	0.2522747594247397	0.3337131739652572
O	0.8809400199999970	0.2520500119999980	0.1697999980000020
O	0.8868555436552696	0.2570665334588739	0.4956854763796667
O	0.6275799869999972	0.4220199880000024	0.2460899949999984
O	0.6216359429551016	0.4181495147254733	0.4142971906933203
O	0.3799849677674681	0.5877847986551139	0.3375464130681831
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O	0.1297000049999966	0.7572699790000001	0.2492299970000005
O	0.1371769927181669	0.7523079666159082	0.4176373879203532

O	0.3828529864454635	0.9231303211096895	0.3353522713649368
O	0.3803899879999975	0.9225900169999974	0.1709299979999983
O	0.3779613820562426	0.9137105323958036	0.5003908375399669
O	0.8762661004362198	0.5884378486289836	0.3311098733172987
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O	0.8717536082248418	0.9198707824138282	0.3365839653409779
O	0.8778399830000012	0.9210100170000004	0.1696500030000010
O	0.8763999369062044	0.9162132455997160	0.4994596505403375
Co	0.3731015420229007	0.0905223312070887	0.4302591509905362
Co	0.3799799980000031	0.0872400029999980	0.2470700000000008
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Co	0.1152003455940910	0.2665960881261499	0.4939307449291661
Co	0.1278931362799747	0.2521859844714892	0.3341817089737582
Co	0.3772873694734986	0.4174780233656976	0.4193523992457390
Co	0.3765200080000000	0.4212099909999978	0.2435899970000008
Co	0.8790996259290607	0.0835380306834650	0.4237979165518756
Co	0.8753799799999982	0.0866900010000009	0.2461100069999986
Co	0.6244699949999983	0.2516300079999993	0.1762599950000023
Co	0.6592130001534749	0.2692429286563344	0.5005994456097235
Co	0.6261854565379091	0.2499064301444962	0.3364154929980864
Co	0.8803134011763649	0.4209232953832249	0.4151192659291885
Co	0.8762099739999982	0.4209499959999974	0.2424499990000015
Co	0.1210800039999995	0.5911999940000001	0.1736499969999983
Co	0.1222333579669300	0.5815142742238749	0.5034223519165739
Co	0.1287075937521762	0.5894689989985553	0.3334097840303930
Co	0.3788296402864432	0.7580045344140359	0.4209184806377149
Co	0.3790099920000003	0.7569699880000016	0.2464600059999995
Co	0.1244399990000034	0.9229400159999983	0.1736100019999967
Co	0.1258568097300198	0.9078772313736206	0.4996495722375103
Co	0.1297441588676193	0.9215045609627226	0.3361576833149910
Co	0.6225600240000020	0.5913599730000030	0.1737499979999981
Co	0.6638904123023959	0.5831965378983782	0.5020374841994374
Co	0.6279904521390882	0.5862302882789429	0.3350415023173737
Co	0.8825088444306652	0.7548089133459904	0.4207732280115025
Co	0.8755000230000007	0.7549399729999990	0.2450000050000014
Co	0.6251699919999965	0.9188799860000003	0.1722500030000020
Co	0.6295686550885727	0.9181398229287983	0.4983922873456532
Co	0.6270739121798379	0.9184583352882685	0.3386151255535633
Rh	0.4489342772638822	0.4477930075147354	0.5695828127435519
N	0.3141378059424412	0.5941991833183293	0.6361939670629303
N	0.2187677917043122	0.6160383256442867	0.5908845900610583
H	0.5776181046549324	0.5637355566569634	0.6012369294698209
H	0.5965470006987083	0.3353889043428407	0.5872380569965517

3

E= -372.86559

O	0.1275400070000003	0.0867199970000030	0.2486699970000004
O	0.1320064705236730	0.0756200916210462	0.4311316523736057
O	0.3706513831583804	0.2498777700077361	0.3339809109224598
O	0.3789100050000016	0.2519800070000002	0.1704400030000031
O	0.3659125668708819	0.2699075571075786	0.5013065107512716

O	0.1285700050000003	0.4216499919999990	0.2459899930000020
O	0.1294864616953919	0.4248181403168339	0.4183491354738165
O	0.6293500069999993	0.0836099980000000	0.2534199950000016
O	0.6268597410329015	0.1000176261038124	0.4280716220773538
O	0.8824347134909645	0.2505888258923030	0.3344055108393059
O	0.8809400199999970	0.2520500119999980	0.1697999980000020
O	0.8802155606814362	0.2590274586440284	0.4988670962775585
O	0.6275799869999972	0.4220199880000024	0.2460899949999984
O	0.6209065353604962	0.4157204577863660	0.4119621939660178
O	0.3782828985408031	0.5884717792049262	0.3345729609819173
O	0.3827799860000027	0.5909299850000025	0.1701100020000013
O	0.1297000049999966	0.7572699790000001	0.2492299970000005
O	0.1360269482505791	0.7508670977390154	0.4171682303516800
O	0.3823556315653965	0.9235896903287424	0.3358333341343485
O	0.3803899879999975	0.9225900169999974	0.1709299979999983
O	0.3919778402107827	0.9145228166078962	0.4989010993606759
O	0.8780876591319453	0.5854768920923485	0.3316863110762277
O	0.8804000020000018	0.5905299779999993	0.1686600000000027
O	0.8768729090860963	0.5831325944834234	0.4909695776516301
O	0.6277800200000030	0.7563300130000030	0.2522000069999990
O	0.6190607883560240	0.7398084616621501	0.4239491953948412
O	0.8752580323773327	0.9203110295687934	0.3367795324317829
O	0.8778399830000012	0.9210100170000004	0.1696500030000010
O	0.8672858017052478	0.9137582927681793	0.5002130302058153
Co	0.3806401190111175	0.0884521711227717	0.4268421843117782
Co	0.3799799980000031	0.0872400029999980	0.2470700000000008
Co	0.1260699930000015	0.2518900040000034	0.1730300039999975
Co	0.1211500556152874	0.2605869832902409	0.4965008564273201
Co	0.1261097884065697	0.2498804027499962	0.3351487554049267
Co	0.3757116487073504	0.4184451290437530	0.4131751547336777
Co	0.3765200080000000	0.4212099909999978	0.2435899970000008
Co	0.8807516292375310	0.0840219086540953	0.4281459437216916
Co	0.8753799799999982	0.0866900010000009	0.2461100069999986
Co	0.6244699949999983	0.2516300079999993	0.1762599950000023
Co	0.6387147498010902	0.2776360284857715	0.5048485533565786
Co	0.6285239555261247	0.2475181679345970	0.3360267262999238
Co	0.8766014705187025	0.4156375704586682	0.4170121920718476
Co	0.8762099739999982	0.4209499959999974	0.2424499990000015
Co	0.1210800039999995	0.5911999940000001	0.1736499969999983
Co	0.1069687432272546	0.5715948572046151	0.5062698925667695
Co	0.1267914765702333	0.5880960099526931	0.3342514964277399
Co	0.3789612831473885	0.7519184916580894	0.4203272883194039
Co	0.3790099920000003	0.7569699880000016	0.2464600059999995
Co	0.1244399990000034	0.9229400159999983	0.1736100019999967
Co	0.1438024875699306	0.8987977569476451	0.5056130475545638
Co	0.1299583749414505	0.9206580457031259	0.3383092368347210
Co	0.6225600240000020	0.5913599730000030	0.1737499979999981
Co	0.6517712388938752	0.5741645740090960	0.4987020765159181
Co	0.6300537321390376	0.5853608279839080	0.3337903329904192
Co	0.8823538810174669	0.7549094476562862	0.4216483929209148
Co	0.8755000230000007	0.7549399729999990	0.2450000050000014
Co	0.6251699919999965	0.9188799860000003	0.1722500030000020
Co	0.6338784412604600	0.9178713545757532	0.4945467019562450
Co	0.6297932948315635	0.9187841058555537	0.3381817674566610
Rh	0.3803198415734740	0.4794221361938733	0.5536383801446981
N	0.3285823029267863	0.6717242183229989	0.5924439789788921
N	0.1912508813425734	0.7086980319527009	0.5729701529875282
H	0.3937061833265411	0.7534209502856508	0.6183552970195260

H 0.5846100777786539 0.4470013127670442 0.5739830098284838

4

E= -379.10080

O	0.1275400070000003	0.0867199970000030	0.2486699970000004
O	0.1330531845752307	0.0705984591700999	0.4332478457719424
O	0.3686126494902542	0.2490354915332930	0.3352987670280002
O	0.3789100050000016	0.2519800070000002	0.1704400030000031
O	0.3714016207022708	0.2752388387993269	0.5026663869701282
O	0.1285700050000003	0.4216499919999990	0.2459899930000020
O	0.1258326255795428	0.4236932885538818	0.4178387576523764
O	0.6293500069999993	0.0836099980000000	0.2534199950000016
O	0.6281695354558053	0.0995375436162639	0.4245834225887474
O	0.8830388081058865	0.2512596737746085	0.3337920314795907
O	0.8809400199999970	0.2520500119999980	0.1697999980000020
O	0.8777948723215564	0.2577892409873493	0.4980643532865207
O	0.6275799869999972	0.4220199880000024	0.2460899949999984
O	0.6208133112434572	0.4181235696275725	0.4111697424522098
O	0.3772438949370787	0.5877413249681723	0.3346212033647445
O	0.3827799860000027	0.5909299850000025	0.1701100020000013
O	0.1297000049999966	0.7572699790000001	0.2492299970000005
O	0.1414458155173098	0.7384843629996313	0.4229385066318742
O	0.3785220533710709	0.9220196344581275	0.3356700507836699
O	0.3803899879999975	0.9225900169999974	0.1709299979999983
O	0.4070899855272992	0.9160182631288780	0.4994658727567448
O	0.8787051277876883	0.5862052048319535	0.3308614077374009
O	0.8804000020000018	0.5905299779999993	0.1686600000000027
O	0.8742405085050212	0.5864162285433544	0.4894665793286884
O	0.6277800200000030	0.7563300130000030	0.2522000069999990
O	0.6212990249775892	0.7418880020611210	0.4209805451579770
O	0.8803028919634388	0.9201238886548497	0.3370433966161263
O	0.8778399830000012	0.9210100170000004	0.1696500030000010
O	0.8686424920462205	0.9141923323063043	0.4987959020168198
Co	0.3818746652279829	0.0874265483264384	0.4289198638545476
Co	0.3799799980000031	0.0872400029999980	0.2470700000000008
Co	0.1260699930000015	0.2518900040000034	0.1730300039999975
Co	0.1222762584420649	0.2590158725974508	0.4943462029673645
Co	0.1261993968508941	0.2510158742047003	0.3344159406427434
Co	0.3755179627359597	0.4210189077520062	0.4136985036590076
Co	0.3765200080000000	0.4212099909999978	0.2435899970000008
Co	0.8790500111143060	0.0873206602527500	0.4254159623840133
Co	0.8753799799999982	0.0866900010000009	0.2461100069999986
Co	0.6244699949999983	0.2516300079999993	0.1762599950000023
Co	0.6367914376167787	0.2829494415297356	0.5037608134202756
Co	0.6268239116972745	0.2491060518047217	0.3356189951460753
Co	0.8744172163918749	0.4167347066241294	0.4173704416094783
Co	0.8762099739999982	0.4209499959999974	0.2424499990000015
Co	0.1210800039999995	0.5911999940000001	0.1736499969999983
Co	0.1111201030274456	0.5728383902409292	0.5055994370645274
Co	0.1274709281179177	0.5868657448276051	0.3340882780392220
Co	0.3811851800515277	0.7546672131744498	0.4239099098408926
Co	0.3790099920000003	0.7569699880000016	0.2464600059999995
Co	0.1244399990000034	0.9229400159999983	0.1736100019999967
Co	0.1035938826810991	0.8954577857449239	0.5067245568966803

Co	0.1317441395020614	0.9188208477195199	0.3396680619634644
Co	0.6225600240000020	0.5913599730000030	0.1737499979999981
Co	0.6484696210449983	0.5795902361358807	0.4991274337768252
Co	0.6289733597742083	0.5863785549808789	0.3332297408306796
Co	0.8793623973782488	0.7520600067311243	0.4184188488479043
Co	0.8755000230000007	0.7549399729999990	0.2450000050000014
Co	0.6251699919999965	0.9188799860000003	0.1722500030000020
Co	0.6365035388189537	0.9198020595628853	0.4944631215352297
Co	0.6276536186851918	0.9199650170883553	0.3382256142328227
Rh	0.3782854859019132	0.4898296376191072	0.5544577188035393
N	0.3131737806123390	0.6874419903108359	0.5897628790831884
N	0.1764142241212492	0.7243798651515022	0.5691714899955050
H	0.3800102137053972	0.7757150468211786	0.6083721250375846
H	0.5876521010733714	0.4534692604017157	0.5688749123887763
H	0.0435720104670482	0.4712164776161039	0.5712949122402713
H	0.1477761215803849	0.4554087948531698	0.5750617541870067

5

E= -380.77669

O	0.1275400070000003	0.0867199970000030	0.2486699970000004
O	0.1332999019027649	0.0851691244193061	0.4428405372239372
O	0.3734375127999449	0.2490627577127620	0.3361508884631748
O	0.3789100050000016	0.2519800070000002	0.1704400030000031
O	0.4098424047358999	0.2745785526610162	0.5057840998177553
O	0.1285700050000003	0.4216499919999990	0.2459899930000020
O	0.1306847151376644	0.4181491293887952	0.4145453055505683
O	0.6293500069999993	0.0836099980000000	0.2534199950000016
O	0.6269812190314341	0.0889863694735799	0.4200808712215947
O	0.8832056338928915	0.2510018559638475	0.3339461601524547
O	0.8809400199999970	0.2520500119999980	0.1697999980000020
O	0.8689432539204096	0.2587246724708012	0.4973023452082159
O	0.6275799869999972	0.4220199880000024	0.2460899949999984
O	0.6236108916653126	0.4211083724061433	0.4129460507196092
O	0.3760598251121483	0.5869067223417639	0.3361525957116752
O	0.3827799860000027	0.5909299850000025	0.1701100020000013
O	0.1297000049999966	0.7572699790000001	0.2492299970000005
O	0.1351553823580721	0.7530989899196334	0.4192664662982930
O	0.3754779679615912	0.9228196595578940	0.3360335221249663
O	0.3803899879999975	0.9225900169999974	0.1709299979999983
O	0.4061963202676687	0.9119619537834274	0.5001547659492247
O	0.8787740421181185	0.5867605823463974	0.3317268099825144
O	0.8804000020000018	0.5905299779999993	0.1686600000000027
O	0.8708006755861822	0.5840430696478225	0.4918805156479841
O	0.6277800200000030	0.7563300130000030	0.2522000069999990
O	0.6181353351406407	0.7416356248889153	0.4201099956715941
O	0.8817094532797622	0.9214687338046340	0.3367957870183718
O	0.8778399830000012	0.9210100170000004	0.1696500030000010
O	0.8641067782525303	0.9145208276781462	0.4987615926610598
Co	0.3749196313933954	0.0878100900919026	0.4323506658323767
Co	0.3799799980000031	0.0872400029999980	0.2470700000000008
Co	0.1260699930000015	0.2518900040000034	0.1730300039999975
Co	0.1032615948512081	0.2746651088375303	0.5034630976388360
Co	0.1284962744558872	0.2514895009560326	0.3353471776355819
Co	0.3773410202478105	0.4171088805223059	0.4175812883592441

Co	0.3765200080000000	0.4212099909999978	0.2435899970000008
Co	0.8817811701515946	0.0859089631053612	0.4252381473622014
Co	0.8753799799999982	0.0866900010000009	0.2461100069999986
Co	0.6244699949999983	0.2516300079999993	0.1762599950000023
Co	0.6366443773665682	0.2595986747084201	0.4977360192640411
Co	0.6270149666038408	0.2486246410156783	0.3352530214308861
Co	0.8755571017839673	0.4175029003074670	0.4156338788977346
Co	0.8762099739999982	0.4209499959999974	0.2424499990000015
Co	0.1210800039999995	0.5911999940000001	0.1736499969999983
Co	0.1009822866496908	0.5787019985510329	0.5025009975550270
Co	0.1290921186868566	0.5874392128145705	0.3340480114735456
Co	0.3763720674199180	0.7559344038909830	0.4225987656599665
Co	0.3790099920000003	0.7569699880000016	0.2464600059999995
Co	0.1244399990000034	0.9229400159999983	0.1736100019999967
Co	0.1036595500575369	0.9008624455953154	0.5089141791666543
Co	0.1305210581781100	0.9203063744673411	0.3389940629366676
Co	0.6225600240000020	0.5913599730000030	0.1737499979999981
Co	0.6447501327807000	0.5770659698343390	0.4952010355981369
Co	0.6280935981091841	0.5867788630345858	0.3328992855442539
Co	0.8770244620211017	0.7537302512590653	0.4193418036056573
Co	0.8755000230000007	0.7549399729999990	0.2450000050000014
Co	0.6251699919999965	0.9188799860000003	0.1722500030000020
Co	0.6345169482338382	0.9167653527395629	0.4956421965034325
Co	0.6258336611745543	0.9198124027633711	0.3379005863633668
Rh	0.3569531129847359	0.4801007162459018	0.5611841320971719
N	0.3006759967047916	0.6820219009156482	0.5938908942438332
N	0.1501635784014573	0.7361498657439959	0.5823242732373974
H	0.0772346773336166	0.6974312351113696	0.6233384967326990
H	0.3756211833100412	0.7641130480629809	0.5751369106955179
H	0.5460187822776180	0.5351163244437979	0.5759914794193489
H	0.1600132045706682	0.4182158751052397	0.5694638719405288

6

E= -380.76300

O	0.1286000010000024	0.0870800020000004	0.2544000150000016
O	0.1380434375174238	0.0883381345391644	0.4462656015077101
O	0.3738850676810574	0.2490323498659688	0.3386188731479332
O	0.3790900110000024	0.2518799899999991	0.1727299899999977
O	0.4179025125128358	0.2729817674697267	0.5083864504298510
O	0.1318700019999994	0.4249500040000029	0.2448000010000015
O	0.1293111469614519	0.4215047350859398	0.4141205377170514
O	0.6326100229999980	0.0850500020000027	0.2500300109999998
O	0.6291001036809866	0.0915926533946014	0.4207622342872420
O	0.8843408452574758	0.2509286044637721	0.3353139977573167
O	0.8879100079999986	0.2527300120000007	0.1709900050000002
O	0.8697993594301450	0.2611107421800193	0.4985872869554663
O	0.6310999989999999	0.4188300069999968	0.2489400059999980
O	0.6265793475732916	0.4221975487014712	0.4116353582713383
O	0.3784665721257405	0.5896866885437647	0.3343318098650957
O	0.4014700059999967	0.5909299850000025	0.1691199990000030
O	0.1325500009999985	0.7533400060000019	0.2446900010000022
O	0.1380091200517558	0.7550902366752853	0.4177622471451881
O	0.3773028459159308	0.9228479430841945	0.3358530564919626
O	0.3817099930000012	0.9268699880000000	0.1710900069999965

O	0.4107439148948564	0.9076099585430621	0.5009178671921445
O	0.8827033877066364	0.5878153992709114	0.3306757976241100
O	0.8701800110000022	0.5896999839999992	0.1678400039999985
O	0.8719848181927540	0.5855366809026404	0.4929952052062032
O	0.6315600280000027	0.7610700130000012	0.2522400020000006
O	0.6229767966744612	0.7447004386560824	0.4177363927155179
O	0.8852297696400945	0.9221865459871171	0.3370368991656015
O	0.8830299970000013	0.9218299979999998	0.1695500020000011
O	0.8684843893695092	0.9157347764261972	0.4990646723697724
Co	0.3784354096594144	0.0881226587794864	0.4341634746876806
Co	0.3802999850000006	0.0868600099999980	0.2498299929999988
Co	0.1303600070000002	0.2505899969999987	0.1755699960000001
Co	0.1010101957407111	0.2791804919777449	0.5039108985172021
Co	0.1299817232379654	0.2520432752963094	0.3380244800435914
Co	0.3802646066924883	0.4212653611301311	0.4161179663189685
Co	0.3782500029999980	0.4255700109999978	0.2429900019999991
Co	0.8850256132541391	0.0875712240157578	0.4267863907381147
Co	0.8786200280000003	0.0867599990000016	0.2464999999999975
Co	0.6224600079999973	0.2529399989999987	0.1760800030000027
Co	0.6392593174904817	0.2678865524228478	0.4996523223442815
Co	0.6296231140053954	0.2485414092761657	0.3351254268525808
Co	0.8769436331490281	0.4208079787326636	0.4156416750864991
Co	0.8791599870000013	0.4187900129999989	0.2442999929999985
Co	0.1000099999999975	0.5893099899999967	0.1727599949999998
Co	0.1050605774349566	0.5806617023619984	0.5054443165888843
Co	0.1318692526720163	0.5883968068717829	0.3336676695855148
Co	0.3802035190332061	0.7532129482177388	0.4219173247546477
Co	0.3801800009999994	0.7552999850000006	0.2439399960000017
Co	0.1291400049999964	0.9265599849999973	0.1753199990000027
Co	0.1129667626339009	0.9000786182564479	0.5085547599328351
Co	0.1337233593781031	0.9208248598744376	0.3391960729326891
Co	0.6285300250000034	0.5910000209999993	0.1727000030000028
Co	0.6458854284419825	0.5770171185991395	0.4924513075537081
Co	0.6311561128980971	0.5892093228003908	0.3313604568048913
Co	0.8807830720463607	0.7542411049725245	0.4200780365848146
Co	0.8786000010000024	0.7581800219999977	0.2458100019999989
Co	0.6265699859999998	0.9184200170000025	0.1712100060000026
Co	0.6398031803157328	0.9171379255681157	0.4944603610875976
Co	0.6279628456759238	0.9225095689395328	0.3370319462210714
Rh	0.3651295498462369	0.4758848570500271	0.5541543012706538
N	0.3164774786100711	0.6889413464808799	0.5995072058881030
N	0.1557420942802233	0.7393885446907694	0.5824645947944006
H	0.3853275817779394	0.7705824013761938	0.5745945194725095
H	0.3345456399531893	0.6927081185219621	0.6558307608951368
H	0.0890658844227641	0.7261753517357592	0.6292735957767069
H	0.1674060015818675	0.4164740676828524	0.5691093279272369

7

E= -380.38845

O	0.1286000010000024	0.0870800020000004	0.2544000150000016
O	0.1398083916865412	0.0834470560957398	0.4402729920554441
O	0.3735479398651066	0.2484534502745896	0.3388439212237437
O	0.3790900110000024	0.2518799899999991	0.1727299989999977
O	0.3857395249692677	0.2961628656747105	0.5099229528989775

O	0.1318700019999994	0.4249500040000029	0.2448000010000015
O	0.1272890130250793	0.4184619957633512	0.4092440567776726
O	0.6326100229999980	0.0850500020000027	0.2500300109999998
O	0.6265042586575149	0.0972710396832722	0.4232549859484241
O	0.8837073769924731	0.2507078338200734	0.3341878620609781
O	0.8879100079999986	0.2527300120000007	0.1709900050000002
O	0.8795999751484663	0.2654299591565404	0.4991704932658497
O	0.6310999989999999	0.4188300069999968	0.2489400059999980
O	0.6286178000934899	0.4237664147266385	0.4102701293022726
O	0.3768890106181168	0.5906431029492838	0.3341354278257331
O	0.4014700059999967	0.5909299850000025	0.1691199990000030
O	0.1325500009999985	0.7533400060000019	0.2446900010000022
O	0.1393258369735189	0.7554975863143194	0.4221627376208926
O	0.3771920689640788	0.9217165037117082	0.3370819719365512
O	0.3817099930000012	0.9268699880000000	0.1710900069999965
O	0.4118649926863943	0.9145877899621936	0.5022851341137206
O	0.8847364970215971	0.5901883996822328	0.3311807828433120
O	0.8701800110000022	0.5896999839999992	0.1678400039999985
O	0.8748085061442745	0.5909878097420571	0.4954917593512167
O	0.6315600280000027	0.7610700130000012	0.2522400020000006
O	0.6243386173535855	0.7476121359644435	0.4181273018870870
O	0.8849902076252026	0.9229387663364175	0.3385541201409031
O	0.8830299970000013	0.9218299979999998	0.1695500020000011
O	0.8704567074311097	0.9192015164610319	0.5005262789653998
Co	0.3809573194613767	0.0874984453411139	0.4300152492219927
Co	0.3802999850000006	0.0868600009999980	0.2498299929999988
Co	0.1303600070000002	0.2505899969999987	0.1755699960000001
Co	0.1294457558893322	0.2765188363046072	0.5000373963545596
Co	0.1288635659711741	0.2501333333149745	0.3355909885862788
Co	0.3818436322161559	0.4257986752544604	0.4148012263318184
Co	0.3782500029999980	0.4255700109999978	0.2429900019999991
Co	0.8824619216813187	0.0949061973690945	0.4279835469427166
Co	0.8786200280000003	0.0867599990000016	0.2464999999999975
Co	0.6224600079999973	0.2529399989999987	0.1760800030000027
Co	0.6342568400105255	0.2853408073843493	0.5042031450009227
Co	0.6308579993442244	0.2493477245497774	0.3359895578543649
Co	0.8768970062794833	0.4203445326611305	0.4167472207929814
Co	0.8791599870000013	0.4187900129999989	0.2442999929999985
Co	0.1000099999999975	0.5893099899999967	0.1727599949999998
Co	0.1062604181284102	0.5752739721109225	0.4904522385957275
Co	0.1316159618693367	0.5892299042279658	0.3314673761800768
Co	0.3819765254933885	0.7476106493228561	0.4264269881400541
Co	0.3801800009999994	0.7552999850000006	0.2439399960000017
Co	0.1291400049999964	0.9265599849999973	0.1753199990000027
Co	0.1025352826890718	0.9059094676305487	0.5066632493492371
Co	0.1336649297578016	0.9221427988773269	0.3405418757632174
Co	0.6285300250000034	0.5910000209999993	0.1727000030000028
Co	0.6457934282869428	0.5747626678166754	0.4983509366259858
Co	0.6315103889239857	0.5904541039819224	0.3321676853058591
Co	0.8776594852991242	0.7548622618795521	0.4194836227901924
Co	0.8786000010000024	0.7581800219999977	0.2458100019999989
Co	0.6265699859999998	0.9184200170000025	0.1712100060000026
Co	0.6409682195751290	0.9196888583062657	0.4934712819599157
Co	0.6270742750430432	0.9232041574597387	0.3375728739926775
Rh	0.3572144984946395	0.5072826028330749	0.5520236110583224
N	0.3271270102907902	0.7173942689149513	0.6026189668763098
N	0.1696987562670159	0.7881415532733196	0.6069558930474328
H	0.3883808325671047	0.7974487183765535	0.5700774648786674

H	0.3722079780056945	0.7129966702826726	0.6554814209104566
H	0.1687623628151499	0.8616069702510499	0.6506666931454632
H	0.0897309071819837	0.7064283915936961	0.6191607753579319

8

E= -382.17519

O	0.1286000010000024	0.0870800020000004	0.2544000150000016
O	0.1281935442766104	0.0774006008972933	0.4313813863322209
O	0.3732522570767330	0.2510141124352070	0.3387038530088740
O	0.3790900110000024	0.2518799899999991	0.1727299989999977
O	0.3373122391449108	0.2618976086324781	0.5089597092834814
O	0.1318700019999994	0.4249500040000029	0.2448000010000015
O	0.1300187325699381	0.4314852723930647	0.4208255865493620
O	0.6326100229999980	0.0850500020000027	0.2500300109999998
O	0.6217630715671176	0.1035619361954583	0.4266510858806836
O	0.8854503391742633	0.2523651617038278	0.3356452739816305
O	0.8879100079999986	0.2527300120000007	0.1709900050000002
O	0.8781971836665082	0.2604610822625917	0.4992527664876742
O	0.6310999899999999	0.4188300069999968	0.2489400059999980
O	0.6293801952617037	0.4221773283088954	0.4122963593582120
O	0.3774703555100831	0.5882377800064899	0.3342711134189899
O	0.4014700059999967	0.5909299850000025	0.1691199990000030
O	0.1325500009999985	0.7533400060000019	0.2446900010000022
O	0.1400797298123072	0.7520715319377052	0.4173171645393134
O	0.3792244144477815	0.9234751689891382	0.3347057473913077
O	0.3817099930000012	0.9268699880000000	0.1710900069999965
O	0.4030621569521330	0.9084639067789981	0.4995120527703215
O	0.8836271486125902	0.5873209170445103	0.3294580698903723
O	0.8701800110000022	0.5896999839999992	0.1678400039999985
O	0.8788954508665874	0.5882834575349636	0.4907728037797706
O	0.6315600280000027	0.7610700130000012	0.2522400020000006
O	0.6225729624699200	0.7439692549279786	0.4183077088703087
O	0.8780481195698610	0.9212885553627341	0.3362546455733815
O	0.8830299970000013	0.9218299979999998	0.1695500020000011
O	0.8618610362390904	0.9182160171101016	0.4969768775242110
Co	0.3734862559392537	0.0855687660899245	0.4326447747181560
Co	0.3802999850000006	0.0868600009999980	0.2498299929999988
Co	0.1303600070000002	0.2505899969999987	0.1755699960000001
Co	0.1094060349085904	0.2650557224218806	0.4975764937234920
Co	0.1296163472142601	0.2506724386552869	0.3380567388850453
Co	0.3765390965839058	0.4232441813685242	0.4171169381489249
Co	0.3782500029999980	0.4255700109999978	0.2429900019999991
Co	0.8764031535101890	0.0888127711815886	0.4240794132519551
Co	0.8786200280000003	0.0867599990000016	0.2464999999999975
Co	0.6224600079999973	0.2529399989999987	0.1760800030000027
Co	0.6471641038149281	0.2708607613756120	0.5022946294255238
Co	0.6261486734845507	0.2515843833256953	0.3356788718519061
Co	0.8790594565387823	0.4222616271687044	0.4160767396193772
Co	0.8791599870000013	0.4187900129999989	0.2442999929999985
Co	0.1000099999999975	0.5893099899999967	0.1727599949999998
Co	0.1150482385417949	0.5922141487493271	0.5036205667386159
Co	0.1311060159234184	0.5904151640611898	0.3333052669360541
Co	0.3809006217377511	0.7555245830984803	0.4212153159867889
Co	0.3801800009999994	0.7552999850000006	0.2439399960000017

Co	0.1291400049999964	0.9265599849999973	0.1753199990000027
Co	0.1000382009548142	0.9040493571434853	0.5065167106198382
Co	0.1324882496509889	0.9215041242368880	0.3394468066905992
Co	0.6285300250000034	0.5910000209999993	0.1727000030000028
Co	0.6516881021968347	0.5781511409301270	0.5013413831298373
Co	0.6304766573192878	0.5878264689895395	0.3329826277805879
Co	0.8785141695119333	0.7538828295656599	0.4179207192107479
Co	0.8786000010000024	0.7581800219999977	0.2458100019999989
Co	0.6265699859999998	0.9184200170000025	0.1712100060000026
Co	0.6324487067302094	0.9179202686483910	0.4936905388669023
Co	0.6267861141374335	0.9204319265881994	0.3370758969850082
Rh	0.4210150461547201	0.4474402765290851	0.5554232938949112
N	0.5303652767882399	0.6324370167285036	0.5912847110576601
N	0.1277554843647961	0.7444111565808216	0.5832885301478056
H	0.4787624991252140	0.7345126145580995	0.5841096652239892
H	0.5918587070603534	0.6313590135344673	0.6401098834322370
H	0.2307420577974865	0.7500187711783785	0.6121137154605232
H	0.0388237761251541	0.7358183189396669	0.6212330301563314

9

E= -389.24398

O	0.1286000010000024	0.0870800020000004	0.2544000150000016
O	0.1313691276257258	0.0762854074602862	0.4307184950523740
O	0.3734907692282029	0.2530463158881022	0.3364465516560235
O	0.3790900110000024	0.2518799899999991	0.1727299989999977
O	0.3458532744355893	0.2694055158643647	0.5014791288291914
O	0.1318700019999994	0.4249500040000029	0.2448000010000015
O	0.1348079763571726	0.4316597721283297	0.4194412169552522
O	0.6326100229999980	0.0850500020000027	0.2500300109999998
O	0.6253696519045739	0.0999625377689943	0.4274584247797741
O	0.8844533909521817	0.2539752028634544	0.3364637560111295
O	0.8879100079999986	0.2527300120000007	0.1709900050000002
O	0.8825682119936188	0.2604932669715250	0.4987722924713236
O	0.6310999899999999	0.4188300069999968	0.2489400059999980
O	0.6210325187453259	0.4230519086889518	0.4155430078297582
O	0.3796847951168163	0.5870550564197150	0.3355744650809497
O	0.4014700059999967	0.5909299850000025	0.1691199990000030
O	0.1325500009999985	0.7533400060000019	0.2446900010000022
O	0.1406226978929542	0.7526920477317859	0.4154754453340382
O	0.3819005076094010	0.9238620409462459	0.3353863214631059
O	0.3817099930000012	0.9268699880000000	0.1710900069999965
O	0.4026943335533074	0.9067712342314138	0.4992712700664620
O	0.8828377262361429	0.5855653842373834	0.3298200762128990
O	0.8701800110000022	0.5896999839999992	0.1678400039999985
O	0.8899974777515037	0.5862043008873686	0.4899388262276996
O	0.6315600280000027	0.7610700130000012	0.2522400020000006
O	0.6276660092833122	0.7443015070425512	0.4176274276531738
O	0.8793115184326801	0.9223077112501703	0.3357201222773497
O	0.8830299970000013	0.9218299979999998	0.1695500020000011
O	0.8668399953797922	0.9166581815113329	0.4976392342683252
Co	0.3761681691014611	0.0834977920093368	0.4318167106217000
Co	0.3802999850000006	0.0868600009999980	0.2498299929999988
Co	0.1303600070000002	0.2505899969999987	0.1755699960000001
Co	0.1129432918425457	0.2633956097780293	0.4954077476914750

Co	0.1303698086477794	0.2508348817794426	0.3373338597811378
Co	0.3788461638128056	0.4225112091317074	0.4190648635005941
Co	0.3782500029999980	0.4255700109999978	0.2429900019999991
Co	0.8793222587556330	0.0866961354588827	0.4245722369136082
Co	0.8786200280000003	0.0867599990000016	0.2464999999999975
Co	0.6224600079999973	0.2529399899999987	0.1760800030000027
Co	0.6518459526850739	0.2730891963120464	0.5000230095404126
Co	0.6256696941775235	0.2521157364483562	0.3365075200049638
Co	0.8805574961210270	0.4223582457914284	0.4164742161721164
Co	0.8791599870000013	0.4187900129999989	0.2442999929999985
Co	0.1000099999999975	0.5893099899999967	0.1727599949999998
Co	0.1249523710884884	0.5891687205094269	0.5011878674759443
Co	0.1318245051505437	0.5895247628153832	0.3327693018594821
Co	0.3833683280667051	0.7517252698090870	0.4207423438389412
Co	0.3801800009999994	0.7552999850000006	0.2439399960000017
Co	0.1291400049999964	0.9265599849999973	0.1753199990000027
Co	0.1070009834312382	0.9005590554080798	0.5064949526855703
Co	0.1338089191698870	0.9217238606973144	0.3388556666074222
Co	0.6285300250000034	0.5910000209999993	0.1727000030000028
Co	0.6652053119883879	0.5905600216960500	0.5057473749691439
Co	0.6308544850025465	0.5872709182622019	0.3334865444882746
Co	0.8827716623341314	0.7545299335705081	0.4177194943151576
Co	0.8786000010000024	0.7581800219999977	0.2458100019999989
Co	0.6265699859999998	0.9184200170000025	0.1712100060000026
Co	0.6341456400558757	0.9146104693229770	0.4949932747061636
Co	0.6287476060437966	0.9204377043514729	0.3369947417941681
Rh	0.4325080815612236	0.4446244073527124	0.5627826342341762
N	0.5358972866261246	0.6473071935056365	0.5920428813077574
N	0.1371859970831167	0.7367815694115476	0.5819333498987831
H	0.4678243108030835	0.7394871322251650	0.5829597550971308
H	0.5823224023339905	0.6534115761339339	0.6441850032118949
H	0.2389510097254123	0.7442566330468464	0.6115555239486117
H	0.0475799541013726	0.7231425625580132	0.6191554493511248
H	0.4540678765692764	0.4031328834061995	0.6527602067179085
H	0.5297723563996684	0.3470711444843169	0.6269612580476870

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E= -389.29873

O	0.1286000010000024	0.0870800020000004	0.2544000150000016
O	0.1292476538028014	0.0752975206418660	0.4282156499679146
O	0.3784335536896111	0.2518207653172277	0.3360802621453571
O	0.3790900110000024	0.2518799899999991	0.1727299989999977
O	0.3390495518109281	0.2638659733623386	0.4993193602541783
O	0.1318700019999994	0.4249500040000029	0.2448000010000015
O	0.1307853629387158	0.4308926685060643	0.4170633704684847
O	0.6326100229999980	0.0850500020000027	0.2500300109999998
O	0.6268843573270468	0.1026673036853950	0.4284334519782619
O	0.8803423490737832	0.2551656123710053	0.3369616469687108
O	0.8879100079999986	0.2527300120000007	0.1709900050000002
O	0.8838494340741132	0.2590035118139385	0.4990473895263116
O	0.6310999899999999	0.4188300069999968	0.2489400059999980
O	0.6168198108104762	0.4294242415587365	0.4251145969202814
O	0.3810019530127983	0.5885889647035750	0.3344650961825837
O	0.4014700059999967	0.5909299850000025	0.1691199990000030

O	0.1325500009999985	0.7533400060000019	0.2446900010000022
O	0.1402909145472263	0.7531216014534291	0.4143320095756418
O	0.3828669035695950	0.9241370828705217	0.3351659815624917
O	0.3817099930000012	0.9268699880000000	0.1710900069999965
O	0.4028765829898164	0.9085968647842019	0.4989787618805953
O	0.8798320255668975	0.5855608743674087	0.3306611515026889
O	0.8701800110000022	0.5896999839999992	0.1678400039999985
O	0.8965532201936630	0.5866267976054019	0.4910649462215835
O	0.6315600280000027	0.7610700130000012	0.2522400020000006
O	0.6265623095709528	0.7473275863970104	0.4169925417998496
O	0.8781902020912169	0.9220796479843860	0.3352350980894189
O	0.8830299970000013	0.9218299979999998	0.1695500020000011
O	0.8674091199485815	0.9157657090373207	0.4975110321626626
Co	0.3765186034496215	0.0847946325324269	0.4314435516480409
Co	0.3802999850000006	0.0868600099999980	0.2498299929999988
Co	0.1303600070000002	0.2505899969999987	0.1755699960000001
Co	0.1128934103258375	0.2622673038030475	0.4962837821275686
Co	0.1301778718798264	0.2500310389750429	0.3376165159978002
Co	0.3706893686768596	0.4235484677796378	0.4156881750093914
Co	0.3782500029999980	0.4255700109999978	0.2429900019999991
Co	0.8799059736831648	0.0859176895799144	0.4242527961738286
Co	0.8786200280000003	0.0867599990000016	0.2464999999999975
Co	0.6224600079999973	0.2529399989999987	0.1760800030000027
Co	0.6565155033434731	0.2662506974463403	0.5044964895209424
Co	0.6265087270518164	0.2530621928545096	0.3383143681351480
Co	0.8806841412576388	0.4228270111378194	0.4177615606482934
Co	0.8791599870000013	0.4187900129999989	0.2442999929999985
Co	0.1000099999999975	0.5893099899999967	0.1727599949999998
Co	0.1371985412409290	0.5864867492669251	0.5011538806514888
Co	0.1306077226478525	0.5904463304115706	0.3321066962305232
Co	0.3812775348816300	0.7530879436007042	0.4214121416826261
Co	0.3801800009999994	0.7552999850000006	0.2439399960000017
Co	0.1291400049999964	0.9265599849999973	0.1753199990000027
Co	0.1107068652654821	0.9005812711028260	0.5058600417725481
Co	0.1343891444869327	0.9221282610193077	0.3382235061357418
Co	0.6285300250000034	0.5910000209999993	0.1727000030000028
Co	0.6749719245146563	0.6000154751893761	0.5008990505981817
Co	0.6298277409564702	0.5868358348713563	0.3340010403923985
Co	0.8859797442993010	0.7554219654444210	0.4178106046627135
Co	0.8786000010000024	0.7581800219999977	0.2458100019999989
Co	0.6265699859999998	0.9184200170000025	0.1712100060000026
Co	0.6340107886443048	0.9174030108959412	0.4952344633830662
Co	0.6285606005038248	0.9210971761689918	0.3364901424723792
Rh	0.4356577470472286	0.4448043038205022	0.5547638067797501
N	0.5503044375386955	0.6316372583323858	0.5926308365179497
N	0.1433264326219403	0.7359395486491583	0.5804872711460157
H	0.4834816390031724	0.7259519069520370	0.5933315697140260
H	0.6057563035386929	0.6216105602288936	0.6426608530322985
H	0.2437282454757584	0.7460786910226805	0.6108824015660382
H	0.0531298896854563	0.7181129176336173	0.6169567502812369
H	0.3435291709922884	0.4130436719294218	0.6270623725209299
H	0.5628640565987718	0.3345052559305643	0.5957655140954079

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O	0.1286000010000024	0.0870800020000004	0.2544000150000016
O	0.1294348948053750	0.0765006006601050	0.4299160315547997
O	0.3756430507578922	0.2524483820783697	0.3383708058452820
O	0.3790900110000024	0.2518799899999991	0.1727299989999977
O	0.3332097136385369	0.2619931714576971	0.5045107548882133
O	0.1318700019999994	0.4249500040000029	0.2448000010000015
O	0.1324935573162779	0.4329200219612349	0.4195782025707656
O	0.6326100229999980	0.0850500020000027	0.2500300109999998
O	0.6251070783287019	0.1083598445499579	0.4277353917493822
O	0.8841233675562080	0.2534305471017107	0.3362497200851481
O	0.8879100079999986	0.2527300120000007	0.1709900050000002
O	0.8852908611773650	0.2562974766544713	0.4989817522754742
O	0.6310999989999999	0.4188300069999968	0.2489400059999980
O	0.6262355971286608	0.4284820483913747	0.4162985481928536
O	0.3790324306922810	0.5895367880701460	0.3343831798064436
O	0.4014700059999967	0.5909299850000025	0.1691199990000030
O	0.1325500009999985	0.7533400060000019	0.2446900010000022
O	0.1389807098341210	0.7538493906124271	0.4153979731620255
O	0.3812180212392303	0.9251964443183369	0.3350304557745949
O	0.3817099930000012	0.9268699880000000	0.1710900069999965
O	0.4040531187081651	0.9110518611421951	0.4981780307185552
O	0.8830834451111850	0.5855469603047022	0.3293601409471616
O	0.8701800110000022	0.5896999839999992	0.1678400039999985
O	0.8842428895335256	0.5848435440345565	0.4913942248442726
O	0.6315600280000027	0.7610700130000012	0.2522400020000006
O	0.6251432485576719	0.7462730719049678	0.4172258077876413
O	0.8769989790112225	0.9212176056445851	0.3364326438380877
O	0.8830299970000013	0.9218299979999998	0.1695500020000011
O	0.8629591681481251	0.9150814426437691	0.4997145615204401
Co	0.3751831481532862	0.0867628215337502	0.4315246416723992
Co	0.3802999850000006	0.0868600009999980	0.2498299929999988
Co	0.1303600070000002	0.2505899969999987	0.1755699960000001
Co	0.1103487042575827	0.2672814524763606	0.4964628133410997
Co	0.1297987069654494	0.2504181111271654	0.3378693767224396
Co	0.3769000533003287	0.4266971357651345	0.4176979534060600
Co	0.3782500029999980	0.4255700109999978	0.2429900019999991
Co	0.8790967357205421	0.0856204235823286	0.4240501300807833
Co	0.8786200280000003	0.0867599990000016	0.2464999999999975
Co	0.6224600079999973	0.2529399989999987	0.1760800030000027
Co	0.6592409483876165	0.2712568652393406	0.5036604590935582
Co	0.6264200833263539	0.2544628574616243	0.3369950049769402
Co	0.8824500290231984	0.4230997703105493	0.4170103331647986
Co	0.8791599870000013	0.4187900129999989	0.2442999929999985
Co	0.1000099999999975	0.5893099899999967	0.1727599949999998
Co	0.1283255211253103	0.5884816725396441	0.5026445112947054
Co	0.1309888512391877	0.5914737295102986	0.3327109570830816
Co	0.3811203085766863	0.7524870507905813	0.4218662744182788
Co	0.3801800009999994	0.7552999850000006	0.2439399960000017
Co	0.1291400049999964	0.9265599849999973	0.1753199990000027
Co	0.1002800631072920	0.9017374831978863	0.5046249134471360
Co	0.1331739193530764	0.9217066202264526	0.3387447799647632
Co	0.6285300250000034	0.5910000209999993	0.1727000030000028
Co	0.6462481686247196	0.5688910170532696	0.5019042341282151

Co	0.6307709337504954	0.5891640851429469	0.3328596862117273
Co	0.8787971916866100	0.7498248605207011	0.4192552079193878
Co	0.8786000010000024	0.7581800219999977	0.2458100019999989
Co	0.6265699859999998	0.9184200170000025	0.1712100060000026
Co	0.6312567938973070	0.9203180703312127	0.4897541389366737
Co	0.6273700409012882	0.9199263829231021	0.3363036939573101
Rh	0.4270286895842933	0.4336146380760943	0.5578041770779064
N	0.6741134859676988	0.6833609992100573	0.5970568859325790
N	0.1624676263762922	0.7417148512572498	0.5786475872117024
H	0.5877539130572249	0.7525906929107579	0.6160809565463994
H	0.7725547967665678	0.7458083791954985	0.5848783647855011
H	0.2779924101665147	0.7668430683357464	0.5880700965819262
H	0.1087209359424732	0.7279583599892399	0.6289203383011143
H	0.7025788192313389	0.6115863055742397	0.6389875637324044
H	0.5731220701856712	0.3312055275282260	0.5928042542017413

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O	0.1286000010000024	0.0870800020000004	0.2544000150000016
O	0.1277147413318963	0.0752632843074765	0.4323614525950197
O	0.3726839880180172	0.2492227086868894	0.3384582072203199
O	0.3790900110000024	0.2518799899999991	0.1727299989999977
O	0.3402624738460449	0.2620255133838643	0.5069017391511800
O	0.1318700019999994	0.4249500040000029	0.2448000010000015
O	0.1321713463822781	0.4295916189085479	0.4208055096286956
O	0.6326100229999980	0.0850500020000027	0.2500300109999998
O	0.6247315526104787	0.1023354199305852	0.4268798891008088
O	0.8867109477903483	0.2522753841407823	0.3353125948307383
O	0.8879100079999986	0.2527300120000007	0.1709900050000002
O	0.8807720513669017	0.2595134498331879	0.4990088039000006
O	0.6310999899999999	0.4188300069999968	0.2489400059999980
O	0.6297027959811201	0.4185753770088523	0.4111813486747506
O	0.3790507974853542	0.5874431981670827	0.3348621124394687
O	0.4014700059999967	0.5909299850000025	0.1691199990000030
O	0.1325500009999985	0.7533400060000019	0.2446900010000022
O	0.1403517112295536	0.7521653669893775	0.4163785172136182
O	0.3811884671652628	0.9224383328336045	0.3347722815371319
O	0.3817099930000012	0.9268699880000000	0.1710900069999965
O	0.4050186643199489	0.9099556908125217	0.4978354028176900
O	0.8843703062695989	0.5876705774125442	0.3303854848958175
O	0.8701800110000022	0.5896999839999992	0.1678400039999985
O	0.8841981731059361	0.5874692106301835	0.4917289178611399
O	0.6315600280000027	0.7610700130000012	0.2522400020000006
O	0.6236285712227265	0.7410848848988806	0.4196816293678111
O	0.8772493911927745	0.9210374793771554	0.3364741680333948
O	0.8830299970000013	0.9218299979999998	0.1695500020000011
O	0.8622364891473905	0.9160146178635015	0.4975899625307483
Co	0.3746226835218326	0.0837176966492292	0.4312906547028731
Co	0.3802999850000006	0.0868600009999980	0.2498299929999988
Co	0.1303600070000002	0.2505899969999987	0.1755699960000001
Co	0.1130365400177455	0.2612044215539838	0.4971236235464239
Co	0.1302342601362848	0.2511497008829570	0.3376536255619874
Co	0.3801341378738262	0.4212950420192521	0.4176708760455126
Co	0.3782500029999980	0.4255700109999978	0.2429900019999991

Co	0.8769733078330720	0.0872392083884684	0.4238706058817944
Co	0.8786200280000003	0.0867599990000016	0.2464999999999975
Co	0.6224600079999973	0.2529399899999987	0.1760800030000027
Co	0.6498225713907615	0.2715308970629163	0.5022592164665243
Co	0.6257722033129178	0.2492144567063314	0.3355270382974944
Co	0.8815994916494507	0.4201814726131356	0.4167046280534054
Co	0.8791599870000013	0.4187900129999989	0.2442999929999985
Co	0.1000099999999975	0.5893099899999967	0.1727599949999998
Co	0.1197223129736509	0.5907964155529773	0.5022392678705461
Co	0.1323654968175434	0.5894664836213523	0.3333165275427690
Co	0.3819529683526909	0.7525822923820178	0.4225815100363602
Co	0.3801800009999994	0.7552999850000006	0.2439399960000017
Co	0.1291400049999964	0.9265599849999973	0.1753199990000027
Co	0.0974402711231953	0.9005028543528504	0.5065630777291474
Co	0.1338062377392332	0.9211651998543564	0.3394347161359921
Co	0.6285300250000034	0.5910000209999993	0.1727000030000028
Co	0.6578362128577844	0.5794898329642358	0.4971145848626536
Co	0.6301192825168220	0.5862936878278776	0.3324193715688324
Co	0.8803222316651335	0.7532038410588504	0.4179636404463585
Co	0.8786000010000024	0.7581800219999977	0.2458100019999989
Co	0.6265699859999998	0.9184200170000025	0.1712100060000026
Co	0.6321301136590018	0.9169729425455558	0.4948821243317559
Co	0.6276975586933127	0.9201841105123033	0.3371961417752177
Rh	0.4182789429443491	0.4498950283083151	0.5556736014431436
N	0.1579993574593040	0.7413692164464364	0.5801823466957450
H	0.2736463392646277	0.7618879033908721	0.5920502636849453
H	0.0984862102906719	0.7297937206589586	0.6291241204001464
H	0.5741497668510133	0.5450551349670784	0.5871635777563541

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O	0.3726800080000032	0.2492199999999975	0.3384599989999916
O	0.3790900110000024	0.2518799909999991	0.1727299999999946
O	0.3402599999999970	0.2620300059999997	0.5069000120000019
O	0.1318700029999994	0.4249500040000029	0.2448000019999963
O	0.1321700079999991	0.4295899870000000	0.4208100149999897
O	0.6326100239999980	0.0850500020000027	0.2500300119999997
O	0.6247299910000024	0.1023399989999979	0.4268800029999896
O	0.8867099889999998	0.2522799970000023	0.3353100129999948
O	0.8879100089999984	0.2527300120000007	0.1709900059999971
O	0.8807700280000006	0.2595100109999996	0.4990099979999912
O	0.6310999999999999	0.4188300079999968	0.2489400069999927
O	0.6297000059999966	0.4185799969999983	0.4111799909999938
O	0.3790449870000019	0.5874400140000020	0.3348599979999964
O	0.4014700069999967	0.5909299850000025	0.1691199999999999
O	0.1325500019999985	0.7533400060000019	0.2446900019999969
O	0.1403499990000014	0.7521700260000017	0.4163799889999956
O	0.3811900029999968	0.9224399920000010	0.3347699949999924
O	0.3817099930000012	0.9268699880000000	0.1710900079999935
O	0.4050199999999967	0.9099599720000029	0.4978399879999885
O	0.8843700290000029	0.5876700289999980	0.3303900069999959
O	0.8701800110000022	0.5896999849999992	0.1678400049999955

O	0.8841999770000015	0.5874699959999993	0.4917300059999904
O	0.6315600280000027	0.7610700130000011	0.2522400020000005
O	0.6236299870000011	0.7410900009999998	0.4196799999999958
O	0.8772500169999979	0.9210399990000013	0.3364700089999931
O	0.8830299970000013	0.9218299989999997	0.1695500029999981
O	0.8622400160000012	0.9160199760000012	0.4975900059999888
Co	0.3746199910000030	0.0837199990000030	0.4312900019999930
Co	0.3802999850000006	0.0868600019999980	0.2498299939999935
Co	0.1303600070000002	0.2505899979999987	0.1755699969999969
Co	0.1130400009999980	0.2612000119999997	0.4971199939999878
Co	0.1302299950000005	0.2511500129999965	0.3376500019999940
Co	0.3801299939999970	0.4212900109999999	0.4176700129999949
Co	0.3782500039999980	0.4255700119999978	0.2429900029999938
Co	0.8769699930000030	0.0872400039999980	0.4238699979999897
Co	0.8786200280000003	0.0867599990000016	0.2465000009999923
Co	0.6224600089999973	0.2529399999999987	0.1760800039999995
Co	0.6498200300000007	0.2715300029999987	0.5022600299999980
Co	0.6257699739999970	0.2492100009999979	0.3355300139999972
Co	0.8816000220000006	0.4201799939999978	0.4167099899999903
Co	0.8791599870000013	0.4187900139999989	0.2442999939999932
Co	0.1000100009999975	0.5893099909999967	0.1727599959999967
Co	0.1197199979999971	0.5907999879999969	0.5022400029999999
Co	0.1323699959999977	0.5894700299999975	0.3333199929999939
Co	0.3819499919999989	0.7525799879999972	0.4225800049999895
Co	0.3801800019999994	0.7552999850000006	0.2439399969999964
Co	0.1291400059999964	0.9265599859999973	0.1753199999999996
Co	0.0974399970000022	0.9005000000000010	0.5065600280000025
Co	0.1338099990000003	0.9211699960000033	0.3394399889999963
Co	0.6285300250000034	0.5910000219999993	0.1727000039999997
Co	0.6578400140000012	0.5794900060000003	0.4971199939999878
Co	0.6301199799999998	0.5862900029999984	0.3324199919999959
Co	0.8803200130000022	0.7531999950000028	0.4179599889999926
Co	0.8786000010000024	0.7581800229999977	0.2458100029999937
Co	0.6265699869999998	0.9184200170000026	0.1712100069999995
Co	0.6321300270000023	0.9169700159999968	0.4948799919999872
Co	0.6276999719999984	0.9201800230000003	0.3371999869999956
Rh	0.4246299869999997	0.4534899890000032	0.5583099729999944
N	0.1580000070279134	0.7413700229652170	0.5801799895618462
H	0.2736499918243888	0.7618899948084942	0.5920500168993364
H	0.0984900004622716	0.7297899722186773	0.6291199927663020
H	0.2276699991065200	0.4828900106310145	0.5665299895296861

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O	0.1286000010000024	0.0870800020000004	0.2544000150000016
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O	0.3767093330353000	0.2535728705673938	0.3378476229749290
O	0.3790900110000024	0.2518799899999991	0.1727299989999977
O	0.3313096678707374	0.2564080704871019	0.5072535279029073
O	0.1318700019999994	0.4249500040000029	0.2448000010000015
O	0.1314509204090439	0.4322320433601642	0.4193687906230386
O	0.6326100229999980	0.0850500020000027	0.2500300109999998
O	0.6225085535319346	0.0951015996375939	0.4310494400083955
O	0.8830384077225423	0.2535076582110131	0.3347389415437262

O	0.8879100079999986	0.2527300120000007	0.1709900050000002
O	0.8856414883844619	0.2565357642169167	0.4985162150203173
O	0.6310999989999999	0.4188300069999968	0.2489400059999980
O	0.6310520797777930	0.4223732573543409	0.4089147098150619
O	0.3782130045379668	0.5897453235439324	0.3360407342651369
O	0.4014700059999967	0.5909299850000025	0.1691199990000030
O	0.1325500009999985	0.7533400060000019	0.2446900010000022
O	0.1358246890467666	0.7490932891158554	0.4198756667661666
O	0.3814323865269842	0.9227701375527384	0.3361418495948877
O	0.3817099930000012	0.9268699880000000	0.1710900069999965
O	0.3684011643870025	0.9086731122441662	0.5028588921119272
O	0.8836226053401256	0.5909411015997140	0.3312536543904040
O	0.8701800110000022	0.5896999839999992	0.1678400039999985
O	0.8772468627780237	0.5856591147291985	0.4943091653603643
O	0.6315600280000027	0.7610700130000012	0.2522400020000006
O	0.6207232442369949	0.7509248681562803	0.4219952021991222
O	0.8771878999041737	0.9208828171757468	0.3373249461834210
O	0.8830299970000013	0.9218299979999998	0.1695500020000011
O	0.8781413202073247	0.9168896361734210	0.5000945339908276
Co	0.3772463189442305	0.0900682646983239	0.4316393845788420
Co	0.3802999850000006	0.0868600009999980	0.2498299929999988
Co	0.1303600070000002	0.2505899969999987	0.1755699960000001
Co	0.1100049379354702	0.2662141449393941	0.4978909208819609
Co	0.1308009793378731	0.2543431195015805	0.3365397079398691
Co	0.3809236109005955	0.4229107288820207	0.4210843988408866
Co	0.3782500029999980	0.4255700109999978	0.2429900019999991
Co	0.8776378129638340	0.0870510429611102	0.4238053976113883
Co	0.8786200280000003	0.0867599990000016	0.2464999999999975
Co	0.6224600079999973	0.2529399989999987	0.1760800030000027
Co	0.6567493348241019	0.2809415953266115	0.4998339391028949
Co	0.6257123940118274	0.2498506225997990	0.3356852931005740
Co	0.8796140251522503	0.4225588013540603	0.4158375124522948
Co	0.8791599870000013	0.4187900129999989	0.2442999929999985
Co	0.1000099999999975	0.5893099899999967	0.1727599949999998
Co	0.1047073195990810	0.5850124550314596	0.5010811531566580
Co	0.1323688356198913	0.5893474111641301	0.3333826382784582
Co	0.3788436231730067	0.7526990577195373	0.4226366167421841
Co	0.3801800009999994	0.7552999850000006	0.2439399960000017
Co	0.1291400049999964	0.9265599849999973	0.1753199990000027
Co	0.1237161373834419	0.9209359058331309	0.4937216542911138
Co	0.1318154179263142	0.9187735620767928	0.3361180934721758
Co	0.6285300250000034	0.5910000209999993	0.1727000030000028
Co	0.6457249750236682	0.5849708560660690	0.5026622743447861
Co	0.6297817047163741	0.5890711493648697	0.3329768116733764
Co	0.8781128197509949	0.7545754959214657	0.4209116322597926
Co	0.8786000010000024	0.7581800219999977	0.2458100019999989
Co	0.6265699859999998	0.9184200170000025	0.1712100060000026
Co	0.6349135744981599	0.9166067302364850	0.4978168543581563
Co	0.6271805193411968	0.9209715820257994	0.3377438230520101
Rh	0.4433652208347679	0.4314398495216623	0.5580879780118274
N	0.1871143718325114	0.6723384810005933	0.6006939626982891
H	0.2696926547700775	0.7533966844649350	0.5895159125356750
H	0.1008334890059937	0.7151973207045473	0.6341268360427347
H	0.2459406632613073	0.5910715444810200	0.6298426713309593

E= -379.76512

O	0.1275400070000003	0.0867199970000030	0.2486699970000004
O	0.1331688978593805	0.0776685699616894	0.4369766246607267
O	0.3705522823920090	0.2496568774179489	0.3347996798228715
O	0.3789100050000016	0.2519800070000002	0.1704400030000031
O	0.3894063213975667	0.2721212118944854	0.5026452173104831
O	0.1285700050000003	0.4216499919999990	0.2459899930000020
O	0.1311211522610086	0.4220248608527736	0.4200994504920944
O	0.6293500069999993	0.0836099980000000	0.2534199950000016
O	0.6288323267309888	0.0933515758508967	0.4223470789775264
O	0.8842242473855183	0.2510206282635135	0.3346330141514464
O	0.8809400199999970	0.2520500119999980	0.1697999980000020
O	0.8743796100190813	0.2570869929428568	0.4987341442429414
O	0.6275799869999972	0.4220199880000024	0.2460899949999984
O	0.6203476998971861	0.4162699487444580	0.4132040433725879
O	0.3762887718097645	0.5865137880300877	0.3350997805665534
O	0.3827799860000027	0.5909299850000025	0.1701100020000013
O	0.1297000049999966	0.7572699790000001	0.2492299970000005
O	0.1344969914410823	0.7520443028892192	0.4166100494445785
O	0.3791993163437714	0.9231811048166834	0.3363170812818165
O	0.3803899879999975	0.9225900169999974	0.1709299979999983
O	0.4099344533535629	0.9115752140096327	0.4988128837207628
O	0.8787983216225952	0.5833730331787180	0.3312746820750443
O	0.8804000020000018	0.5905299779999993	0.1686600000000027
O	0.8705497001865791	0.5838201176120914	0.4898743282697876
O	0.6277800200000030	0.7563300130000030	0.2522000069999990
O	0.6213238402789641	0.7400917662791660	0.4194600105178355
O	0.8787256815912347	0.9213013361015612	0.3362658766024759
O	0.8778399830000012	0.9210100170000004	0.1696500030000010
O	0.8676625016234754	0.9133847326411288	0.4985829256086249
Co	0.3784533136260760	0.0833829002247012	0.4298612358428465
Co	0.3799799980000031	0.0872400029999980	0.2470700000000008
Co	0.1260699930000015	0.2518900040000034	0.1730300039999975
Co	0.1210909047291338	0.2619232897144966	0.5001796735428630
Co	0.1283087660274952	0.2508171473673298	0.3354699304954964
Co	0.3767245506033465	0.4216075996995549	0.4177812929812271
Co	0.3765200080000000	0.4212099909999978	0.2435899970000008
Co	0.8806617794043082	0.0865263068020379	0.4251071208553238
Co	0.8753799799999982	0.0866900010000009	0.2461100069999986
Co	0.6244699949999983	0.2516300079999993	0.1762599950000023
Co	0.6332801358805397	0.2627672185633547	0.5008026016727674
Co	0.6246917338854936	0.2482682723898225	0.3354601596068176
Co	0.8750428998548561	0.4141836902764830	0.4173550855574700
Co	0.8762099739999982	0.4209499959999974	0.2424499990000015
Co	0.1210800039999995	0.5911999940000001	0.1736499969999983
Co	0.0974263504251419	0.5686882321027810	0.5060543645777125
Co	0.1276554261325927	0.5872269533149767	0.3343199409487613
Co	0.3773089285446529	0.7502493944525213	0.4225077129478200
Co	0.3790099920000003	0.7569699880000016	0.2464600059999995
Co	0.1244399990000034	0.9229400159999983	0.1736100019999967
Co	0.0995554321169751	0.8956706418587199	0.5059785894227131
Co	0.1320998381501937	0.9211165137399420	0.3386458217248033
Co	0.6225600240000020	0.5913599730000030	0.1737499979999981
Co	0.6449411659949129	0.5761852719972497	0.4968172152211284

Co	0.6281443627894890	0.5840106321274562	0.3330602179186481
Co	0.8785371673814175	0.7512520431752090	0.4172952056258930
Co	0.8755000230000007	0.7549399729999990	0.2450000050000014
Co	0.6251699919999965	0.9188799860000003	0.1722500030000020
Co	0.6372138503150767	0.9144682460951261	0.4940820616822236
Co	0.6275296912295121	0.9191950594271038	0.3376551800485969
Rh	0.3655195768545257	0.4846226975206806	0.5620300278114090
N	0.3075050068796835	0.6875711597640825	0.5855715292060100
N	0.1684356537025704	0.7239610507295674	0.5707511758938209
H	0.3838493753347858	0.7755667423111282	0.5944634430927400
H	0.5656103199969910	0.5107490130573640	0.5811145395933814
H	0.2410562771182991	0.3918214079899979	0.6300220924562828
H	0.3340219742504156	0.3914895071214076	0.6491652246320211

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E= -380.19059

O	0.1275400070000003	0.0867199970000030	0.2486699970000004
O	0.1345705511937768	0.0873207708862345	0.4439841613593981
O	0.3714215956590673	0.2495123974385086	0.3365246041882216
O	0.3789100050000016	0.2519800070000002	0.1704400030000031
O	0.4072610121293469	0.2839854033139877	0.5038875532581999
O	0.1285700050000003	0.4216499919999990	0.2459899930000020
O	0.1293389252935506	0.4211524611800949	0.4165916565135514
O	0.6293500069999993	0.0836099980000000	0.2534199950000016
O	0.6273822456615943	0.0906235830930112	0.4192805272142596
O	0.8837470018115593	0.2526289670425807	0.3339609939659918
O	0.8809400199999970	0.2520500119999980	0.1697999980000020
O	0.8680110295006834	0.2598396340594311	0.4971359835906821
O	0.6275799869999972	0.4220199880000024	0.2460899949999984
O	0.6229841414633142	0.4234701797312497	0.4123591182552879
O	0.3748796081265758	0.5874921561173800	0.3362573458551790
O	0.3827799860000027	0.5909299850000025	0.1701100020000013
O	0.1297000049999966	0.7572699790000001	0.2492299970000005
O	0.1321533258570383	0.7571895905073668	0.4175668842119207
O	0.3759251717415145	0.9242117391029154	0.3363119225756423
O	0.3803899879999975	0.9225900169999974	0.1709299979999983
O	0.4049547370728049	0.9153868958239152	0.4999117591450220
O	0.8785033508957416	0.5872329827395821	0.3314727274530840
O	0.8804000020000018	0.5905299779999993	0.1686600000000027
O	0.8671993757247116	0.5856198589646500	0.4910868869726284
O	0.6277800200000030	0.7563300130000030	0.2522000069999990
O	0.6181749306967448	0.7444605631117195	0.4196841403581056
O	0.8812128406061863	0.9231631518852909	0.3364779911880576
O	0.8778399830000012	0.9210100170000004	0.1696500030000010
O	0.8648967820533323	0.9169699293152502	0.4989158973706934
Co	0.3774034104511700	0.0873825209385701	0.4295714947099985
Co	0.3799799980000031	0.0872400029999980	0.2470700000000008
Co	0.1260699930000015	0.2518900040000034	0.1730300039999975
Co	0.1033934649498870	0.2731480832514891	0.5043888923029318
Co	0.1283697466607360	0.2533297708128280	0.3359466127400949
Co	0.3744599800292919	0.4232558935125266	0.4171857077530334
Co	0.3765200080000000	0.4212099909999978	0.2435899970000008
Co	0.8817714360002648	0.0872218076143999	0.4248672565034943
Co	0.8753799799999982	0.0866900010000009	0.2461100069999986

Co	0.6244699949999983	0.2516300079999993	0.1762599950000023
Co	0.6347210152862837	0.2632566404147467	0.4968376697531587
Co	0.6256424319990807	0.2507397029285028	0.3350709290361102
Co	0.8739027116740019	0.4191077450173825	0.4155121653428288
Co	0.8762099739999982	0.4209499959999974	0.2424499990000015
Co	0.1210800039999995	0.5911999940000001	0.1736499969999983
Co	0.0955307683554415	0.5734415637548623	0.5049058183882623
Co	0.1273845771277197	0.5888769483202432	0.3346262576846569
Co	0.3738247045524480	0.7531524804042765	0.4243127352173046
Co	0.3790099920000003	0.7569699880000016	0.2464600059999995
Co	0.1244399990000034	0.9229400159999983	0.1736100019999967
Co	0.1029753954692332	0.9037710565775761	0.5084951243135808
Co	0.1310273226995314	0.9206340984976294	0.3380834958556055
Co	0.6225600240000020	0.5913599730000030	0.1737499979999981
Co	0.6420648262863110	0.5801902837331441	0.4955049626541129
Co	0.6281189160334633	0.5882391222861024	0.3328046392774665
Co	0.8768944900971590	0.7558629249263475	0.4192094432252355
Co	0.8755000230000007	0.7549399729999990	0.2450000050000014
Co	0.6251699919999965	0.9188799860000003	0.1722500030000020
Co	0.6328393748320509	0.9177875197394251	0.4949478499377437
Co	0.6253135838125368	0.9209117219363657	0.3376697488564794
Rh	0.3608511144423922	0.4860416395016252	0.5631958671456162
N	0.2964125174695273	0.6884756151210605	0.5915147988340399
N	0.1639608461696281	0.7352121738758589	0.5716921747739950
H	0.1655735477928462	0.4174632631099101	0.5721592561662130
H	0.3763800319181581	0.7698605413898049	0.6066792793584016
H	0.5479801810417225	0.5324972290164147	0.5812253889888537
H	0.3905135939498894	0.4218067086550809	0.6441767366460369

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E= -380.46306

O	0.1275400070000003	0.0867199970000030	0.2486699970000004
O	0.1357159403524617	0.0804130214004543	0.4451234146687907
O	0.3722546961437855	0.2482884230559527	0.3366394434087843
O	0.3789100050000016	0.2519800070000002	0.1704400030000031
O	0.4108715959739929	0.2766664272036911	0.5073066847098849
O	0.1285700050000003	0.4216499919999990	0.2459899930000020
O	0.1310912405408451	0.4208602840345258	0.4161895859657082
O	0.6293500069999993	0.0836099980000000	0.2534199950000016
O	0.6252490650266356	0.0881065784150656	0.4211759046644832
O	0.8838356981575914	0.2501315999515573	0.3345471085437953
O	0.8809400199999970	0.2520500119999980	0.1697999980000020
O	0.8710262642217480	0.2567221893277843	0.4971920480197644
O	0.6275799869999972	0.4220199880000024	0.2460899949999984
O	0.6242229762637060	0.4204272997429567	0.4130117210365841
O	0.3773607452856031	0.5868770612048241	0.3360059694035196
O	0.3827799860000027	0.5909299850000025	0.1701100020000013
O	0.1297000049999966	0.7572699790000001	0.2492299970000005
O	0.1318461159429229	0.7532699020024579	0.4148542147322134
O	0.3758965784025998	0.9234033134792485	0.3370347261469396
O	0.3803899879999975	0.9225900169999974	0.1709299979999983
O	0.4064683197746658	0.9071736087600742	0.5031989016783449
O	0.8777062791431035	0.5853550894798144	0.3306407504162051
O	0.8804000020000018	0.5905299779999993	0.1686600000000027

O	0.8732870635586504	0.5828096907895608	0.4902893859642571
O	0.6277800200000030	0.7563300130000030	0.2522000069999990
O	0.6182093817672866	0.7419696092191037	0.4196424984009524
O	0.8797925953257192	0.9225646953901422	0.3362274545146699
O	0.8778399830000012	0.9210100170000004	0.1696500030000010
O	0.8659554887988443	0.9130299105555445	0.4984090212805105
Co	0.3757975653217306	0.0839582841374373	0.4341618772034671
Co	0.3799799980000031	0.0872400029999980	0.2470700000000008
Co	0.1260699930000015	0.2518900040000034	0.1730300039999975
Co	0.1058646944695014	0.2714787685068730	0.5023432109548486
Co	0.1284306269644668	0.2518047909720506	0.3357036088288332
Co	0.3787062808616634	0.4161826066936765	0.4165232721358946
Co	0.3765200080000000	0.4212099909999978	0.2435899970000008
Co	0.8830920842767715	0.0836239897153604	0.4257862670956920
Co	0.8753799799999982	0.0866900010000009	0.2461100069999986
Co	0.6244699949999983	0.2516300079999993	0.1762599950000023
Co	0.6379463680171096	0.2608793345835974	0.4974652180661256
Co	0.6276097183827209	0.2476246874967155	0.3356878036079938
Co	0.8768416835162958	0.4175085733935273	0.4156925072756805
Co	0.8762099739999982	0.4209499959999974	0.2424499990000015
Co	0.1210800039999995	0.5911999940000001	0.1736499969999983
Co	0.1072139117807634	0.5801321534675926	0.5046923460825194
Co	0.1284499868840546	0.5871655702209588	0.3337987066703838
Co	0.3744107542822491	0.7534538921294166	0.4239228381244250
Co	0.3790099920000003	0.7569699880000016	0.2464600059999995
Co	0.1244399990000034	0.9229400159999983	0.1736100019999967
Co	0.1052675585182974	0.8941117819351678	0.5110946194998156
Co	0.1307711248068404	0.9201776353266226	0.3381572410038305
Co	0.6225600240000020	0.5913599730000030	0.1737499979999981
Co	0.6489713842747652	0.5784383560091793	0.4946350919112169
Co	0.6282241719958300	0.5863932171215679	0.3327266447867481
Co	0.8788606623345462	0.7523917562680950	0.4185494118427155
Co	0.8755000230000007	0.7549399729999990	0.2450000050000014
Co	0.6251699919999965	0.9188799860000003	0.1722500030000020
Co	0.6357693855109466	0.9138535705888275	0.4956383965894307
Co	0.6254878610853465	0.9199608310409784	0.3379732364471819
Rh	0.3552677007515203	0.4824857919205474	0.5588079914180353
N	0.2920461330246681	0.6879976756817832	0.6050095673345839
N	0.1459859978153305	0.7236169267188213	0.5726633823005770
H	0.3732218186849083	0.7684869259919358	0.5898033106720858
H	0.5440358237473182	0.5415410129419499	0.5736302776653156
H	0.1635856824651021	0.4197301519228498	0.5697994571682409
H	0.2823892617434932	0.6776946578650520	0.6616947352654396

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E= -387.38076

O	0.1251389610388525	0.0872464354008946	0.2537484331762992
O	0.1343024331708584	0.0843755042644004	0.4442988949382903
O	0.3712371829541546	0.2512131874415965	0.3372068646330528
O	0.3756629646878086	0.2519519600343487	0.1719715469927579
O	0.4077027080222667	0.2781103359167082	0.5059043318003328
O	0.1270223742838144	0.4229238639533020	0.2457778103255566
O	0.1309749691080025	0.4234182195859179	0.4177538889096428
O	0.6285498457530246	0.0879446337289817	0.2492195948314467

O	0.6249062715477625	0.0901403246675665	0.4194834292751517
O	0.8830841054903702	0.2517385954853036	0.3353664477086409
O	0.8788875699347563	0.2522458935689964	0.1701834857197964
O	0.8692129456744919	0.2590645229811185	0.4974432538820335
O	0.6268349436855192	0.4196428376797813	0.2481413970193830
O	0.6219568692012342	0.4241058489635615	0.4136068029541110
O	0.3746001772199564	0.5887087983732286	0.3357321725180105
O	0.3884902692628424	0.5885361305695368	0.1693004883950291
O	0.1267492212731220	0.7536752796667748	0.2442855447336633
O	0.1296796208722421	0.7558110658972957	0.4123592642686907
O	0.3754330864147191	0.9245125724317558	0.3369811908714269
O	0.3777913135349020	0.9247184743597858	0.1718397694192727
O	0.4064934791287552	0.9099164405582457	0.5025870201034596
O	0.8779524341924404	0.5857025965896744	0.3296068805677640
O	0.8718124658922208	0.5877846512093625	0.1669232527227265
O	0.8758069510296667	0.5853833490084071	0.4897720375528872
O	0.6262888656829948	0.7561314073560469	0.2499613598767750
O	0.6180558367425069	0.7447792545950399	0.4179170859573558
O	0.8766898688339666	0.9231128584865607	0.3346882153156195
O	0.8758507580003151	0.9219028402350525	0.1686282932597423
O	0.8648572601552680	0.9156777757620228	0.4973144488374124
Co	0.3752204477546273	0.0865622008123503	0.4334907276793388
Co	0.3768061164981356	0.0872965555636818	0.2489348136964942
Co	0.1298549195321113	0.2507389100257529	0.1755562921702878
Co	0.1034224972474257	0.2721232304178110	0.5027639814212175
Co	0.1278914888247342	0.2516967938101458	0.3380469481552326
Co	0.3769824638674357	0.4220654120111139	0.4191709787456511
Co	0.3744417756693475	0.4226711608433895	0.2443857059931960
Co	0.8813354413356721	0.0860080982623591	0.4250588824875357
Co	0.8767499522009153	0.0870210860048286	0.2460668434921408
Co	0.6256480373351936	0.2544546883878293	0.1744166423087106
Co	0.6353471845269316	0.2624913527518496	0.4957969667744354
Co	0.6253715941695842	0.2503154535899614	0.3345377882900016
Co	0.8756186084762424	0.4200748847926615	0.4156650143251505
Co	0.8757575352073788	0.4194894509377491	0.2431047037487997
Co	0.1075937744449622	0.5876329837465966	0.1718804689154461
Co	0.1140005065548175	0.5804269391624074	0.5021663816932803
Co	0.1273287567648451	0.5884040879636687	0.3325986083977379
Co	0.3728644768601886	0.7545480801957352	0.4237585874329555
Co	0.3735932612604748	0.7546693879229772	0.2447736433765297
Co	0.1224328734909199	0.9249590034486447	0.1751537796228236
Co	0.1044832871023139	0.8974265949729375	0.5098017670620042
Co	0.1295965984582624	0.9212296381935324	0.3374550974173621
Co	0.6211838922411228	0.5892706000483071	0.1722705282039666
Co	0.6515298740178109	0.5828954353795601	0.4936623860927399
Co	0.6267631595507035	0.5882497910796320	0.3315760341504454
Co	0.8789346318359093	0.7543117584730354	0.4176875860979017
Co	0.8742686859934251	0.7547976213188847	0.2436019085757116
Co	0.6232917622511811	0.9218989370805425	0.1741661771920788
Co	0.6348446460086200	0.9158810183210300	0.4943051711326613
Co	0.6241400978783775	0.9211148481959377	0.3361643335021710
Rh	0.3571787946477327	0.4828335437786739	0.5666928770410000
N	0.2901211405841869	0.6934003182371657	0.6061635328282553
N	0.1487968486819478	0.7253591566284218	0.5693453534945558
H	0.3730760630915443	0.7717588502854904	0.5899939603600295
H	0.5450044579543113	0.5514213233614170	0.5726769954354949
H	0.1644580613700454	0.4247092016031320	0.5717521029671474
H	0.2750750669296258	0.6914382099157624	0.6627502221376846

H	0.4473025473006769	0.4135067626175588	0.6581738993458360
H	0.3596030292914198	0.3795610430862006	0.6585390866696802

19

E= -387.88416

O	0.1251399960000015	0.0872500019999976	0.2537499960000034
O	0.1334077673653188	0.0870847963312335	0.4430878251446442
O	0.3699214428767337	0.2507095713240255	0.3371418206355410
O	0.3756600019999965	0.2519499960000005	0.1719699949999978
O	0.3983838055422406	0.2765036799621383	0.5031501260732143
O	0.1270200009999982	0.4229199890000004	0.2457800059999968
O	0.1277552781499228	0.4273284337722518	0.4171465745654522
O	0.6285499930000000	0.0879499990000028	0.2492199989999975
O	0.6244469382079288	0.0906400282475563	0.4209945953572651
O	0.8831363365260917	0.2517212511559899	0.3352054251987553
O	0.8788899779999966	0.2522499860000025	0.1701799929999979
O	0.8689723965033299	0.2592381333708219	0.4988474052754467
O	0.6268399949999974	0.4196400049999980	0.2481400070000035
O	0.6240174901638191	0.4215784608946612	0.4121769719691937
O	0.3744996736385158	0.5879483490100652	0.3346342480508873
O	0.3884899910000001	0.5885400180000033	0.1693000049999966
O	0.1267500069999983	0.7536799909999985	0.2442899939999990
O	0.1344833388294113	0.7584849421225641	0.4140837974963646
O	0.3760406635354571	0.9237284754764095	0.3364712974545615
O	0.3777900039999977	0.9247199890000033	0.1718399969999993
O	0.4044985693908976	0.9061154121733679	0.5014849600282785
O	0.8791192593248954	0.5875463960034935	0.3299101049752640
O	0.8718100190000015	0.5877900119999993	0.1669200059999980
O	0.8722699487313875	0.5862457189053926	0.4907515648505830
O	0.6262900230000028	0.7561299799999972	0.2499600049999984
O	0.6202825465423359	0.7434584199044902	0.4178265189340144
O	0.8779094411265898	0.9229828197725392	0.3359736942240352
O	0.8758500220000016	0.9218999739999987	0.1686300040000006
O	0.8645935037715463	0.9147450346813328	0.4982148692906500
Co	0.3748027253884966	0.0856673369819548	0.4320862941867101
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Co	0.1298599989999971	0.2507399919999997	0.1755599979999971
Co	0.1079815690759205	0.2742288083694842	0.5025660923472679
Co	0.1275745059001746	0.2518603196713107	0.3381327990147248
Co	0.3769376912544520	0.4253519207021713	0.4176926036527857
Co	0.3744400140000010	0.4226700070000007	0.2443899960000024
Co	0.8793393038954185	0.0883813222257859	0.4262082517138434
Co	0.8767499920000006	0.0870200020000027	0.2460699980000030
Co	0.6256499890000029	0.2544499930000015	0.1744199990000013
Co	0.6300806828203066	0.2674111752547036	0.4978762726045414
Co	0.6254790528840147	0.2493265467558313	0.3348433556055864
Co	0.8744548043146843	0.4193436959495076	0.4167457978132145
Co	0.8757600189999977	0.4194900099999970	0.2431100009999980
Co	0.1075899969999980	0.5876299740000022	0.1718800069999986
Co	0.1113442101069791	0.5807504633990209	0.4999820464939000
Co	0.1256953142701130	0.5895109243836237	0.3326293804397087
Co	0.3773595878697403	0.7473982619693398	0.4232586930895494
Co	0.3735899930000031	0.7546700239999993	0.2447700049999995
Co	0.1224299969999976	0.9249600169999965	0.1751500069999992

Co	0.1013720128607867	0.8995523046581846	0.5047772625259530
Co	0.1303133528839240	0.9226941395782623	0.3374376677130551
Co	0.6211799980000023	0.5892699959999987	0.1722699999999975
Co	0.6461697136745423	0.5789635203398824	0.4957058287229199
Co	0.6281357993855160	0.5878101812191477	0.3316795165085066
Co	0.8767494374068234	0.7530926257528547	0.4177585968358752
Co	0.8742700219999975	0.7548000219999977	0.2435999960000004
Co	0.6232900019999974	0.9218999739999987	0.1741700019999968
Co	0.6344194006698964	0.9147986260832148	0.4936852671468385
Co	0.6246490630531351	0.9209477530914240	0.3365090567361609
Rh	0.3632444317202931	0.4886211023650526	0.5602909073756958
N	0.3067311958443142	0.6983102957210098	0.6010022587978701
N	0.1473292615889999	0.7284638271689526	0.5779532144229160
H	0.3728415144818847	0.7807511587421591	0.5738460153479491
H	0.5618029274371984	0.5179476651205793	0.5793591925040475
H	0.0734944009443355	0.7081001530076955	0.6217270121779431
H	0.3184980000185799	0.7081552906437935	0.6574377874600816
H	0.3507348677079839	0.4024743824280186	0.6505148727041397
H	0.2568250968809125	0.3924578844076542	0.6335334920539678

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E= -388.41589

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O	0.1383537961878593	0.0912839783150154	0.4451649167407886
O	0.3750288586435139	0.2494679633164059	0.3375401453004991
O	0.3790900110000024	0.2518799899999991	0.1727299899999977
O	0.4092309486025012	0.2868019428051992	0.5040967728017394
O	0.1318700019999994	0.4249500040000029	0.2448000010000015
O	0.1326545684996104	0.4237938993756702	0.4161771612980398
O	0.6326100229999980	0.0850500020000027	0.2500300109999998
O	0.6277787452826087	0.0919206947962539	0.4205519645363885
O	0.8861713033508224	0.2521789379277937	0.3353942129515744
O	0.8879100079999986	0.2527300120000007	0.1709900050000002
O	0.8712003739087019	0.2618603239078682	0.4982798928176732
O	0.6310999989999999	0.4188300069999968	0.2489400059999980
O	0.6277235751964353	0.4250747364267304	0.4122982692729537
O	0.3774162690860791	0.5885412107067399	0.3348537934491486
O	0.4014700059999967	0.5909299850000025	0.1691199990000030
O	0.1325500009999985	0.7533400060000019	0.2446900010000022
O	0.1362116484625924	0.7581971709005834	0.4162650429023318
O	0.3782650823537471	0.9230284166316293	0.3363669129873575
O	0.3817099930000012	0.9268699880000000	0.1710900069999965
O	0.4095568084499209	0.9084869982283004	0.5010754060330819
O	0.8836293609459593	0.5875512136493785	0.3305679060094711
O	0.8701800110000022	0.5896999839999992	0.1678400039999985
O	0.8748017428265054	0.5871249811041666	0.4919388581690865
O	0.6315600280000027	0.7610700130000012	0.2522400020000006
O	0.6230184637412536	0.7445298256919193	0.4180507716365365
O	0.8838199744820223	0.9230907224844405	0.3366617398933408
O	0.8830299970000013	0.9218299979999998	0.1695500020000011
O	0.8678187724127687	0.917222429310056	0.4986367942979826
Co	0.3781839171984375	0.0876175393890482	0.4326733549055329
Co	0.3802999850000006	0.0868600009999980	0.2498299929999988
Co	0.1303600070000002	0.2505899969999987	0.1755699960000001

Co	0.1068210930001692	0.2795775926638085	0.5051606826724221
Co	0.1309750875452846	0.2527874609947947	0.3383093640047309
Co	0.3793177089803139	0.4248825234490476	0.4165353179377903
Co	0.3782500029999980	0.4255700109999978	0.2429900019999991
Co	0.8847587336984166	0.0889653011486057	0.4263533512034400
Co	0.8786200280000003	0.0867599990000016	0.2464999999999975
Co	0.6224600079999973	0.2529399989999987	0.1760800030000027
Co	0.6374082139362255	0.2656400300217248	0.4966187683802347
Co	0.6282475131911927	0.2502396382127051	0.3349344660649183
Co	0.8783885046328219	0.4204503512096990	0.4161019559719089
Co	0.8791599870000013	0.4187900129999989	0.2442999929999985
Co	0.1000099999999975	0.5893099899999967	0.1727599949999998
Co	0.1077193950757026	0.5806787226078155	0.5036443745479984
Co	0.1310342128602452	0.5899755035823941	0.3330610609026859
Co	0.3777279927223217	0.7477158442394797	0.4239548264068850
Co	0.3801800009999994	0.7552999850000006	0.2439399960000017
Co	0.1291400049999964	0.9265599849999973	0.1753199990000027
Co	0.1110513582573494	0.9032940278247067	0.5066230834536269
Co	0.1344532638263013	0.9220673150921376	0.3383985156111846
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Co	0.6493199413139721	0.5814881262647292	0.4948718825959014
Co	0.6314767050544354	0.5892117122569833	0.3316742667350559
Co	0.8810711638539103	0.7557465911018461	0.4191804404560876
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Co	0.6265699859999998	0.9184200170000025	0.1712100060000026
Co	0.6386876863982187	0.9162285163972742	0.4938928708952251
Co	0.6271148895591638	0.9223357810686347	0.3370936149529822
Rh	0.3694661738094844	0.4914271224599395	0.5623710152636775
N	0.3100205980979347	0.7011728974398876	0.6035279241489762
N	0.1521646652238192	0.7428712911768350	0.5812497707324414
H	0.3804197968445623	0.7804453047543584	0.5770100749788138
H	0.3230055362272068	0.7100706492552520	0.6599112106923001
H	0.0791277148118807	0.7266117466416044	0.6256723253453731
H	0.1720110492690765	0.4257575592949570	0.5714518595393809
H	0.3953138033714799	0.4329459062557766	0.6446115388622389
H	0.5577843024270899	0.5318206542995582	0.5803647710757194

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O	0.3837853386613957	0.2472912759920869	0.1712500669107724
O	0.3883494301677536	0.2923441680883856	0.5030437616777214
O	0.1332487558054825	0.4220482712726795	0.2408932313804084
O	0.1271139309100935	0.4124483134393336	0.4071793526425926
O	0.6319169687396741	0.0799328006580626	0.2510692728079758
O	0.6256193894355265	0.0951468416164196	0.4249824499987692
O	0.8828578612280351	0.2469260902161039	0.3334899894003865
O	0.8867006452313323	0.2478962981649908	0.1704037995309975
O	0.8747431260725761	0.2616597429900554	0.4990162083503588
O	0.6327087895514532	0.4160447599783696	0.2489146057775008
O	0.6297229948472218	0.4225244940991419	0.4129462029386722
O	0.3770768829094724	0.5857364801452909	0.3336324137837506

O	0.4030167459345127	0.5891607681803276	0.1691090040723171
O	0.1330999958008258	0.7495997592799882	0.2460339686411519
O	0.1388646522821419	0.7559798050874368	0.4210648066462728
O	0.3783360982918055	0.9190729071485667	0.3370266961387613
O	0.3842067282879623	0.9219060422136541	0.1713926249221594
O	0.4086850618522623	0.9084057697101212	0.5027879720494797
O	0.8849727983607518	0.5869931047475692	0.3310187831418630
O	0.8706996090242449	0.5863884709202918	0.1678761406806675
O	0.8818744273921497	0.5886155047830520	0.4935595375441633
O	0.6326919506011736	0.7573974500310049	0.2530989154566551
O	0.6225317155564895	0.7418618768207150	0.4197655767484536
O	0.8837863637993906	0.9203847831099613	0.3385533664376357
O	0.8842790966176314	0.9171889705045907	0.1699225771851787
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Co	0.1297942216430426	0.2468405858326165	0.1742026141967732
Co	0.1339018928747513	0.2817576171781859	0.5040992301836642
Co	0.1297248469032758	0.2442122625780625	0.3351852106619093
Co	0.3778711016497995	0.4245229898835928	0.4126298031794248
Co	0.3798890430766702	0.4206222916247636	0.2407661161157175
Co	0.8836223252482148	0.0920615353584005	0.4284225390304691
Co	0.8781015083102469	0.0820123593710118	0.2469043801238002
Co	0.6262308950570541	0.2483364836115133	0.1763509571991812
Co	0.6322630513999985	0.2741609134980393	0.4997212062869289
Co	0.6289328461344668	0.2474015379630500	0.3357517896120069
Co	0.8786234179706542	0.4152586977807364	0.4168956291598088
Co	0.8800737915285280	0.4146535858486644	0.2441031702965989
Co	0.0998150843636277	0.5885755487931126	0.1714654910801731
Co	0.1115753163333785	0.5738064833871842	0.4873498411822738
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Co	0.3809756966056317	0.7402313564754629	0.4262622634389487
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Co	0.1298381273228520	0.9209533246385397	0.1755398992477098
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Co	0.1341877102919573	0.9200886040982016	0.3403795979297027
Co	0.6296275871477974	0.5884037343277594	0.1729898722161665
Co	0.6567028144866351	0.5767754324261696	0.5005048775671882
Co	0.6320997935314978	0.5863504373538238	0.3327121936621826
Co	0.8780346225148973	0.7524650401563023	0.4188433909493913
Co	0.8789172533215497	0.7549879372587095	0.2467426797092455
Co	0.6273354920589053	0.9149393404390558	0.1717278668959434
Co	0.6381487829226534	0.9167931312254312	0.4943282671388984
Co	0.6272343177886082	0.9185714987090844	0.3384755174516038
Rh	0.3559350012274717	0.5039686703440811	0.5546905579242598
N	0.3152843757844558	0.7138325510734803	0.6045021552455683
N	0.1579983056977395	0.7820460885495890	0.6058559340290118
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H	0.1505622659700635	0.8526944704352658	0.6505629933951409
H	0.0778773155656621	0.6985792945785522	0.6145043332652871
H	0.3361623513508523	0.4335245049220828	0.6348677737117285
H	0.5682909985262082	0.5133757841191336	0.5796302225518486

E= -389.57717

O	0.1290100069999980	0.0825499970000010	0.2527300120000007
O	0.1321605216140494	0.0736675266999449	0.4311252682200747
O	0.3736215792689204	0.2469169040101490	0.3365976775720159
O	0.3837899859999965	0.247289999999996	0.1712500009999971
O	0.3452090957760406	0.2651924599212088	0.5044566157662707
O	0.1332499979999966	0.4220499990000022	0.2408899959999999
O	0.1315154789122494	0.4266130757436036	0.4170559237431948
O	0.6319199799999993	0.0799299999999974	0.2510699930000015
O	0.6234020689165026	0.0995472792171038	0.4282714042719261
O	0.8866328707880388	0.2477215004961295	0.3343792972408572
O	0.8866999749999991	0.2478999940000008	0.1703999940000003
O	0.8858358343803455	0.2556291758525183	0.4977587426731044
O	0.6327099800000013	0.4160499870000010	0.2489199939999978
O	0.6279107065359527	0.4134925068788682	0.4092371474928950
O	0.3791166898628892	0.5851682368658518	0.3346003916841178
O	0.4030199939999974	0.5891600249999982	0.1691100000000034
O	0.1331000030000027	0.7495999929999968	0.2460300030000013
O	0.1412225868928569	0.7485889687668689	0.4190315445112642
O	0.3811148757691651	0.9182410826419602	0.3367058053278287
O	0.3842099909999988	0.9219099880000030	0.1713899969999986
O	0.4049025394839833	0.9015161398306291	0.5031621917877744
O	0.8856630488826047	0.5838016773945072	0.3300068734126405
O	0.8707000019999995	0.5863900180000030	0.1678799990000002
O	0.8814110279429699	0.5819422745501187	0.4917225314750823
O	0.6326900119999976	0.7573999760000021	0.2531000079999970
O	0.6221132906357357	0.7352681262439021	0.4210642766146014
O	0.8780181808551493	0.9171524098188139	0.3369494062838966
O	0.8842800259999990	0.9171900150000027	0.1699199970000009
O	0.8596383690718618	0.9138041527319370	0.4960977299788969
Co	0.3769377815717987	0.0794125235249764	0.4329567571958242
Co	0.3801800009999994	0.0831900020000020	0.2492700069999998
Co	0.1297899930000028	0.2468399999999988	0.1741999979999989
Co	0.11765922261861990	0.2639092747006156	0.4979240469703828
Co	0.1317949916590611	0.2490942432267622	0.3366459595135370
Co	0.3788023249179484	0.4179545351299205	0.4167500717051008
Co	0.3798899949999992	0.4206199939999991	0.2407699970000010
Co	0.8787758122456332	0.0852546838106937	0.4236708723275341
Co	0.8780999780000016	0.0820100010000004	0.2469000070000007
Co	0.6262300010000033	0.2483399959999986	0.1763499979999992
Co	0.6557314011021917	0.2745332380193702	0.5021728475307735
Co	0.6275314963861247	0.2441994652917104	0.3351540877163349
Co	0.8826795425363816	0.4172939851749274	0.4152479021925597
Co	0.8800699709999975	0.4146499929999976	0.2441000040000034
Co	0.0998200029999978	0.5885800120000013	0.1714700010000030
Co	0.1159031849638464	0.5898214252415200	0.5049698498258298
Co	0.1338982584396492	0.5861962401413648	0.3329056448409999
Co	0.3812736811222980	0.7476041837107198	0.4243668120631304
Co	0.3815400000000011	0.7524899840000003	0.2451699969999979
Co	0.1298400009999980	0.9209499959999974	0.1755399999999980
Co	0.0966753317311735	0.9037981214328824	0.5049433869220923
Co	0.1342703294928854	0.9180358976262307	0.3395762539970812
Co	0.6296300289999976	0.5884000060000005	0.1729899939999981
Co	0.6547899867961813	0.5661992183558658	0.4952622343355370

Co	0.6301316740062385	0.5828683550745524	0.3319547339752112
Co	0.8795431073430156	0.7486547044992238	0.4185448636503334
Co	0.8789200189999988	0.7549899819999979	0.2467399980000025
Co	0.6273400190000018	0.9149400000000014	0.1717299969999999
Co	0.6321708109084380	0.9150249672334201	0.4934731669710050
Co	0.6271306465526352	0.9162551032767391	0.3381205043964792
Rh	0.4088362523016549	0.4528610287999776	0.5585017705294233
N	0.4423565690123634	0.6465224376432203	0.6246330731302214
N	0.1057161302534727	0.7505732170325349	0.5848265302686956
H	0.4263582094546240	0.7413275706643048	0.5929900938053981
H	0.5504421553550644	0.6525429001015044	0.6491647289020051
H	0.1922059224741642	0.7705549078027026	0.6224910216202997
H	0.0024585435111673	0.7451542259671764	0.6137278811401753
H	0.3611290529855369	0.6455686286331591	0.6665824107562895
H	0.6128595556185535	0.4241906065117680	0.5659794828365041

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E= -379.90253

O	0.1262255566144977	0.0824954872792097	0.2517205562282868
O	0.1350274030883012	0.0874334735964516	0.4407640859633972
O	0.3744632722613044	0.2450165798694079	0.3364215348086277
O	0.3804382726500826	0.2473940369869968	0.1712561251688470
O	0.4011889180277112	0.2773754671220455	0.5068822810364145
O	0.1306043234277268	0.4221341333798878	0.2400786593020815
O	0.1261817990973305	0.4110582292834683	0.4064002428321069
O	0.6299972608921398	0.0799191391227948	0.2497724765159430
O	0.6278274562714568	0.0908820055148272	0.4211465566174926
O	0.8803713056716980	0.2473209233158731	0.3327955824304895
O	0.8837393975626860	0.2485559289558580	0.1697498450636743
O	0.8718814447594817	0.2600402272707115	0.4981667036396099
O	0.6295629329167344	0.4157875600739749	0.2490668601192683
O	0.6238117085383815	0.4214353094830369	0.4130860142996762
O	0.3745098908410975	0.5859012891438279	0.3333268614744251
O	0.4011565102194525	0.5891067461544630	0.1683065862801216
O	0.1302639481527976	0.7492942905285987	0.2453644261794470
O	0.1379423433031955	0.7528859751040470	0.4212304532410164
O	0.3738356620899223	0.9185626511393093	0.3360072505700061
O	0.3811925277747968	0.9217465047414003	0.1708489211978002
O	0.4074349657513535	0.9133483032470735	0.5006375302093576
O	0.8818114412601661	0.5861300302732093	0.3308140204816365
O	0.8667468402765239	0.5867742106712219	0.1676555959324886
O	0.8778382747238677	0.5863487782900278	0.4929199545473296
O	0.6299085584348840	0.7584798265549347	0.2535192520270125
O	0.6199799273211544	0.7410268232234822	0.4200648943093960
O	0.8839662639084109	0.9191880851153418	0.3378019388496402
O	0.8814103115305971	0.9167458083615502	0.1692328979859550
O	0.8678876294010718	0.9146892553900313	0.4995713721304390
Co	0.3761025084703211	0.0878384020899939	0.4324427069384303
Co	0.3778630287570764	0.0826898327640805	0.2488154219698785
Co	0.1271522667821796	0.2469423591624698	0.1733577154851006
Co	0.1142207180458380	0.2787643189549679	0.5064858341549757
Co	0.1274905951954531	0.2428564565667586	0.3345138774154987
Co	0.3750761905294046	0.4191531282419378	0.4133244823427908
Co	0.3769966253335496	0.4214734204809283	0.2406493004157701

Co	0.8827856488511419	0.0890069234656615	0.4264066964338761
Co	0.8757468773639784	0.0819072358076187	0.2457023335205948
Co	0.6226969123078171	0.2490745790267794	0.1756952034335898
Co	0.6338540573054211	0.2676033467749078	0.4982812954278530
Co	0.6266752470484461	0.2468770972784538	0.3343727644254778
Co	0.8745561124008592	0.4143747437230808	0.4151288325743804
Co	0.8773184939952389	0.4150104728540142	0.2435034197247181
Co	0.0955690571143425	0.5886422718762334	0.1710450557223586
Co	0.1058425693456257	0.5675707083717197	0.4877085473218512
Co	0.1301801359679377	0.5844986728530712	0.3301783569933815
Co	0.3791126238593187	0.7530534744553806	0.4248798229999088
Co	0.3787464584068254	0.7518022236870546	0.2446375886152711
Co	0.1277209111038022	0.9206785675006223	0.1748991279434991
Co	0.1020415541963316	0.9033687670314927	0.5064881051147172
Co	0.1317464899981158	0.9184322958905029	0.3397944464058409
Co	0.6262010235757915	0.5888219717172118	0.1725030545410859
Co	0.6521795061383312	0.5760375944312415	0.4990195939611029
Co	0.6281995161201709	0.5859832259526306	0.3326830553053972
Co	0.8761622768284839	0.7522884592101853	0.4189281856512076
Co	0.8760825311894707	0.7552314851874046	0.2465880117581362
Co	0.6246338853305441	0.9139615218536393	0.1710384469987620
Co	0.6358032087247666	0.9171777818559144	0.4950350531267588
Co	0.6251182867670022	0.9194016843261912	0.3377912917449244
Rh	0.3449785893711910	0.4829457508975116	0.5547258044902373
N	0.2995822967869179	0.6795074036904412	0.5962828630777859
N	0.1574233355404774	0.7672761153439893	0.6004709418891925
H	0.1656778172196919	0.8346573206015704	0.6464712346746239
H	0.3862265919524112	0.7572259877403528	0.5883114486869893
H	0.5571572574574386	0.5223140267379458	0.5757977996764021
H	0.0655126918494685	0.6961633094029747	0.6106828855956604

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E= -386.83880

O	0.1262300010000033	0.0825000029999998	0.2517200110000033
O	0.1324523713566603	0.0705941239270017	0.4343354962781841
O	0.3716594284772100	0.2451078779262308	0.3348444412530397
O	0.3804399970000034	0.2473900020000031	0.1712599990000001
O	0.3673813550688246	0.2746897166015476	0.5009752675473674
O	0.1306000049999980	0.4221299889999983	0.2400799990000024
O	0.1272706816247194	0.4137495616749069	0.4090672584067925
O	0.6299999949999986	0.0799200009999979	0.2497700010000017
O	0.6293776526945668	0.0996546145304064	0.4243489357747208
O	0.8825480091391162	0.2487957837054838	0.3327306514606516
O	0.8837400079999966	0.2485599959999973	0.1697500049999974
O	0.8803348158939324	0.2572425380198381	0.4974467905552497
O	0.6295599939999974	0.4157899920000006	0.2490700040000036
O	0.6217904547697363	0.4172452906175414	0.4115728065481659
O	0.3743724539847790	0.5846394155738777	0.3332080461911606
O	0.4011600019999975	0.5891100170000030	0.1683100010000018
O	0.1302600060000003	0.7492899889999975	0.2453600019999982
O	0.1376297270765990	0.7480755293725677	0.4221624921933838
O	0.3767414242925430	0.9170659240467803	0.3362650949855358
O	0.3811900019999968	0.9217500090000001	0.1708499940000010
O	0.4124917158752762	0.9166180847185936	0.4982532494432628

O	0.8832450225510449	0.5843726542474904	0.3308567911773129
O	0.8667500020000034	0.5867699980000012	0.1676599979999978
O	0.8740508001125763	0.5825336908067589	0.4935339924066596
O	0.6299099920000018	0.7584800119999997	0.2535200120000027
O	0.6217931553346829	0.7373468096167828	0.4211619234107022
O	0.8792210861489319	0.9172568741845046	0.3381145204089389
O	0.8814100029999992	0.9167500140000016	0.1692299990000024
O	0.8678523861559077	0.9122051569439558	0.5000736618191127
Co	0.3787822057487051	0.0860942303939686	0.4286683705281756
Co	0.3778600099999991	0.0826900010000031	0.2488200069999991
Co	0.1271499989999967	0.2469400020000023	0.1733600049999993
Co	0.1232916899531485	0.2606313231361538	0.4957246538589900
Co	0.1284068895154684	0.2462030610298429	0.3329724876875933
Co	0.3760562176004649	0.4217884763968171	0.4159008132049521
Co	0.3770000040000028	0.4214699859999982	0.2406499980000021
Co	0.8800899554816140	0.0869817248652658	0.4252378825474980
Co	0.8757500050000004	0.0819099989999970	0.2457000019999995
Co	0.6226999759999998	0.2490800019999995	0.1756999939999986
Co	0.6328124979504357	0.2807756500246204	0.5030822477826273
Co	0.6270932952517115	0.2465394053331306	0.3346422535295988
Co	0.8731221341102672	0.4146461149367384	0.4162617226273925
Co	0.8773199919999968	0.4150100049999992	0.2434999939999969
Co	0.0955699980000020	0.5886399749999995	0.1710499969999972
Co	0.1039512091119728	0.5669783272983370	0.4896900699756540
Co	0.1304159820316806	0.5847056555257236	0.3304709641427015
Co	0.3791793075183994	0.7465511560681732	0.4260466036915305
Co	0.3787499960000034	0.7518000009999994	0.2446399929999998
Co	0.1277199980000034	0.9206799860000032	0.1748999949999970
Co	0.0979431539384344	0.8983722491105458	0.5073283881917838
Co	0.1318420368690314	0.9178554808485169	0.3403617087544439
Co	0.6262000199999989	0.5888199810000003	0.1724999990000029
Co	0.6401917591101191	0.5731560325234236	0.5002396179787194
Co	0.6279080898878302	0.5847066991255938	0.3324265617618569
Co	0.8766561944417814	0.7490154430733544	0.4191533751061192
Co	0.8760799770000034	0.7552300099999982	0.2465900030000014
Co	0.6246299740000012	0.9139599800000013	0.1710399990000013
Co	0.6392130210483988	0.9185267025814882	0.4923376028388125
Co	0.6248819005490955	0.9193184071675403	0.3379502718358502
Rh	0.3551219995332967	0.4954610977396093	0.5612244861488110
N	0.3225363199123421	0.7025689095118008	0.5917158060132233
N	0.1755299737437088	0.7797159381341700	0.6041042447676577
H	0.1911786199338077	0.8524006338872703	0.6475988002930350
H	0.3922306763052726	0.7857028620855296	0.5692303312125871
H	0.5791177609156579	0.4457286985872539	0.5674301273729930
H	0.0929651151207913	0.7042648249227105	0.6213119362190794
H	0.2076875560997423	0.4154727085736016	0.6213345874223141
H	0.2948826270931693	0.3806392452931247	0.6381323216078102

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E= -379.72516

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O	0.3719858168051630	0.2493694129646405	0.3356985180258752
O	0.3789100050000016	0.2519800070000002	0.1704400030000031

O	0.4106629788100634	0.2651677096396303	0.5025392387288902
O	0.1285700050000003	0.4216499919999990	0.2459899930000020
O	0.1318969415778538	0.4185144247374628	0.4145107972985048
O	0.6293500069999993	0.0836099980000000	0.2534199950000016
O	0.6259591385186590	0.0902730201332599	0.4213494644525036
O	0.8829044385824328	0.2507769966292738	0.3344280443992777
O	0.8809400199999970	0.2520500119999980	0.1697999980000020
O	0.8682056884866857	0.2608964830681651	0.4979998800579450
O	0.6275799869999972	0.4220199880000024	0.2460899949999984
O	0.6255142504304981	0.4194923599770745	0.4108712772457572
O	0.3772535081371434	0.5895497026498046	0.3359331581840398
O	0.3827799860000027	0.5909299850000025	0.1701100020000013
O	0.1297000049999966	0.7572699790000001	0.2492299970000005
O	0.1332459386633857	0.7540190764257306	0.4173963558601120
O	0.3758520558649548	0.9232512685792527	0.3370172500488603
O	0.3803899879999975	0.9225900169999974	0.1709299979999983
O	0.4070054033458720	0.9055043791013291	0.5020104014566789
O	0.8786145755352389	0.5861878462963266	0.3311516675743960
O	0.8804000020000018	0.5905299779999993	0.1686600000000027
O	0.8795078961165708	0.5822890984122040	0.4924885170679688
O	0.6277800200000030	0.7563300130000030	0.2522000069999990
O	0.6202278035038523	0.7397076733962038	0.4209364289805376
O	0.8802521890772661	0.9214696532264049	0.3364115069760379
O	0.8778399830000012	0.9210100170000004	0.1696500030000010
O	0.8610241060145596	0.9171245654622302	0.4965528275431334
Co	0.3725659711060999	0.0807034438446361	0.4329964426476118
Co	0.3799799980000031	0.0872400029999980	0.2470700000000008
Co	0.1260699930000015	0.2518900040000034	0.1730300039999975
Co	0.1018759683940745	0.2793909384179276	0.5023840915449218
Co	0.1284414296225418	0.2523757499421492	0.3359033869718743
Co	0.3788681181165631	0.4191559400541615	0.4151335752624368
Co	0.3765200080000000	0.4212099909999978	0.2435899970000008
Co	0.8809020363458463	0.0885330329469278	0.4248299923144205
Co	0.8753799799999982	0.0866900010000009	0.2461100069999986
Co	0.6244699949999983	0.2516300079999993	0.1762599950000023
Co	0.6357196472320839	0.2649820942487269	0.4992133850129463
Co	0.6269825575105201	0.2470380499391107	0.3353624527633368
Co	0.8802178432771760	0.4197918659000515	0.4157723774509765
Co	0.8762099739999982	0.4209499959999974	0.2424499990000015
Co	0.1210800039999995	0.5911999940000001	0.1736499969999983
Co	0.1132174111470504	0.6015167355161311	0.5168086054769939
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Co	0.3753971665669250	0.7518192649845563	0.4247546042406291
Co	0.3790099920000003	0.7569699880000016	0.2464600059999995
Co	0.1244399990000034	0.9229400159999983	0.1736100019999967
Co	0.0905943768710041	0.8955557727552330	0.5109971030479794
Co	0.1304416234659611	0.9207611289034616	0.3390245018567887
Co	0.6225600240000020	0.5913599730000030	0.1737499979999981
Co	0.6533958523903277	0.5689784859400353	0.4930594484237946
Co	0.6283855711015887	0.5871331246549476	0.3324825533508949
Co	0.8776284723087793	0.7504548472622117	0.4188608375878947
Co	0.8755000230000007	0.7549399729999990	0.2450000050000014
Co	0.6251699919999965	0.9188799860000003	0.1722500030000020
Co	0.6323210936116984	0.9156072293863765	0.4947680500777252
Co	0.6258448332983578	0.9197461086229156	0.3383771083746190
Rh	0.3739395236665636	0.4577636149048130	0.5573014185719166
N	0.3933568794278059	0.6470821049003977	0.6269559953889737
N	0.1134890211029984	0.7539314419441869	0.5723265834947847

H	0.4018118012610296	0.7424323895509605	0.5955068807640856
H	0.4886575062054586	0.6401642786786473	0.6613760048461079
H	0.1722204791027597	0.4242438013958235	0.5701918271651926
H	0.2942039104197179	0.6598576899390729	0.6584795889950128

26

E= -387.24699

O	0.1275400070000003	0.0867199970000030	0.2486699970000004
O	0.1314714006232237	0.0818623233802239	0.4457521106593442
O	0.3719858168051630	0.2493694129646405	0.3356985180258752
O	0.3789100050000016	0.2519800070000002	0.1704400030000031
O	0.4106629788100634	0.2651677096396303	0.5025392387288902
O	0.1285700050000003	0.4216499919999990	0.2459899930000020
O	0.1318969415778538	0.4185144247374628	0.4145107972985048
O	0.6293500069999993	0.0836099980000000	0.2534199950000016
O	0.6259591385186590	0.0902730201332599	0.4213494644525036
O	0.8829044385824328	0.2507769966292738	0.3344280443992777
O	0.8809400199999970	0.2520500119999980	0.1697999980000020
O	0.8682056884866857	0.2608964830681651	0.4979998800579450
O	0.6275799869999972	0.4220199880000024	0.2460899949999984
O	0.6255142504304981	0.4194923599770745	0.4108712772457572
O	0.3772535081371434	0.5895497026498046	0.3359331581840398
O	0.3827799860000027	0.5909299850000025	0.1701100020000013
O	0.1297000049999966	0.7572699790000001	0.2492299970000005
O	0.1332459386633857	0.7540190764257306	0.4173963558601120
O	0.3758520558649548	0.9232512685792527	0.3370172500488603
O	0.3803899879999975	0.9225900169999974	0.1709299979999983
O	0.4070054033458720	0.9055043791013291	0.5020104014566789
O	0.8786145755352389	0.5861878462963266	0.3311516675743960
O	0.8804000020000018	0.5905299779999993	0.1686600000000027
O	0.8795078961165708	0.5822890984122040	0.4924885170679688
O	0.6277800200000030	0.7563300130000030	0.2522000069999990
O	0.6202278035038523	0.7397076733962038	0.4209364289805376
O	0.8802521890772661	0.9214696532264049	0.3364115069760379
O	0.8778399830000012	0.9210100170000004	0.1696500030000010
O	0.8610241060145596	0.9171245654622302	0.4965528275431334
Co	0.3725659711060999	0.0807034438446361	0.4329964426476118
Co	0.3799799980000031	0.0872400029999980	0.2470700000000008
Co	0.1260699930000015	0.2518900040000034	0.1730300039999975
Co	0.1018759683940745	0.2793909384179276	0.5023840915449218
Co	0.1284414296225418	0.2523757499421492	0.3359033869718743
Co	0.3788681181165631	0.4191559400541615	0.4151335752624368
Co	0.3765200080000000	0.4212099909999978	0.2435899970000008
Co	0.8809020363458463	0.0885330329469278	0.4248299923144205
Co	0.8753799799999982	0.0866900010000009	0.2461100069999986
Co	0.6244699949999983	0.2516300079999993	0.1762599950000023
Co	0.6357196472320839	0.2649820942487269	0.4992133850129463
Co	0.6269825575105201	0.2470380499391107	0.3353624527633368
Co	0.8802178432771760	0.4197918659000515	0.4157723774509765
Co	0.8762099739999982	0.4209499959999974	0.2424499990000015
Co	0.1210800039999995	0.5911999940000001	0.1736499969999983
Co	0.1132174111470504	0.6015167355161311	0.5168086054769939
Co	0.1290599035171749	0.5867563005767639	0.3351619273559263
Co	0.3753971665669250	0.7518192649845563	0.4247546042406291
Co	0.3790099920000003	0.7569699880000016	0.2464600059999995

Co	0.1244399990000034	0.9229400159999983	0.1736100019999967
Co	0.0905943768710041	0.8955557727552330	0.5109971030479794
Co	0.1304416234659611	0.9207611289034616	0.3390245018567887
Co	0.6225600240000020	0.5913599730000030	0.1737499979999981
Co	0.6533958523903277	0.5689784859400353	0.4930594484237946
Co	0.6283855711015887	0.5871331246549476	0.3324825533508949
Co	0.8776284723087793	0.7504548472622117	0.4188608375878947
Co	0.8755000230000007	0.7549399729999990	0.2450000050000014
Co	0.6251699919999965	0.9188799860000003	0.1722500030000020
Co	0.6323210936116984	0.9156072293863765	0.4947680500777252
Co	0.6258448332983578	0.9197461086229156	0.3383771083746190
Rh	0.3739395236665636	0.4577636149048130	0.5573014185719166
N	0.3933568794278059	0.6470821049003977	0.6269559953889737
N	0.1134890211029984	0.7539314419441869	0.5723265834947847
H	0.4018118012610296	0.7424323895509605	0.5955068807640856
H	0.4886575062054586	0.6401642786786473	0.6613760048461079
H	0.1722204791027597	0.4242438013958235	0.5701918271651926
H	0.2942039104197179	0.6598576899390729	0.6584795889950128

27

E= -388.69637

O	0.1286000010000024	0.0870800020000004	0.2544000150000016
O	0.1323534389608454	0.0870754457629856	0.4441279262541546
O	0.3735016761932076	0.2511447655714533	0.3359377796732198
O	0.3790900110000024	0.2518799899999991	0.1727299989999977
O	0.4027908734644413	0.2748122026360625	0.5023170438281199
O	0.1318700019999994	0.4249500040000029	0.2448000010000015
O	0.1340343820127627	0.4238362063503872	0.4154220898566617
O	0.6326100229999980	0.0850500020000027	0.2500300109999998
O	0.6257819889505413	0.0948991234636268	0.4198214076488695
O	0.8855243028625974	0.2534907856250770	0.3349133759553732
O	0.8879100079999986	0.2527300120000007	0.1709900050000002
O	0.8720721275735005	0.2649207880410884	0.4984377749449496
O	0.6310999899999999	0.4188300069999968	0.2489400059999980
O	0.6278100548640786	0.4236905604893104	0.4113500699769891
O	0.3780774329911611	0.5913884501891057	0.3350902510559994
O	0.4014700059999967	0.5909299850000025	0.1691199990000030
O	0.1325500009999985	0.7533400060000019	0.2446900010000022
O	0.1369856394376548	0.7540889837560488	0.4192965201597308
O	0.3761633842208874	0.9231881768179986	0.3370809712197445
O	0.3817099930000012	0.9268699880000000	0.1710900069999965
O	0.4046989333334156	0.9114052997934571	0.5015153843482210
O	0.8825814977469781	0.5891381594327042	0.3304261614960177
O	0.8701800110000022	0.5896999839999992	0.1678400039999985
O	0.8788147167957682	0.5892552365188685	0.4907104504737170
O	0.6315600280000027	0.7610700130000012	0.2522400020000006
O	0.6199447091563488	0.7429666502236331	0.4202511045235077
O	0.8837215376437587	0.9228825035932525	0.3361947906916342
O	0.8830299970000013	0.9218299979999998	0.1695500020000011
O	0.8589169233455287	0.9215331828380519	0.4957068343259252
Co	0.3742781711783039	0.0862485367055515	0.4320134722881380
Co	0.3802999850000006	0.0868600009999980	0.2498299929999988
Co	0.1303600070000002	0.2505899969999987	0.1755699960000001
Co	0.1108177590280463	0.2840289293970800	0.5032522165230277

Co	0.1297299427890997	0.2533507708355502	0.3378027033889448
Co	0.3810621047310134	0.4210704050404627	0.4151520132642508
Co	0.3782500029999980	0.4255700109999978	0.2429900019999991
Co	0.8809432693225618	0.0940707127783339	0.4252664840321596
Co	0.8786200280000003	0.0867599990000016	0.2464999999999975
Co	0.6224600079999973	0.2529399989999987	0.1760800030000027
Co	0.6350340667919628	0.2692838243330309	0.4984869970101516
Co	0.6283521282066181	0.2507726450509469	0.3344293912951568
Co	0.8813717919635254	0.4219563471734853	0.4162958710774115
Co	0.8791599870000013	0.4187900129999989	0.2442999929999985
Co	0.1000099999999975	0.5893099899999967	0.1727599949999998
Co	0.1080982467324605	0.6018701666380896	0.5109764855675699
Co	0.1323613693013384	0.5893510428494216	0.3342606089458793
Co	0.3779423542532216	0.7544797896980090	0.4246562919052189
Co	0.3801800009999994	0.7552999850000006	0.2439399960000017
Co	0.1291400049999964	0.9265599849999973	0.1753199990000027
Co	0.0960692083121353	0.9078874862511161	0.5105093583331346
Co	0.1324578548619249	0.9208162369470198	0.3398385267126328
Co	0.6285300250000034	0.5910000209999993	0.1727000030000028
Co	0.6525241701817608	0.5781707491278958	0.4939440869578942
Co	0.6305840039149575	0.5900082648581974	0.3318057333088474
Co	0.8785997355299068	0.7566715107421208	0.4180382739616230
Co	0.8786000010000024	0.7581800219999977	0.2458100019999989
Co	0.6265699859999998	0.9184200170000025	0.1712100060000026
Co	0.6308404853973942	0.9209466033843244	0.4938183455733132
Co	0.6273364682166471	0.9231897922367330	0.3368409031699927
Rh	0.3824449877645725	0.4748384737498354	0.5604926025658252
N	0.3792652833089254	0.6658916040989349	0.6259975365096121
N	0.0920241404073522	0.7578357566601105	0.5807052571868282
H	0.4343566185258129	0.7522809285369229	0.5992982225567876
H	0.4300755172489675	0.6506717141568232	0.6768744260631252
H	-0.0167918346725674	0.7492420969627422	0.6052844683392592
H	0.1789110021451266	0.4427270081736184	0.5675251831080744
H	0.2622514850013591	0.7024823404421116	0.6299220733189946
H	0.5808393980240236	0.4856819831158969	0.5727966586810657

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E= -376.73894

O	0.1286000010000024	0.0870800020000004	0.2544000150000016
O	0.1305841117250025	0.0810095846844238	0.4306482263184053
O	0.3721143152809994	0.2523587393064713	0.3362671518149210
O	0.3790900110000024	0.2518799899999991	0.1727299989999977
O	0.3498555238014827	0.2695058216919910	0.5039439312925548
O	0.1318700019999994	0.4249500040000029	0.2448000010000015
O	0.1349102635254066	0.4350363923400305	0.4205651109664981
O	0.6326100229999980	0.0850500020000027	0.2500300109999998
O	0.6261589525279142	0.1038301093965850	0.4270070491498584
O	0.8849482825664289	0.2540708988801818	0.3355187275251463
O	0.8879100079999986	0.2527300120000007	0.1709900050000002
O	0.8873373345115543	0.2622326754183322	0.4980943295799224
O	0.6310999989999999	0.4188300069999968	0.2489400059999980
O	0.6227853241439929	0.4196939526163906	0.4115404963188528
O	0.3787593514196954	0.5898232420950492	0.3344534638570055
O	0.4014700059999967	0.5909299850000025	0.16911999900000030

O	0.1325500009999985	0.7533400060000019	0.2446900010000022
O	0.1407099385929031	0.7542089880714092	0.4178658698511065
O	0.3814770080248232	0.9241680485633230	0.3352156410684043
O	0.3817099930000012	0.9268699880000000	0.1710900069999965
O	0.4032909270861977	0.9129168519359433	0.4988374310134987
O	0.8829698765242531	0.5872643779730823	0.3311225748392660
O	0.8701800110000022	0.5896999839999992	0.1678400039999985
O	0.8802956399946805	0.5880929282957367	0.4920278929227411
O	0.6315600280000027	0.7610700130000012	0.2522400020000006
O	0.6217705738341853	0.7400622845289420	0.4219898680054776
O	0.8780775982302924	0.9212328753191910	0.3359994124163589
O	0.8830299970000013	0.9218299979999998	0.1695500020000011
O	0.8607865128796992	0.9194444880291230	0.4962672725760615
Co	0.3766223189169970	0.0863404566538527	0.4310541170098875
Co	0.3802999850000006	0.0868600009999980	0.2498299929999988
Co	0.1303600070000002	0.2505899969999987	0.1755699960000001
Co	0.1187649573920227	0.2680717560180663	0.4979801465659318
Co	0.1293897435732787	0.2533550094981505	0.3374174090821448
Co	0.3793865742355723	0.4226920665601195	0.4156002976326795
Co	0.3782500029999980	0.4255700109999978	0.2429900019999991
Co	0.8788263471464578	0.0902612545384359	0.4235223028714966
Co	0.8786200280000003	0.0867599990000016	0.2464999999999975
Co	0.6224600079999973	0.2529399989999987	0.1760800030000027
Co	0.6580849879888797	0.2775914979007365	0.5026489707549389
Co	0.6260897031521007	0.2503323006123615	0.3355499760359211
Co	0.8824461663834924	0.4225652502657971	0.4164664386746547
Co	0.8791599870000013	0.4187900129999989	0.2442999929999985
Co	0.1000099999999975	0.5893099899999967	0.1727599949999998
Co	0.1121243196842222	0.5989268214432025	0.5048583751915737
Co	0.1326278821405708	0.5913508728642008	0.3337630735394450
Co	0.3816266487345846	0.7573320474321367	0.4227087878319188
Co	0.3801800009999994	0.7552999850000006	0.2439399960000017
Co	0.1291400049999964	0.9265599849999973	0.1753199990000027
Co	0.0984108201040715	0.9101112474182699	0.5059511937747411
Co	0.1332508963149671	0.9225790455168356	0.3393428309013911
Co	0.6285300250000034	0.5910000209999993	0.1727000030000028
Co	0.6542264480287707	0.5731010291626928	0.4987830326120876
Co	0.6313268015381261	0.5875597710370437	0.3327687595309617
Co	0.8784363662264799	0.7554430331222144	0.4187997421300997
Co	0.8786000010000024	0.7581800219999977	0.2458100019999989
Co	0.6265699859999998	0.9184200170000025	0.1712100060000026
Co	0.6310283022152556	0.9199805811504741	0.4945754910489299
Co	0.6280572304097209	0.9207744878773574	0.3372411563466389
Rh	0.4095555759240671	0.4520889043027811	0.5624138338272917
N	0.1278406903587177	0.7564856404392342	0.5837120675482536
H	0.2356757958968958	0.7655703063952835	0.6079652799629882
H	0.0456373997268244	0.7511792055403177	0.6250308121152590
H	0.6129629257784341	0.4221743966537866	0.5682637767603274
H	0.4420734676069941	0.6256323605242283	0.5829258736712907
H	0.4261502721809884	0.5704961041110442	0.6307256994042364

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E= -376.42003

O	0.1286000010000024	0.0870800020000004	0.2544000150000016
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O	0.3790900110000024	0.2518799899999991	0.1727299989999977
O	0.3066536488511737	0.2120401773652648	0.5351234170868548
O	0.1318700019999994	0.4249500040000029	0.2448000010000015
O	0.1310626128088374	0.4239102174471713	0.4167850227237881
O	0.6326100229999980	0.0850500020000027	0.2500300109999998
O	0.6191014443600904	0.0977832946112899	0.4328144685719976
O	0.8789428616465805	0.2511400224767529	0.3346105996267948
O	0.8879100079999986	0.2527300120000007	0.1709900050000002
O	0.8877562642486274	0.2592513314865250	0.4974907921799657
O	0.6310999899999999	0.4188300069999968	0.2489400059999980
O	0.6300003823720411	0.4236181873996234	0.4092005584510474
O	0.3797743109981469	0.5905784310679537	0.3343959610668875
O	0.4014700059999967	0.5909299850000025	0.1691199990000030
O	0.1325500009999985	0.7533400060000019	0.2446900010000022
O	0.1358558544817624	0.7428249170277480	0.4220157195924240
O	0.3846666212837139	0.9175184422443132	0.3338940590580215
O	0.3817099930000012	0.9268699880000000	0.1710900069999965
O	0.3699120129841655	0.9050037292570933	0.5022664554251535
O	0.8828715671702102	0.5901123346848177	0.3308923663696929
O	0.8701800110000022	0.5896999839999992	0.1678400039999985
O	0.8755310404394873	0.5853050510411666	0.4940609738340315
O	0.6315600280000027	0.7610700130000012	0.2522400020000006
O	0.6199384160574363	0.7461264848881970	0.4265494342022611
O	0.8733870136507971	0.9192743251198523	0.3377689519790581
O	0.8830299970000013	0.9218299979999998	0.1695500020000011
O	0.8770223533743188	0.9185107299175069	0.5003926569247323
Co	0.3728505700882149	0.0950226303606439	0.4401830009531523
Co	0.3802999850000006	0.0868600009999980	0.2498299929999988
Co	0.1303600070000002	0.2505899969999987	0.1755699960000001
Co	0.1101500541364134	0.2735811125795241	0.5122986059750481
Co	0.1290872118777655	0.2503189116736104	0.3385338642059600
Co	0.3765457033150699	0.4267266645074556	0.4141607580237924
Co	0.3782500029999980	0.4255700109999978	0.2429900019999991
Co	0.8817189498066632	0.0876245495024476	0.4242605415584338
Co	0.8786200280000003	0.0867599990000016	0.2464999999999975
Co	0.6224600079999973	0.2529399989999987	0.1760800030000027
Co	0.6610355633327460	0.2775717574474123	0.4997461116833905
Co	0.6250428839549979	0.2488000270121959	0.3363137823633935
Co	0.8810434977649119	0.4219627037559678	0.4145845771111277
Co	0.8791599870000013	0.4187900129999989	0.2442999929999985
Co	0.1000099999999975	0.5893099899999967	0.1727599949999998
Co	0.1057637050198790	0.5760786343447142	0.5038121602242223
Co	0.1307584273208489	0.5884422921985982	0.3336859509713411
Co	0.3774191533208879	0.7565493544887926	0.4206468581215290
Co	0.3801800009999994	0.7552999850000006	0.2439399960000017
Co	0.1291400049999964	0.9265599849999973	0.1753199990000027
Co	0.1239914550638765	0.9202045186563497	0.4944187478535448
Co	0.1337310899976616	0.9168477655357675	0.3361772909843337
Co	0.6285300250000034	0.5910000209999993	0.1727000030000028
Co	0.6436191426677428	0.5709307472377699	0.5020331293223255
Co	0.6317059301042889	0.5899971379271411	0.3329779817562562
Co	0.8790015033205631	0.7541073147323893	0.4218595883447611
Co	0.8786000010000024	0.7581800219999977	0.2458100019999989
Co	0.6265699859999998	0.9184200170000025	0.1712100060000026
Co	0.6351486108519343	0.9177447160033053	0.4964631576047918
Co	0.6267438594849277	0.9204400270179238	0.3380306411499924

Rh	0.4101450920320814	0.4091294697264174	0.5498401731016419
N	0.1718369583114806	0.6781921054837442	0.6044223588058630
H	0.2549279440027178	0.7594664203072413	0.5954041722614861
H	0.0820604004387246	0.7200681499562562	0.6359317065063057
H	0.6059645860078261	0.4091259452333603	0.5711149054995960
H	0.4662715642506454	0.5880113525608435	0.5585826521948871
H	0.2286335781555469	0.5969913232084757	0.6340699301946571

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