

Electronic supplementary information for:

Exploring nickel-catalyzed organochalcogen synthesis *via* cross-coupling of benzonitrile and alkyl chalcogenols with computational tools

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Gibbs Energy Calculation

The final Gibbs energies at a given temperature, based on the rigid rotor/harmonic oscillator approach to statistical mechanics, were obtained with the following formula:

$$G_T^\circ = E_{BS2} + H_{corr,BS1} - TS_{BS1} + RT \ln (C^\circ/C^{1atm})$$

where E_{BS2} is the electronic energy, including the solvent and dispersion terms, obtained with the large basis sets scheme (BS2). $H_{corr,BS1}$ is the thermal correction to enthalpy and contains the zero-point energy plus the vibrational, rotational and translational energies computed with the BS1 scheme. Finally, TS_{BS1} accounts for the entropic correction obtained from the BS1 scheme. Gibbs energies as output by Gaussian16, which refer to an ideal gas ($P = 1$ atm) standard state, were corrected to use a standard state in which the species in solution have a standard concentration of 1 M. This procedure was carried out by adding an additional term to the computed Gibbs energy of each species. This correction is computed as $RT \ln(C^\circ/C_{1atm})$, where C° is the standard reference state concentration (1 M), and C_{1atm} is the concentration of an ideal gas under the standard $P = 1$ atm conditions at a given temperature. Therefore, for an ideal gas at 1 atm and at 110°C: $C_{1atm} = 1/V_m = P/RT = 0.0042$ M; numerically, this correction term equals to 2.62 kcal mol⁻¹ per molecule.

The E_{BS2} , $H_{corr,BS1}$, TS_{BS1} and G° terms for the different species can be found in table S1.

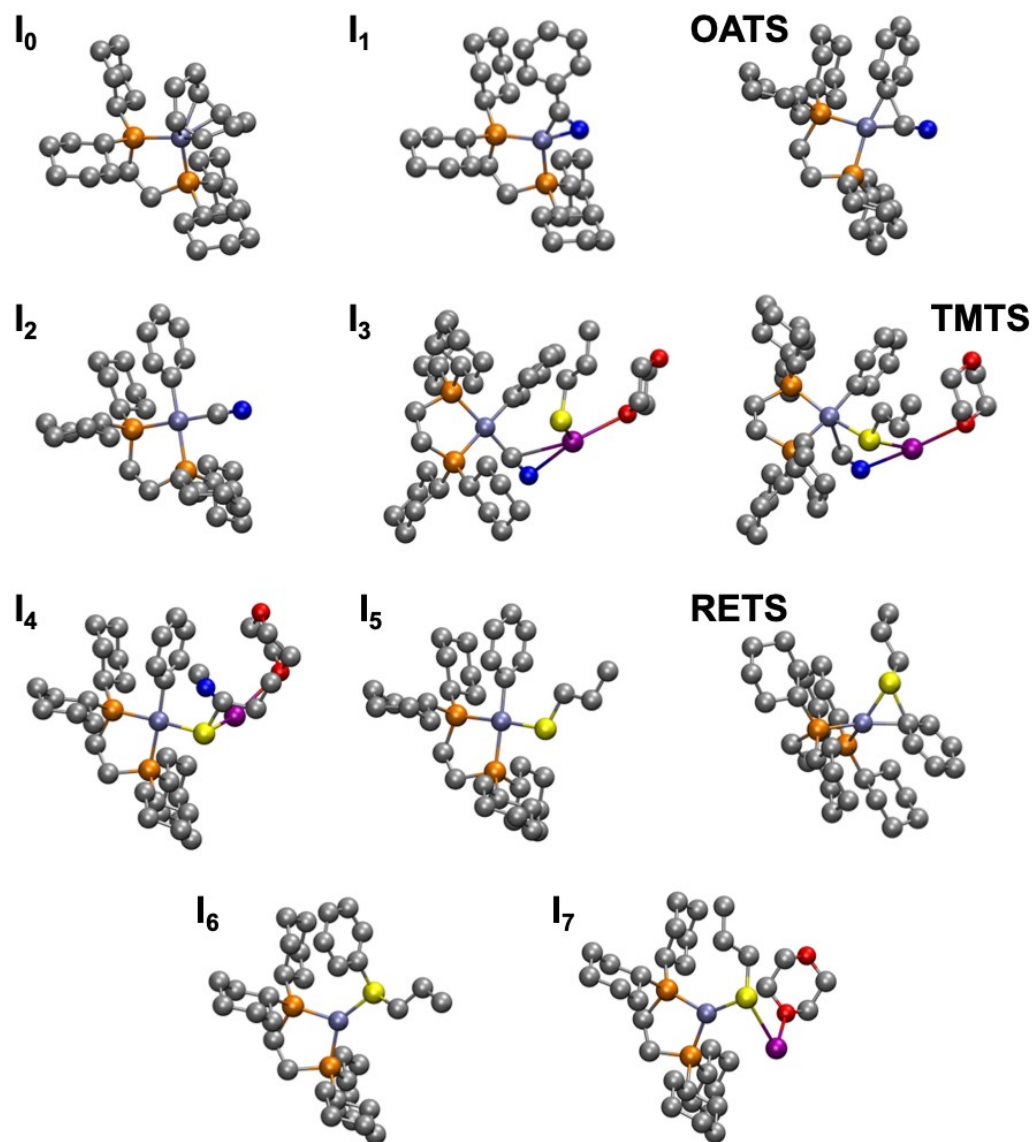


Figure S1. 3D representation of species in the Ni-catalyzed process.

Table S1. Energy terms (E_{BS2} , $H_{corr,BS1}$, TS_{BS1} and G° , in Hartrees), for all the species involved in the catalytic cycles.

		E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	G°
	PhCN	-324.6479	0.1063	0.0479	-324.5853
	COD	-312.1943	0.1888	0.0511	-312.0524
	KCN	-1000.7091	0.1417	0.0679	-1000.6312
	<i>t</i> BuOH	-233.8093	0.1433	0.0468	-233.7085
	<i>t</i> BuOK	-1141.0178	0.2628	0.0820	-1140.8328
C-S coupling	HSPr	-517.4435	0.1105	0.0465	-517.3753
	KSPr	-1424.6694	0.2340	0.0819	-1424.5131
	PhSPr	-748.6030	0.1976	0.0625	-748.4637
	I₀	-3523.7728	0.9266	0.1397	-3522.9817
	I₁	-3536.2275	0.8448	0.1428	-3535.5214
	OATS	-3536.2016	0.8416	0.1380	-3535.4938
	I₂	-3536.2330	0.8445	0.1422	-3535.5265
	I₃	-4960.9518	1.0813	0.1940	-4960.0604
	TMTS	-4960.9307	1.0798	0.1889	-4960.0356
	I₄	-4960.9506	1.0814	0.1895	-4960.0545
	I₅	-3960.1958	0.9367	0.1561	-3959.4110
	RETS	-3960.1499	0.9337	0.1551	-3959.3672
	I₆	-3960.1645	0.9353	0.1600	-3959.3850
	I₇	-4636.2556	0.9718	0.1699	-4635.4495
C-Se coupling	HSePr	-2520.8449	0.1092	0.0485	-2520.7800
	KSePr	-3428.0890	0.2336	0.0798	-3427.9310
	PhSePr	-2752.0040	0.1968	0.0646	-2751.8677
	I₃	-6964.3631	1.0806	0.1967	-6963.4749
	TMTS	-6964.3410	1.0791	0.1919	-6963.4496
	I₄	-6964.3620	1.0811	0.1909	-6963.4676
	I₅	-5963.6082	0.9363	0.1563	-5962.8239
	RETS	-5963.5614	0.9332	0.1542	-5962.7783
	I₆	-5963.5659	0.9343	0.1625	-5962.7900
	I₇	-6639.6672	0.9714	0.1741	-6638.8657
C-Te coupling	HTePr	-387.3129	0.1082	0.0501	-387.2505
	KTePr	-1294.5577	0.2338	0.0836	-1294.4034
	PhTePr	-618.4725	0.1963	0.0675	-618.3395
	I₃	-4830.8438	1.0809	0.1949	-4829.9536
	TMTS	-4830.8146	1.0790	0.1916	-4829.9230
	I₄	-4830.8338	1.0804	0.1928	-4829.9420

	I₅	-3830.0819	0.9359	0.1574	-3829.2992
	RETS	-3830.0404	0.9333	0.1552	-3829.2580
	I₆	-3830.0402	0.9345	0.1619	-3829.2635
	I₇	-4506.1410	0.9711	0.1752	-4505.3410
Radical species	I₀_radical	-3523.6385	0.9298	0.0485	-3522.7530
	I₅_Ni(I)	-3443.2980	0.8316	0.1430	-3442.6051
	SPr radical	-516.7996	0.0999	0.0457	-516.7412
	SePr radical	-2520.2131	0.0998	0.0475	-2520.1567
	TePr radical	-386.6953	0.0998	0.0486	-386.6399
	H ₂	-1.1798	0.0136	0.0190	-1.1810
	S ₂ Pr ₂	-1033.6933	0.2048	0.0674	-1033.5518
	Se ₂ Pr ₂	-5040.5123	0.2035	0.0720	-5040.3767
	Te ₂ Pr ₂	-773.4681	0.2029	0.0752	-773.3363

Microkinetic modeling

Methodology

The kinetics modeling, which allows the calculation of the transient concentrations of all the species during the reaction course, was built using the COPASI¹ software using the simple mass action law. The forward and backward rate constants for each step were calculated from the Gibbs free energy differences along the reaction pathway. In these models all the steps have been considered to be reversible although the energy difference between some of them would point to a non-reversible behavior; nevertheless, this assumption did not produce significant differences in the kinetics profiles. In all cases the reaction time and the initial concentrations of copper catalyst and substrate in the model were identical to those used in the experiments, *i.e.* [Ni(COD)₂] = 0.05 M, [PhCN] = 0.333 M, and [HXPr] = 0.367 M, while the concentration of all the remaining species was set to zero. The computed rate constants for all the studied processes can be found in Table S2.

Rate constant calculations

Reactions of type $A + B \rightleftharpoons C$ (or its reversal) proceeding without a barrier on the potential energy surface, *i.e.* the association/dissociation stages, are considered diffusion-controlled elemental steps. Hence, the rate constant in solution for the associative direction is given by the the Stokes-Einstein equation within the von Smoluchowski formulation:²

$$k_{diff} = 8k_B T N_A \cdot 10^3 / 3\eta \quad (M^{-1}s^{-1})$$

where k_B is the Boltzmann constant, T is the temperature, N_A is Avogadro's number and η is the solvent viscosity at that temperature. It must be noted that this expression is used for the association reaction, which may correspond either to the forward (k_f) or backward (k_b) rate constant of the process. Thus, once k_f or k_b is known the other one is easily computed through the formulation of the thermodynamic equilibrium constant K and the computed Gibbs free energy difference between the intermediates involved (ΔG°):

$$\Delta G^\circ = -RT \ln K$$

$$K = \exp\left(\frac{-\Delta G^\circ}{RT}\right)$$

$$K = k_f/k_b$$

For example, in the barrierless reaction $A + B \rightleftharpoons C$, the forward rate constant k_1 is equal to k_{diff} . The equilibrium constant K is computed placing the Gibbs free energy in the expression above and, consequently, $k_b = k_f/K$. In the case of 1,4-dioxane, the viscosity at 110°C could not be found in literature and it had to be estimated with a third-degree polynomial fit of the experimental data,³ Figure S1. Using this polynomial fit, the viscosity of 1,4-dioxane at 110°C (383.15 K) was estimated to be 0.447 mPa·s, yielding a diffusion-controlled rate constant k_{diff} of $1.899 \cdot 10^{10} M^{-1}s^{-1}$.

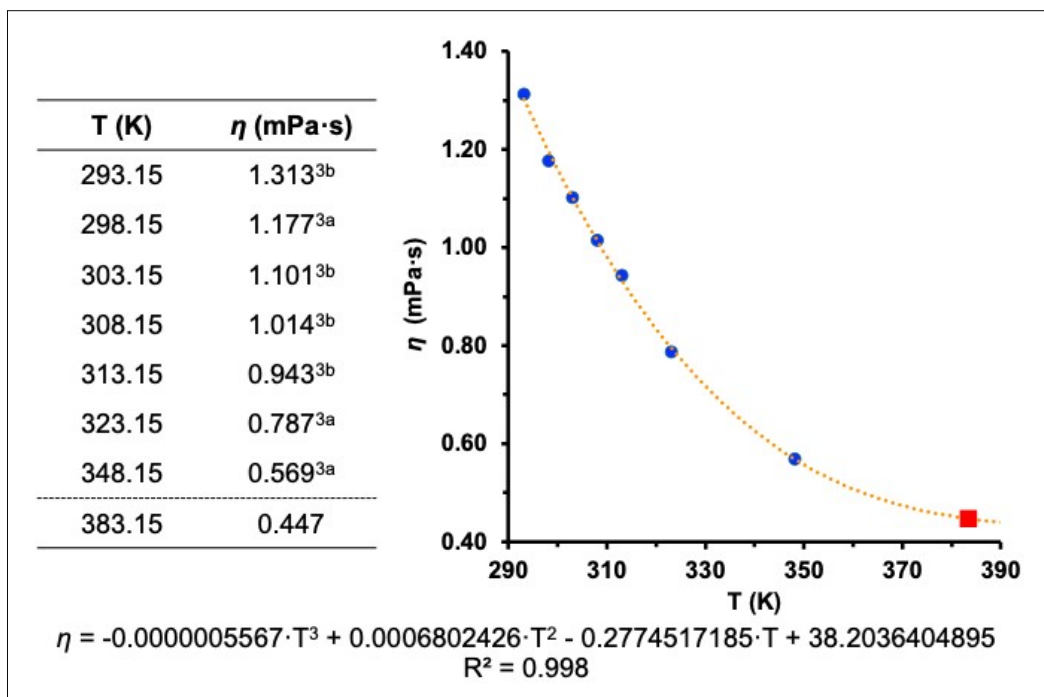


Figure S1. Experimental viscosity (η) data of 1,4-dioxane at different temperatures, third-degree polynomial fit of the data: equation (bottom) and graphical representation (right). The expected viscosity of 1,4-dioxane at the desired temperature (383.15 K) is shown at the bottom of the table and as a red square in the graph. The experimental values for the polynomial fit have been extracted from references 3a and 3b.

On the other hand, the rate constants of all the steps governed by a transition state are computed with the Eyring-Polanyi equation:⁴

$$k = \frac{k_B T}{h} \exp\left(\frac{-\Delta G^\ddagger}{RT}\right)$$

where k_B is the Boltzmann constant, T is the temperature, h is the Planck constant, $\Delta G^\ddagger$ is the activation Gibbs free energy and R is the gas constant. The forward (k_f) and backward (k_b) rate constants are computed independently using their corresponding activation energies. For instance, in a reaction such as $A \rightleftharpoons B$ with a transition state TS_{AB} connecting both species, $\Delta G_{forward}^\ddagger = G_{TSAB}^\circ - G_A^\circ$ while $\Delta G_{backward}^\ddagger = G_{TSAB}^\circ - G_B^\circ$. Additionally, the forward and backward rate constants of all the bimolecular substitution steps, *i.e.* $A + B \rightleftharpoons C + D$, without a transition state have been also calculated using the Eyring-Polanyi equation. These stages are considered fast processes with an associated fictional 2 kcal mol⁻¹ barrier in the endergonic direction of the reversible step. Note that all the bimolecular reactions, where the rate constants are given in M⁻¹s⁻¹, produce a free energy of activation that implicitly contains a reference to a standard state for the translational degrees of freedom of 1 M, so is consistent with the free energies as computed in this work.

Table S2. Computed forward (k_f), backward (k_b) rate constants for all the studied reactions. All the other rate constants are given in s^{-1} except for bimolecular reactions, in which the rate constants are given in $M^{-1}s^{-1}$.

Substrate: propanethiol (HSPr)		
Step	k_f	k_b
$I_0 + PhCN \rightleftharpoons I_1 + COD$	5.766E+11	2.082E+09
$I_1 \rightleftharpoons I_2$	1.075E+03	1.541E+01
$I_2 + KSPr \rightleftharpoons I_3$	1.899E+10	1.084E-02
$I_3 \rightleftharpoons I_4$	1.095E+04	1.321E+06
$I_4 \rightleftharpoons I_5 + KCN$	3.145E+10	1.899E+10
$I_5 \rightleftharpoons I_6$	1.604E-03	3.149E+06
$I_6 + PhCN \rightleftharpoons I_2 + PhSPr$	5.766E+11	1.291E+01
$I_6 + KSPr \rightleftharpoons I_7 + PhSPr$	5.766E+11	1.449E-04
$I_7 + PhCN \rightleftharpoons I_2 + KSPr$	6.472E+06	5.766E+11
$I_0 + KSPr \rightleftharpoons I_7 + COD$	5.766E+11	1.616E+09
Substrate: propaneselenol (HSePr)		
Step	k_f	k_b
$I_0 + PhCN \rightleftharpoons I_1 + COD$	5.766E+11	2.082E+09
$I_1 \rightleftharpoons I_2$	1.075E+03	1.541E+01
$I_2 + KSePr \rightleftharpoons I_3$	1.899E+10	3.120E-06
$I_3 \rightleftharpoons I_4$	6.597E+03	2.761E+06
$I_4 \rightleftharpoons I_5 + KCN$	2.715E+10	1.899E+10
$I_5 \rightleftharpoons I_6$	3.851E-04	5.368E+08
$I_6 + PhCN \rightleftharpoons I_2 + PhSePr$	5.766E+11	2.440E+01
$I_6 + KSePr \rightleftharpoons I_7 + PhSePr$	5.766E+11	2.027E-08
$I_7 + PhCN \rightleftharpoons I_2 + KSePr$	4.791E+02	5.766E+11
$I_0 + KSePr \rightleftharpoons I_7 + COD$	5.766E+11	6.327E+09
Substrate: propanetellurol (HTePr)		
Step	k_f	k_b
$I_0 + PhCN \rightleftharpoons I_1 + COD$	5.766E+11	2.082E+09
$I_1 \rightleftharpoons I_2$	1.075E+03	1.541E+01
$I_2 + KTePr \rightleftharpoons I_3$	1.899E+10	3.538E-09
$I_3 \rightleftharpoons I_4$	8.744E+01	1.282E+06
$I_4 \rightleftharpoons I_5 + KCN$	5.825E+10	1.899E+10
$I_5 \rightleftharpoons I_6$	1.472E-02	8.828E+10
$I_6 + PhCN \rightleftharpoons I_2 + PhTePr$	5.766E+11	8.005E+00
$I_6 + KTePr \rightleftharpoons I_7 + PhTePr$	5.766E+11	1.293E-10
$I_7 + PhCN \rightleftharpoons I_2 + KTePr$	9.315E+00	5.766E+11
$I_0 + KTePr \rightleftharpoons I_7 + COD$	5.766E+11	5.866E+08

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20			H	1.082636	1.072536	1.306401	C	6.537292	3.646397	7.237658	
COD			C	-0.096170	-1.100252	0.000108	H	6.212689	4.637443	7.574469	
C	8.181907	7.066928	6.470353	H	-0.487971	-1.606102	0.884578	C	8.068156	6.797002	6.376907
H	8.169636	6.384625	7.317972	H	-0.487952	-1.606183	-0.884324	H	8.007514	6.217934	7.292884
C	9.379132	7.340743	5.950661	H	0.991529	-1.194247	0.000124	C	7.902824	3.365295	7.886975
H	10.229249	6.839592	6.407323	C	-0.008942	1.076193	-1.259520	H	8.255355	2.378857	7.566620
C	6.810482	7.549423	6.081367	H	-0.396169	0.583080	-2.153196	H	8.641262	4.088053	7.536783
H	6.448952	8.232861	6.861116	H	-0.339652	2.119078	-1.275000	C	4.894868	3.751824	3.215704
H	6.135027	6.686897	6.123813	H	1.082668	1.072421	-1.306351	H	5.404869	4.628075	2.807946
C	9.725043	8.231945	4.782740	O	-1.957290	0.347913	0.000019	H	5.419674	2.880223	2.819744
H	10.774306	8.525101	4.874049	H	-2.267536	1.261855	-0.000013	C	5.504069	2.618592	7.720424
H	9.156971	9.160043	4.809682					H	4.517734	2.826952	7.302333
C	8.184701	7.066929	3.023255	29				H	5.788785	1.619353	7.371965
H	8.196972	6.384627	2.175637	tBuOK_dioxane				C	9.318843	6.931582	7.799837
C	6.987476	7.340744	3.542948	C	-0.619617	0.681214	-0.047224	H	10.141069	6.427171	6.291191
H	6.137359	6.839593	3.086286	C	0.173997	0.733367	1.283254	C	7.419808	2.197981	4.818579
C	9.556126	7.549424	3.412242	H	0.217831	1.767204	1.638707	H	7.091586	1.410295	5.500604
H	9.917656	8.232862	2.632493	H	-0.350141	0.142075	2.039993	H	6.957111	1.990121	3.854942
H	10.231581	6.686897	3.369796	H	1.199304	0.353870	1.196375	C	4.158962	4.967595	5.303267
C	6.641565	8.231945	4.710869	C	-0.654109	-0.790285	-0.533320	H	4.171914	4.967788	6.395673
H	5.592302	8.525101	4.619560	H	-1.185720	-1.402139	0.201400	H	4.636795	5.899413	4.987097
H	7.209637	9.160043	4.683928	H	-1.205124	-0.847456	-1.476700	C	6.878632	7.700178	6.132459
				H	0.341920	-1.222476	-0.687822	H	6.964320	8.625378	6.721674
17				C	0.144601	1.522054	-1.101643	H	5.993091	7.182963	6.509124
KCN_dioxane				H	-0.398900	1.492860	-2.050780	C	9.717105	8.047875	4.848093
K	-7.545266	1.945156	-3.115234	H	0.186575	2.564725	-0.772569	H	10.774760	8.283271	4.996600
O	-8.380393	0.894104	-0.733845	H	1.169410	1.174094	-1.279252	H	9.174249	8.959492	5.106373
C	-8.883961	-0.446908	-0.586117	O	-1.887383	1.162093	0.127789	C	5.408268	2.606934	9.253511
C	-8.714593	1.690325	0.420038	K	-4.073752	2.065315	0.453755	H	5.011983	3.572314	9.590023
H	-8.555608	-1.012767	-1.459772	O	-6.805914	1.778852	0.223391	H	4.691312	1.845496	9.575264
H	-9.980092	-0.422013	-0.571759	C	-7.650245	1.417788	1.331152	C	3.443115	3.735592	2.721665
C	-8.354365	-1.077395	0.688483	C	-7.415247	1.395844	-1.02				

C	10.958337	2.606935	0.240097	H	1.934401	5.065115	2.190980	H	5.765858	3.749665	2.895784
H	11.354624	3.572312	-0.096418	H	3.370990	5.969683	2.651228	C	6.034893	2.402011	7.863545
H	11.675292	1.845493	-0.081655	P	9.475777	3.601078	4.247343	H	5.033663	2.505579	7.440029
C	12.923491	3.735612	6.771944	C	11.114005	3.661157	5.161450	H	6.432871	1.446184	7.506816
H	12.940458	3.744864	7.865882	H	11.618326	2.700043	5.007819	C	7.486352	2.147942	4.808767
H	13.401019	2.799588	6.458144	C	9.951532	3.478181	2.437452	H	7.038566	1.339148	5.388205
C	8.556016	3.374923	0.077828	H	10.417462	4.448708	2.236168	H	7.016224	2.129336	3.824701
H	7.576251	3.155958	-0.357250	C	8.688093	3.394012	1.566710	C	4.469482	5.016366	5.875801
H	8.832585	4.380452	-0.260115	H	8.166049	2.453168	1.773973	H	4.443249	4.673581	6.911444
C	13.657239	4.950109	4.687814	H	8.002525	4.200582	1.836651	H	4.958085	5.991324	5.877880
H	14.167088	4.066387	4.285710	C	10.856801	3.852166	6.666586	C	5.951405	2.361894	9.395662
H	14.191567	5.823434	4.302047	H	10.263527	4.763154	6.802040	H	5.461615	3.276095	9.749705
C	9.596784	2.366736	-0.418011	H	10.257378	3.030602	7.063755	H	5.320747	1.525422	9.709836
H	9.688525	2.415162	-1.506983	C	10.954619	2.380052	2.061568	C	3.802633	4.639871	3.015925
H	9.255254	1.352822	-0.176478	H	11.866690	2.467458	2.656535	H	3.820048	4.985335	1.978366
C	13.722023	4.917291	6.216487	H	10.525415	1.397498	2.283849	H	3.301574	3.664214	3.014724
H	14.761410	4.866858	6.553662	C	8.830777	1.885107	4.692154	C	8.267532	3.370706	9.551876
H	13.306452	5.850958	6.613823	H	9.281611	1.123580	4.053202	H	9.268721	3.244375	9.973064
C	8.298455	6.797007	3.116711	H	9.179175	1.688552	5.706835	H	7.892828	4.334411	9.914664
H	8.359096	6.217943	2.200731	C	12.012158	4.790082	4.631182	C	3.035188	5.171899	5.356343
C	7.047767	6.931587	3.693782	H	12.240884	4.638851	3.574056	H	2.504934	4.216550	5.454887
H	6.225540	6.427181	3.202424	H	11.468822	5.736777	4.704926	H	2.502019	5.894108	5.980562
C	9.487980	7.700180	3.361163	C	11.300859	2.440733	0.567067	C	7.339836	2.250760	10.033036
H	9.402293	8.625382	2.771950	H	11.828497	3.379320	0.360584	H	7.257465	2.269013	11.123156
H	10.373520	7.182966	2.984495	H	11.990667	1.630836	0.312165	H	7.779455	1.281627	9.767794
C	6.649507	8.047878	4.645529	C	12.162325	3.964485	7.461074	C	3.011288	5.613741	3.891592
H	5.591852	8.283275	4.497023	H	11.935318	4.133778	8.517692	H	1.980618	5.693692	3.534560
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				H	8.124133	3.352732	-0.522480	C	11.597342	3.319260	4.744394
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				H	13.910706	3.986303	5.274036	H	10.535484	4.447280	2.096971
				H	13.915814	5.727972	5.037424	C	8.510581	3.895309	1.709365
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				H	10.313141	2.450066	-1.363214	H	8.101049	4.794754	2.175219
				H	9.578500	1.380747	-0.178963	C	11.682677	3.591458	6.257750
				C	13.053248	5.085076	6.920473	H	11.378169	4.626474	6.442476
				H	13.996146	5.123021	7.473612	H	10.984364	2.955115	6.805326
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				C	10.136596	7.681534	3.193253	C	9.000621	1.967339	4.675445
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				C	11.006567	8.690665	2.798117	H	9.437768	1.693681	5.636926
				H	10.205622	6.691201	2.762364	C	12.620325	4.180630	3.984385
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				H	11.595788	10.741462	3.071858	C	13.102791	3.374115	6.790798
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I3_S

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99			
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H	8.738461	1.342667	7.790015
H	9.061890	3.017228	7.384689
C	5.030760	2.424334	3.509745
H	5.669657	3.205882	3.082954
H	5.405139	1.474859	3.120353
C	5.985812	1.607529	8.156798
H	4.966084	1.729283	7.784528
H	6.253145	0.556336	8.003556
C	7.364599	0.520694	5.202805
H	7.001268	-0.102208	6.023496
H	6.792287	0.238667	4.317780
C	4.568140	3.783002	5.584172
H	4.599193	3.799748	6.675364
H	5.189391	4.618982	5.245705
C	6.026183	1.917565	9.660387
H	5.653616	2.935918	9.822644
H	5.350433	1.246639	10.199531
C	3.585682	2.637152	3.046698
H	3.543178	2.626081	1.953326
H	2.965372	1.801953	3.393902
C	8.427616	2.684693	9.242031
H	9.444222	2.553736	9.825137
H	8.166662	3.738849	9.592379
C	3.125516	4.001080	5.114845
H	2.482066	3.226435	5.549446
H	2.758966	4.960869	5.491593
C	7.446277	1.805546	10.224042
H	7.455324	2.073890	11.284591
H	7.775081	0.761049	10.161965
C	3.014004	3.948861	3.589652
H	1.972225	4.070144	3.278183
H	3.572967	4.788527	3.159754
P	9.698712	1.699304	4.014301
C	11.498300	1.434597	4.515001
H	11.716361	0.360666	4.484854
C	9.653309	1.132271	2.217689
H	10.258076	1.889768	1.707089
C	8.222978	1.255066	1.668282
H	7.573487	0.540481	2.185281
H	7.829910	2.250405	1.890616

C	11.697656	1.941110	5.954243
H	11.369053	2.986179	5.997911
H	11.059157	1.390339	6.648425
C	10.241109	-0.248302	1.899074
H	11.270498	-0.325284	2.257421
H	9.667997	-1.021614	2.421208
C	8.863395	0.276643	4.957777
H	9.021449	-0.676301	4.448357
H	9.387581	0.209069	5.912230
C	12.452457	2.166197	3.559020
H	12.364198	1.766498	2.546599
H	12.153491	3.219921	3.506655
C	10.194054	-0.535337	0.391193
H	10.851693	0.172010	-0.127822
H	10.588053	-1.536031	0.188984
C	13.157594	1.842950	6.408760
H	13.257432	2.243857	7.422117
H	13.452366	0.787819	6.458187
C	8.173522	0.969755	0.164059
H	7.141443	1.029512	-0.194470
H	8.736109	1.746964	-0.366425
C	13.913370	2.073575	4.015894
H	14.241869	1.028648	3.962070
H	14.551470	2.637750	3.328893
C	8.772455	-0.401579	-0.163783
H	8.770039	-0.570559	-1.244645
H	8.141282	-1.182687	0.277391
C	14.091652	2.582237	5.448107
H	15.132736	2.471450	5.765465
H	13.863978	3.654457	5.479935
Ni	8.552495	3.449910	4.509864
S	8.622714	5.576354	4.281317
C	10.279903	6.388996	4.548022
H	10.640056	6.094745	5.535187
H	10.915923	5.901442	3.807384
C	10.275776	7.901006	4.382545
H	9.571328	8.342085	5.092825
H	9.912707	8.153488	3.382069
C	11.666587	8.498601	4.601232
H	12.390396	8.091355	3.889777
H	11.652498	9.584251	4.476995
H	12.034597	8.284579	5.608544
C	7.701710	6.347439	5.646741
C	6.584585	7.129479	5.363145
C	8.038661	6.080356	6.974843
C	5.799166	7.627748	6.400445
H	6.323728	7.337977	4.332848
C	7.264925	6.594911	8.006944
H	8.890432	5.449549	7.195109
C	6.136516	7.363864	7.723372
H	4.925179	8.225851	6.170724
H	7.531336	6.381013	9.035410
H	5.526461	7.752726	8.529601

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I7_S

P	7.262474	2.888762	5.310374
C	5.428271	3.210722	4.959483
H	4.849305	2.325057	5.245781
C	7.252595	2.592437	7.180971
H	7.031008	3.585691	7.585320
C	8.666642	2.226128	7.657447
H	8.945740	1.249552	7.246389
H	9.382419	2.950105	7.260523
C	5.234002	3.465132	3.457029
H	5.905713	4.276064	3.164982
H	5.537177	2.592883	2.873639

C	6.216955	1.612053	7.745609
H	5.206146	1.897370	7.444419
H	6.394739	0.610816	7.338869
C	7.427106	1.130437	4.607353
H	6.995333	0.392498	5.287056
H	6.821511	1.108879	3.699961
C	4.929432	4.421071	5.763055
H	5.007478	4.232614	6.835683
H	5.585962	5.271224	5.550137
C	6.294902	1.543120	9.278049
H	6.006840	2.516312	9.693110
H	5.571431	0.814490	9.657523
C	3.792493	3.845069	3.102383
H	3.717323	4.055074	2.030506
H	3.132219	2.992620	3.301406
C	8.746258	2.158863	9.185720
H	9.753071	1.862242	9.495740
H	8.574132	3.160554	9.596503
C	3.485012	4.798280	5.415015
H	2.814761	3.985980	5.720897
H	3.185121	5.682297	5.986125
C	7.706323	1.190128	9.757603
H	7.745553	1.188404	10.851146
H	7.949748	0.170559	9.433763
C	3.316006	5.051029	3.915265
H	2.273181	5.283760	3.680309
H	3.905366	5.931449	3.631443
P	9.855922	2.300991	3.665415
C	11.619873	1.693950	4.011623
H	11.698108	0.643697	3.707361
C	9.748195	2.102612	1.774514
H	10.445061	2.863923	1.396593
C	8.345551	2.496881	1.291341
H	7.627925	1.744717	1.634908
H	8.045871	3.436198	1.758237
C	11.902559	1.798140	5.519522
H	11.724519	2.833408	5.831291
H	11.199036	1.184916	6.086029
C	10.175142	0.771728	1.143944
H	11.183306	0.494324	1.460534
H	9.508163	-0.025526	1.486314
C	8.882191	0.781776	4.273243
H	8.936190	-0.036948	3.552280
H	9.398063	0.440567	5.171708
C	12.659675	2.513288	3.234062
H	12.503559	2.419297	2.155614
H	12.521725	3.570992	3.497630
C	10.115626	0.846756	-0.389582
H	10.864306	1.568443	-0.740039
H	10.389584	-0.119544	-0.823657
C	13.337205	1.388901	5.870883
H	13.503782	1.510325	6.945398
H	13.476192	0.323645	5.649694
C	8.279514	2.587518	-0.235145
H	7.264016	2.841184	-0.554613
H	8.925128	3.407952	-0.573441
C	14.098774	2.107693	3.576680
H	14.268490	1.076962	3.244054
H	14.805612	2.735218	3.024029
C	8.730795	1.275790	-0.886924
H	8.732532	1.369780	-1.976956
H	8.005636	0.490648	-0.642256
C	14.363311	2.204769	5.080992
H	15.379134	1.869928	5.310743
H	14.299244	3.254745	5.389663
Ni	8.955916	4.004503	4.567558
S	9.578606	6.115640	4.870057

C	8.157403	7.114051	5.542057
K	10.735199	5.660549	2.049189
H	8.434223	8.172093	5.502738
H	7.294689	6.975694	4.884538
C	7.780663	6.724149	6.965243
O	8.418289	6.227467	0.789252
H	7.587276	5.649263	6.979122
H	8.641163	6.889985	7.620343
C	6.565050	7.486443	7.494659
C	7.312365	6.099514	1.709869
C	7.984943	6.817442	-0.441019
H	6.748620	8.564965	7.517780
H	5.685432	7.317461	6.866833
H	6.308684	7.173601	8.511083
H	7.715094	5.681942	2.636582
H	6.579187	5.406582	1.283347
C	6.677907	7.451351	1.956683
C	7.335728	8.166889	-0.183085
H	7.275852	6.144128	-0.938747
H	8.866324	6.928275	-1.075959
H	5.793075	7.344966	2.584451
H	7.392830	8.110944	2.465671
O	6.246703	8.047483	0.727090
H	8.085199	8.866709	0.214615
H	6.934792	8.578294	-1.111125

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KSPr

S	8.835808	7.012328	3.940571
C	9.738020	8.626919	3.736509
H	9.076234	9.460176	3.999166
H	10.587088	8.665821	4.428145
C	10.255339	8.844617	2.315134
H	10.908267	8.008764	2.046639
H	9.409128	8.807970	1.622548
C	11.006935	10.168034	2.151524
H	10.364168	11.021945	2.388087
H	11.875784	10.216120	2.815569
H	11.367321	10.300820	1.127309
K	7.844449	7.081520	6.816181
O	6.945458	7.220107	9.402439
C	7.689862	6.765612	10.548408
C	5.616711	7.618514	9.789602
H	8.697505	6.524951	10.204700
H	7.223471	5.855786	10.944871
C	7.730738	7.843162	11.615795
C	5.675591	8.688226	10.864140
H	5.069646	6.741899	10.156409
H	5.118951	7.995943	8.894666
H	8.227937	7.470421	12.512150
H	8.285555	8.715391	11.242626
O	6.411087	8.228667	11.996986
H	6.137901	9.598819	10.457694
H	4.670595	8.931786	11.211188

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OATS_S

Ni	8.634502	5.257137	4.973753
P	7.018643	3.802550	5.543765
C	5.251211	4.079174	4.996076
H	4.709285	3.135451	5.128000
C	6.926357	3.549298	7.392968
H	6.575019	4.522400	7.752599
C	8.328815	3.329128	7.982850
H	8.737510	2.383820	7.610676
H	9.003749	4.118052	7.642941
C	5.232940	4.458352	3.503679

H	5.857288	5.346129	3.362980	C	7.925969	6.960875	5.570880	H	3.267111	17.278230	4.607756
H	5.675455	3.664922	2.897421	C	7.845648	7.246261	6.946869	C	0.087777	17.497002	2.924104
C	5.951441	2.467366	7.875451	C	7.117399	7.723791	4.707602	H	-0.411897	18.109260	3.677480
H	4.948300	2.643178	7.480629	C	6.990293	8.226540	7.433596	H	1.155086	17.506721	3.159702
H	6.272806	1.489998	7.499271	H	8.469370	6.691900	7.638742	C	1.253380	11.919894	9.758997
C	7.467804	2.136262	4.807206	C	6.263523	8.705176	5.193985	H	2.298620	11.589886	9.760730
H	7.056828	1.323226	5.408197	H	7.173118	7.547832	3.639645	H	1.164337	12.682720	10.538223
H	6.970003	2.094274	3.837663	C	6.188481	8.961155	6.561688	C	-0.654785	16.455495	5.911153
C	4.568718	5.172144	5.839256	H	6.947740	8.418906	8.500260	H	0.019944	17.305110	5.755712
H	4.521013	4.874731	6.888160	H	5.651396	9.273396	4.502050	C	-0.394053	15.925723	7.329792
H	5.166146	6.086449	5.797059	H	5.524535	9.728496	6.941104	H	-1.036933	15.059022	7.517030
C	5.905827	2.417796	9.408914	C	9.656908	6.762741	4.902219	H	0.635074	15.569348	7.408176
H	5.484639	3.357912	9.783220	N	10.479412	7.592124	4.801693	C	4.170693	14.549835	2.021481
H	5.232054	1.620003	9.734402					H	4.434463	13.782635	1.301343
C	3.813659	4.755494	3.009184	22				C	0.082127	10.278979	7.588389
H	3.846974	5.050594	1.956459	PhSPr				H	-0.962821	10.608551	7.579255
H	3.211940	3.840078	3.060702	C	8.884716	7.432865	6.084810	H	0.176567	9.509433	6.818284
C	8.281294	3.282016	9.513167	C	8.724910	6.349969	6.959492	C	2.321227	10.226912	4.489790
H	9.282790	3.094374	9.910450	C	8.348460	8.673881	6.436152	H	3.083601	11.007041	4.385800
H	7.971671	4.263386	9.890197	C	8.044119	6.509899	8.157830	H	2.458729	9.787194	5.480387
C	3.152686	5.470641	5.333365	H	9.135536	5.380763	6.700543	C	0.405362	9.675017	8.962238
H	2.519792	4.587338	5.483301	C	7.667516	8.823187	7.642375	H	-0.282906	8.852545	9.178964
H	2.716973	6.275589	5.931681	H	8.451460	9.529640	5.784579	H	1.412336	9.242449	8.932518
C	7.300664	2.214723	10.008587	C	7.510597	7.748553	8.508689	C	-2.098423	16.958938	5.783729
H	7.247905	2.225378	11.100761	H	7.930915	5.661064	8.821731	H	-2.288897	17.354329	4.783354
H	7.673665	1.223942	9.721899	H	7.258226	9.793012	7.900096	H	-2.790428	16.122801	5.928752
C	3.148892	5.847293	3.850409	H	6.980545	7.871493	9.444910	C	2.547836	9.154632	3.418083
H	2.126320	6.024132	3.505117	S	9.779875	7.109014	4.568906	H	3.560720	8.752003	3.510318
H	3.696425	6.787075	3.717927	C	9.809709	8.740900	3.716770	H	1.859989	8.318385	3.591788
P	9.831381	3.572162	4.124297	H	8.782672	9.065184	3.539236	C	0.343851	10.728098	10.072934
C	11.599035	3.344635	4.690356	H	10.299669	9.468357	4.366646	H	-0.689234	11.082424	10.174834
H	11.910351	2.332347	4.406867	C	10.562851	8.617988	2.394110	H	0.617893	10.281436	11.033048
C	9.898770	3.550517	2.255983	H	11.580520	8.264765	2.582706	C	0.228229	15.214285	1.854116
H	10.465617	4.457806	2.022244	H	10.077980	7.866823	1.764252	H	1.301466	15.138943	2.049604
C	8.491829	3.728001	1.662445	C	10.611163	9.955359	1.655099	H	-0.159153	14.192491	1.860954
H	7.874931	2.860381	1.920353	H	9.605721	10.319797	1.427893	C	0.680428	11.394136	2.952278
H	8.010982	4.603256	2.105976	H	11.117439	10.719746	2.250681	H	-0.341028	11.770699	2.864158
C	11.673899	3.477445	6.222471	H	11.150786	9.858863	0.710337	H	1.344648	12.244909	2.766414
H	11.275753	4.457212	6.505687	99				C	-2.398830	18.035167	6.837151
H	11.044464	2.728571	6.708372	RETS_S				H	-1.776715	18.915134	6.635597
C	10.615308	2.348847	1.625484	Ni	1.840652	14.195804	5.126096	H	-3.439660	18.361134	6.751116
H	11.627478	2.248066	2.023454	S	3.768963	14.533031	6.222578	C	3.595140	16.193550	7.024173
H	10.081975	1.426593	1.880314	P	0.766454	12.288371	5.605608	H	4.457550	16.806648	6.750414
C	8.986865	1.970723	4.629391	P	-0.064808	15.214118	4.624910	H	2.695080	16.660485	6.624752
H	9.208368	1.176667	3.914343	C	3.413047	15.141454	4.270768	C	-0.685395	16.997413	8.384077
H	9.443752	1.677826	5.575437	C	3.821346	14.174543	3.313696	H	-0.516217	16.593015	9.386386
C	12.532559	4.368040	4.018945	H	3.868926	13.129687	3.595803	H	0.022025	17.825008	8.256690
H	12.527277	4.241259	2.934616	C	-1.073151	12.695926	5.561509	C	0.918960	10.316440	1.889487
H	12.163009	5.377387	4.222861	H	-1.654518	11.813286	5.284149	H	0.171509	9.521825	2.001920
C	10.668302	2.483495	0.097335	H	-1.351915	12.951988	6.584754	H	0.773381	10.746067	0.893979
H	11.291888	3.346289	-0.163081	C	0.995281	11.472393	7.278100	C	-2.115929	17.530728	8.256057
H	11.152900	1.603509	-0.335316	H	2.031614	11.118229	7.243143	H	-2.820558	16.725479	8.496659
C	13.113102	3.348390	6.732768	C	0.923388	12.529116	8.392879	H	-2.291896	18.328365	8.983480
H	13.128791	3.478160	7.818753	H	-0.084564	12.956193	8.432581	C	0.007037	15.841552	0.474109
H	13.480344	2.334769	6.530940	H	1.604687	13.349246	8.159053	H	0.511308	15.239030	-0.287100
C	8.547390	3.860403	0.137133	C	4.222566	15.892536	1.659196	H	-1.062805	15.826704	0.231887
H	7.534109	3.951041	-0.264647	C	0.931182	10.874013	4.378371	C	-0.127219	18.122403	1.539956
H	9.072779	4.786599	-0.121176	H	0.169083	10.123819	4.616236	H	-1.203655	18.210055	1.347893
C	13.970120	4.237405	4.536112	C	3.921146	16.860609	2.623695	H	0.276156	19.139537	1.530405
H	14.376236	3.263084	4.237067	H	3.965504	17.912477	2.361616	C	0.516530	17.283921	0.433036
H	14.596401	4.998487	4.062750	C	-0.420342	16.047478	2.975580	H	1.603026	17.279912	0.570663
C	9.270983	2.670924	-0.501215	H	-1.507505	16.050878	2.830616	H	0.319428	17.731411	-0.545677
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TMTS_S

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H	9.896647	9.118145	0.403792	C	9.699888	3.706520	5.230408	H	9.037409	3.582660	-3.212671
C	11.575324	5.388734	-2.933532	H	10.257447	2.932080	4.693784	C	15.164205	5.316679	2.706729
H	11.310333	6.334937	-3.413993	H	10.158562	4.662284	4.966804	H	16.229816	5.135239	2.873510
H	12.594253	5.140551	-3.245061	C	5.879034	4.774194	1.296324	H	14.938557	6.301918	3.129545
C	11.861677	9.217392	3.078749	H	6.213281	5.810570	1.255748	C	8.082514	7.048108	3.628613
H	11.680580	9.554446	4.103304	H	6.431737	4.246667	0.516527	C	8.179768	7.164907	5.021839
H	12.895075	8.852662	3.045515	C	7.581190	2.336616	5.144408	C	7.073917	7.792672	2.998438
C	9.175062	4.608697	-2.914015	H	6.532941	2.310236	4.840873	C	7.318592	7.981454	5.752802
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H	8.827136	5.535118	-3.381331	C	8.617099	2.782747	1.957915	C	6.210913	8.615702	3.720823
C	11.879490	9.911325	0.651712	H	8.349786	1.839299	2.436332	H	6.931823	7.720702	1.925916
H	12.913322	9.584517	0.491458	H	8.048431	2.839134	1.029532	C	6.326826	8.713143	5.104805
H	11.698017	10.733303	-0.043011	C	5.340774	4.838444	3.782972	H	7.425188	8.048792	6.830569
C	10.596495	4.307127	-3.398296	H	5.512046	4.350442	4.744433	H	5.440345	9.175776	3.203449
H	10.613737	4.234654	-4.488846	H	5.635557	5.880489	3.900917	H	5.654497	9.349594	5.667928
H	10.912232	3.329700	-3.010216	C	7.692877	2.072838	6.652573	C	5.491812	7.471840	-1.249815
C	11.706025	10.382257	2.097133	H	7.107480	2.827526	7.189969	N	6.512180	7.735196	-0.743877
H	12.424992	11.172555	2.331518	H	7.250036	1.101917	6.892149	K	8.903426	8.784047	-0.134970
H	10.706688	10.817601	2.215599	C	8.42568	4.725211	0.977054	O	7.764865	11.329949	-0.095424
C	5.906052	6.292388	2.193118	H	4.211939	5.212773	0.014977	C	10.192391	9.366775	3.473294
C	5.537056	6.590395	3.510478	H	4.062997	3.680052	0.876176	C	6.382037	11.264267	-0.506024
C	4.872533	6.016294	1.287650	C	9.816504	3.447034	6.735696	C	7.914178	12.245031	1.000757
C	4.203928	6.568046	3.919886	H	10.869325	3.444435	7.031827	H	9.119015	9.469519	3.328639
H	6.299637	6.842885	4.239120	H	9.338671	4.271294	7.277270	H	10.354341	9.133446	4.524797
C	3.538849	5.986540	1.687895	C	3.847264	4.777838	3.439497	C	10.927162	10.642497	3.083311
H	5.109676	5.823231	0.247260	H	3.515064	3.731950	3.436736	H	6.316772	10.528580	-1.306571
C	3.197866	6.252350	3.011935	H	3.277760	5.286617	4.222690	H	6.077380	12.246477	-0.887428
H	3.952430	6.797802	4.949993	C	9.147984	2.125885	7.128128	C	5.507717	10.850304	0.660407
H	2.763623	5.760062	0.963624	H	9.197309	1.982128	8.211019	C	7.029991	11.828652	2.162817
H	2.161206	6.229615	3.326879	H	9.703195	1.295285	6.675606	H	7.651051	13.256892	0.667447
C	7.462680	7.953757	0.823327	C	3.558480	5.402582	2.072746	H	8.966521	12.233935	1.287647
N	7.276168	8.983865	0.315747	H	2.491517	5.335787	1.841552	H	12.006499	10.497609	3.186175
K	8.363975	10.329293	-1.817270	H	3.810578	6.468103	2.099605	H	10.752547	10.862110	2.024007
Se	10.392213	9.074685	-4.067397	P	10.667957	4.621331	1.378283	C	10.486165	11.835289	3.934674
O	10.141925	12.414880	-1.422626	C	12.519330	4.469708	1.655129	H	4.456051	10.871421	0.373650
C	12.149964	9.337676	-3.143331	H	12.790280	3.491832	1.238801	H	5.759788	9.828399	0.962253
C	10.171701	13.440628	-0.421876	C	10.475371	4.925769	-0.456894	O	5.663032	11.752901	1.762695
C	10.876044	12.814339	-2.598140	H	10.968870	5.896379	-0.588819	H	7.360593	10.858248	2.554298
H	12.007928	10.009621	-2.294815	C	8.998619	5.091968	-0.849228	H	7.085971	12.562513	2.968231
H	12.462266	8.371866	-2.738290	H	8.482662	4.135309	-0.725328	H	9.407980	11.998078	3.863754
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H	9.659704	13.045277	0.457258	C	12.828223	4.458194	3.163397	H	10.987641	12.755208	3.622236
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C	11.601489	13.825131	-0.080884	H	12.259657	3.675070	3.669263				
C	12.297301	13.186292	-2.228856	C	11.158320	3.906788	-1.381532	99			
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H	10.851050	11.968466	-3.287888	H	10.682646	2.928731	-1.254874	P	7.062558	3.821924	5.430275
H	13.357124	9.224399	-4.916089	C	10.114821	2.858594	1.670578	C	5.246373	3.965939	4.977155
H	12.933291	10.854972	-4.451907	H	10.390500	2.229608	0.822732	H	4.823797	2.977039	5.194189
C	14.589409	10.027172	-3.331478	H	10.687592	2.502667	2.527761	C	7.075752	3.742408	7.299343
H	11.608870	14.670374	0.609317	C	13.359257	5.543635	0.942802	H	6.648767	4.709760	7.579037
H	12.111787	12.979797	0.399454	H	13.177098	5.531549	-0.133066	C	8.509107	3.700720	7.851401
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H	12.825870	12.304815	-1.844743	C	11.026853	4.332259	-2.850858	H	9.111078	4.489225	7.394582
H	12.832504	13.560456	-3.101906	H	11.582896	5.265134	-3.002145	C	5.095529	4.231339	3.468589
H	14.512817	10.694468	-2.467735	H	11.493719	3.581999	-3.495364	H	5.586612	5.176004	3.227192
H	14.945787	9.059011	-2.966916	C	14.324768	4.258859	3.426866	H	5.602497	3.458729	2.886994
H	15.358547	10.433925	-3.994267	H	14.514030	4.290174	4.503650	C	6.220362	2.635061	7.930101
				H	14.625450	3.261621	3.083030	H	5.195664	2.665939	7.553986
116				C	8.863823	5.529655	-2.310106	H	6.627744	1.655339	7.658958
I4_Se				H	7.808621	5.641042	-2.563304	C	7.440978	2.085962	4.830763
Ni	9.328298	5.979511	2.622027	H	9.316438	6.521981	-2.437808	H	7.007585	1.347306	5.506992
P	8.035107	4.222927	3.004845	C	14.855401	5.333279	1.207785	H	6.924673	1.980357	3.875955
C	6.189236	4.179473	2.681510	H	15.172926	4.382960	0.761280	C	4.471153	5.009577	5.799725
H	5.943554	3.110243	2.658541	H	15.428023	6.120866	0.709846	H	4.527925	4.780332	6.864923
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H	5.627098	1.951003	9.897533	H	8.978136	8.817506	3.641534	H	9.401394	0.194796	5.908960
C	3.622132	4.301724	3.052687	H	9.539643	8.628558	5.296970	C	12.446267	2.127190	3.501332
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H	9.535105	3.771263	9.754544	C	10.677167	10.941672	4.237907	H	10.817026	0.079053	-0.143358
H	8.131357	4.821281	9.652442	H	9.832038	11.276494	3.629801	H	10.547830	-1.623969	0.195050
C	2.999470	5.066369	5.372239	H	10.405393	11.088438	5.287074	C	13.175840	1.858898	6.350833
H	2.511818	4.113364	5.612070	H	11.525406	11.596243	4.018552	H	13.280509	2.277764	7.356370
H	2.484388	5.837659	5.951457	Se	10.307099	6.649715	3.885884	H	13.478950	0.806964	6.415739
C	7.638253	2.753374	10.030830					C	8.144774	0.892830	0.157595
H	7.610426	2.893228	11.115026	99				H	7.110587	0.953336	-0.194576
H	8.090212	1.769884	9.853588	I6_Se				H	8.707454	1.660919	-0.385855
C	2.857798	5.342627	3.873801	P	6.998687	2.327902	5.495619	C	13.911118	2.053159	3.948792
H	1.802490	5.352746	3.586410	C	5.176723	2.459044	5.043081	H	14.246959	1.009853	3.911119
H	3.256857	6.338977	3.654265	H	4.632924	1.618350	5.489282	H	14.539629	2.609545	3.246805
P	9.781123	3.393471	3.961559	C	6.994394	2.513102	7.367824	C	8.734937	-0.485211	-0.157935
C	11.567558	3.072929	4.447912	H	6.688569	3.555520	7.503323	H	8.724012	-0.666982	-1.236639
H	11.701689	1.987774	4.358212	C	8.425028	2.393226	7.915195	H	8.103288	-1.258011	0.296970
C	9.735597	3.233691	2.100340	H	8.785161	1.368437	7.774183	C	14.096443	2.588699	5.370219
H	10.410015	4.035715	1.781590	H	9.093472	3.038446	7.339234	H	15.140791	2.491782	5.681266
C	8.342578	3.574508	1.546765	C	5.030096	2.391662	3.513108	H	13.860188	3.659392	5.384970
H	7.623216	2.815836	1.873080	H	5.673178	3.161925	3.072236	Ni	8.554364	3.412105	4.463030
H	8.008362	4.530895	1.954698	H	5.392817	1.433880	3.133000	C	10.355345	6.456016	4.606362
C	11.780120	3.472032	5.919675	C	6.032639	1.622858	8.163947	H	10.610701	6.090541	5.601258
H	11.579057	4.542549	6.020219	H	5.008913	1.733814	7.799169	H	11.042903	5.998140	3.893660
H	11.067459	2.956019	6.566626	H	6.303827	0.570580	8.025711	C	10.377120	7.973813	4.535150
C	10.236190	1.901580	1.526662	C	7.373697	0.496305	5.207622	H	9.614530	8.380372	5.205114
H	11.229814	1.656219	1.908152	H	7.014524	-0.117465	6.036966	H	10.108397	8.293977	3.524257
H	9.568314	1.093514	1.844396	H	6.796126	0.205545	4.328816	C	11.746614	8.541876	4.914642
C	8.942179	1.866400	4.649456	C	4.594770	3.779836	5.574832	H	12.529068	8.170404	4.247015
H	9.145823	1.000215	4.017768	H	4.632594	3.807801	6.665517	H	11.749926	9.633445	4.857210
H	9.416226	1.672484	5.612548	H	5.221289	4.606700	5.223517	H	12.020579	8.261929	5.935654
C	12.607205	3.762464	3.548474	C	6.085937	1.958576	9.661598	C	7.577477	6.439108	5.605721
H	12.491515	3.449966	2.509406	H	5.709526	2.977602	9.810116	C	6.488307	7.259125	5.324558
H	12.450737	4.842967	3.574766	H	5.419081	1.293483	10.218673	C	7.868767	6.104284	6.927848
C	10.259842	1.946142	-0.007496	C	3.583828	2.612760	3.057927	C	5.684480	7.731803	6.360914
H	10.996263	2.690440	-0.331098	H	3.533411	2.588530	1.965120	H	6.260383	7.521787	4.298442
H	10.593070	0.981645	-0.401717	H	2.958026	1.787986	3.419877	C	7.078365	6.593906	7.960892
C	13.208549	3.168973	6.384761	C	8.481038	2.734903	9.407328	H	8.696720	5.441354	7.145599
H	13.333605	3.498123	7.420318	H	9.501962	2.615819	9.782571	C	5.977829	7.402506	7.679670
H	13.372049	2.084259	6.377662	H	8.216077	3.790053	9.543339	H	4.831284	8.360521	6.134064
C	8.360481	3.619371	0.015653	C	3.151251	4.005822	5.112356	H	7.309917	6.329991	8.986346
H	7.356186	3.832841	-0.361254	H	2.503213	3.242688	5.560354	H	5.354216	7.771534	8.484991
H	8.999721	4.449077	-0.305369	H	2.797125	4.973635	5.480106	Se	8.591429	5.631617	4.126652
C	14.033349	3.448871	4.018224	C	7.512076	1.863492	10.213013				
H	14.228304	2.375645	3.899765	H	7.529945	2.149362	11.268832	103			
H	14.749765	3.970159	3.377132	H	7.846068	0.819916	10.164913	I7_Se			
C	8.885797	2.309488	-0.579783	C	3.029086	3.936649	3.588720	P	7.263452	2.885353	5.265927
H	8.937791	2.381452	-1.669768	H	1.986522	4.064627	3.282656	C	5.427955	3.203664	4.921329
H	8.178884	1.502117	-0.352584	H	3.593530	4.765454	3.145259	H	4.849497	2.340288	5.269186
C	14.244106	3.843281	5.481965	P	9.700280	1.657212	3.988190	C	7.261745	2.622204	7.141782
H	15.256769	3.583825	5.804155	C	11.504094	1.406767	4.477677	H	7.050247	3.623754	7.529340
H	14.148138	4.930401	5.576819	H	11.726510	0.333428	4.463336	C	8.675806	2.255493	7.618601
Ni	8.606825	5.212689	4.662768	C	9.639243	1.071560	2.198897	H	8.947377	1.269810	7.224582
C	7.505584	6.706734	5.223287	H	10.244173	1.820511	1.676164	H	9.393490	2.969174	7.206988
C	7.462207	7.148996	6.553224	C	8.205825	1.195626	1.657941	C	5.193859	3.372882	3.412608
C	6.718090	7.412839	4.300887	H	7.555877	0.491049	2.187733	H	5.852592	4.166675	3.051935
C	6.660039	8.218676	6.949515	H	7.820167	2.195904	1.871275	H	5.479246	2.468263	2.871222
H	8.074145	6.655266	7.300156	C	11.711693	1.938874	5.906570	C	6.220798	1.661115	7.729176
C	5.911955	8.481087	4.685001	H	11.376345	2.982322	5.934875	H	5.210713	1.951552	7.430453
H	6.747921	7.133007	3.253788	H	11.082602	1.395480	6.614998	H	6.385920	0.651092	7.338908
C	5.870786	8.886197	6.017394	C	10.218818	-0.315144	1.892474	C	7.428840	1.116039	4.593175
H	6.653261	8.531524	7.988611	H	11.250308	-0.392078	2.244851	H	6.993539	0.390987	5.284373
H	5.316644	9.001750	3.942044	H	9.645990	-1.079829	2.427453	H	6.827193	1.078633	3.684077
H	5.243830	9.716465	6.320859	C	8.871305	0.248254	4.956813	C	4.955008	4.460536	5.667509

H	5.067306	4.336608	6.746487	C	6.406949	7.422113	7.522402	C	10.612527	10.020625	1.615635
H	5.605299	5.294991	5.384649	C	7.324450	6.076409	1.765344	H	9.599207	10.372381	1.404110
C	6.307099	1.618851	9.262250	C	7.974553	6.838924	-0.376409	H	11.107822	10.777312	2.229981
H	6.028338	2.601466	9.661138	H	6.594941	8.490897	7.662020	H	11.148773	9.960325	0.665651
H	5.580087	0.902602	9.658118	H	5.599146	7.323651	6.791588	Se	9.842272	6.961370	4.529499
C	3.740588	3.730080	3.081621	H	6.041228	7.024043	8.473752				
H	3.631034	3.875920	2.002210	H	7.727795	5.617190	2.672015	99			
H	3.090148	2.889579	3.351335	H	6.562557	5.419635	1.332018	RETS_Se			
C	8.761280	2.216156	9.147383	C	6.737983	7.438443	2.067011	Ni	1.898717	14.146156	5.109368
H	9.767788	1.919659	9.458253	C	7.370914	8.198246	-0.064411	P	0.817182	12.259859	5.566747
H	8.597050	3.226449	9.539624	H	7.236418	6.201011	-0.878415	P	0.005399	15.216698	4.664537
C	3.500660	4.818908	5.342591	H	8.845633	6.943103	-1.026583	C	3.460728	15.050326	4.381373
H	2.840453	4.027842	5.717861	H	5.864897	7.339336	2.712108	C	3.813999	13.951063	3.557416
H	3.219128	5.736408	5.868403	H	7.484673	8.059981	2.578320	H	3.930095	12.962092	3.979800
C	7.718221	1.264427	9.741192	O	6.298045	8.082966	0.865234	C	-1.019712	12.684143	5.533929
H	7.762475	1.281462	10.834380	H	8.148576	8.863653	0.338134	H	-1.604811	11.812418	5.230984
H	7.953245	0.237718	9.434087	H	6.963767	8.649370	-0.971047	H	-1.298718	12.911081	6.563484
C	3.284746	4.981104	3.836258	Se	9.745640	6.115162	5.040939	C	1.018881	11.391548	7.220723
H	2.234135	5.196649	3.620457					H	2.056441	11.040188	7.194894
H	3.860347	5.844753	3.481706	26				C	0.917092	12.401100	8.376581
P	9.869832	2.257454	3.642404	KSePr				H	-0.094106	12.820448	8.412597
C	11.628983	1.640313	3.985843	C	9.475411	7.704802	5.046636	H	1.597314	13.234969	8.196995
H	11.694527	0.584336	3.698888	H	9.592570	7.733947	6.134337	C	4.141920	15.426816	1.667418
C	9.746149	2.059359	1.754895	H	10.478348	7.651844	4.618584	C	0.944342	10.863121	4.312785
H	10.455261	2.806720	1.372113	C	8.777640	8.976985	4.577375	H	0.145911	10.145197	4.529854
C	8.348474	2.478553	1.277954	H	8.639989	8.927202	3.493804	C	3.916790	16.526309	2.509268
H	7.617923	1.742754	1.629213	H	7.771954	9.017727	5.006825	H	3.971620	17.531576	2.105878
H	8.070084	3.425899	1.741454	C	9.552798	10.245828	4.942978	C	-0.368122	16.103052	3.045660
C	11.919310	1.768854	5.490721	H	9.695420	10.332098	6.024662	H	-1.457828	16.136952	2.926307
H	11.748188	2.810363	5.784917	H	10.544165	10.248868	4.480675	C	-1.331926	13.886236	4.631137
H	11.214485	1.169567	6.070556	H	9.028204	11.144957	4.607477	H	-2.307325	14.310395	4.877593
C	10.144738	0.718162	1.127676	K	8.772774	4.684135	7.408958	H	-1.387371	13.564338	3.590547
H	11.148881	0.422993	1.441025	O	7.570407	6.748291	8.701058	C	3.589989	16.350766	3.839943
H	9.464037	-0.064679	1.476350	C	7.511653	7.184287	10.066480	H	3.379745	17.215378	4.453484
C	8.884280	0.756725	4.270006	C	6.823551	7.643515	7.844216	C	0.172721	17.541367	3.023218
H	8.937418	-0.073839	3.562690	H	8.130964	6.501071	10.651584	H	-0.294314	18.142743	3.805718
H	9.395752	0.427891	5.175419	H	6.476976	7.119502	10.425800	H	1.244899	17.520445	3.234340
C	12.671428	2.435800	3.187383	C	8.018166	8.610194	10.193045	C	1.219731	11.736758	9.723813
H	12.510189	2.319611	2.111991	C	7.336200	9.061013	7.994789	H	2.265854	11.409439	9.735061
H	12.542490	3.499844	3.428692	H	5.762665	7.591176	8.116534	H	1.111791	12.467693	10.530697
C	10.078587	0.788758	-0.405699	H	6.951871	7.284571	6.820741	C	-0.578971	16.423727	5.988015
H	10.838357	1.495356	-0.762790	H	7.905087	8.963990	11.219165	H	0.113553	17.265959	5.874287
H	10.332477	-0.183944	-0.837475	H	9.083939	8.648381	9.924087	C	-0.349425	15.834456	7.388215
C	13.352851	1.357281	5.843281	O	7.270535	9.489840	9.359268	H	-1.013528	14.975357	7.531141
H	13.524340	1.498306	6.914543	H	8.370535	9.123852	7.635341	H	0.670424	15.453468	7.465890
H	13.484897	0.287222	5.641773	H	6.723616	9.750459	7.413768	C	4.093329	14.147771	2.202651
C	8.275637	2.563688	-0.248471	Se	8.504112	6.025783	4.520868	H	4.316647	13.289306	1.578364
H	7.263103	2.834907	-0.562817					C	0.101797	10.184720	7.465334
H	8.934050	3.370805	-0.594245	22				H	-0.943268	10.513500	7.448044
C	14.108873	2.027003	3.532959	PhSePr				H	0.212306	9.445543	6.668517
H	14.270258	0.988667	3.220289	C	8.869922	7.357988	6.154096	C	2.298080	10.144142	4.423263
H	14.817490	2.638495	2.964955	C	8.685202	6.302980	7.053826	H	3.102199	10.881623	4.329939
C	8.699027	1.241116	-0.897028	C	8.355076	8.617647	6.462421	H	2.408044	9.686123	5.408926
H	8.696239	1.330433	-1.987409	C	7.996225	6.508893	8.241995	C	0.396921	9.525352	8.819772
H	7.960871	0.470598	-0.644807	H	9.079632	5.318738	6.828048	H	-0.293612	8.693164	8.986737
C	14.380032	2.152345	5.033934	C	7.665791	8.814318	7.657179	H	1.405543	9.096216	8.794282
H	15.394958	1.816534	5.266118	H	8.480341	9.451941	5.786555	C	-2.010627	16.960951	5.861551
H	14.322493	3.208355	5.322418	C	7.482322	7.766294	8.551424	H	-2.180111	17.399329	4.875590
Ni	8.990349	3.969313	4.550721	H	7.861334	5.681861	8.929092	H	-2.721066	16.134018	5.964212
C	8.179278	7.185643	5.714943	H	7.271268	9.797911	7.884162	C	2.471457	9.073917	3.339374
K	10.767298	5.639395	2.009761	H	6.945807	7.924988	9.478648	H	3.460374	8.615203	3.430434
H	8.495142	8.229718	5.774990	C	9.846743	8.737024	3.647988	H	1.738176	8.274530	3.500264
H	7.391892	7.113891	4.962478	H	8.810051	9.037582	3.494670	C	0.308099	10.531330	9.970888
C	7.667601	6.689740	7.057832	H	10.327885	9.444405	4.323822	H	-0.728086	10.878645	10.065115
O	8.415459	6.199159	0.826661	C	10.592245	8.662591	2.318894	H	0.563453	10.046739	10.917741
H	7.466690	5.620292	6.969554	H	11.617790	8.322973	2.489823	C	0.232559	15.287090	1.886081
H	8.457112	6.792846	7.808264	H	10.117150	7.920975	1.670322	H	1.306974	15.175217	2.055181

H	-0.183978	14.277082	1.871164
C	0.729073	11.416648	2.893740
H	-0.271003	11.847054	2.807079
H	1.436085	12.234800	2.723205
C	-2.304705	18.001181	6.952283
H	-1.661197	18.874825	6.794652
H	-3.337022	18.352831	6.864095
C	3.463486	16.568294	7.039905
H	4.316856	17.142632	6.675828
H	2.561180	16.913005	6.536124
C	-0.636752	16.867778	8.481172
H	-0.493197	16.418261	9.468260
H	0.089016	17.684821	8.401750
C	0.915540	10.341677	1.817676
H	0.125513	9.587272	1.915404
H	0.799609	10.791187	0.827051
C	-2.054012	17.435565	8.353926
H	-2.778673	16.636442	8.551716
H	-2.224994	18.207392	9.109926
C	-0.001058	15.960297	0.529718
H	0.472609	15.368792	-0.259358
H	-1.075620	15.977715	0.309821
C	-0.058191	18.212097	1.663107
H	-1.136240	18.329226	1.498073
H	0.368057	19.219890	1.672967
C	0.540762	17.391425	0.518324
H	1.629828	17.359713	0.630108
H	0.332621	17.871351	-0.442549
C	2.278984	9.657979	1.938221
H	3.068983	10.392537	1.742405
H	2.381750	8.874918	1.181474
C	3.322382	16.697403	8.550823
H	2.457430	16.120357	8.888332
H	4.197448	16.263927	9.044320
C	3.167817	18.158257	8.978810
H	2.303571	18.622433	8.496328
H	3.028477	18.239849	10.059732
H	4.050996	18.744384	8.710729
H	4.384405	15.578968	0.623004
Se	3.723129	14.666083	6.494832

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Ni	8.820116	6.053544	2.074916
P	7.805979	4.202534	2.810940
C	5.994786	3.817672	2.492696
H	5.902007	2.736366	2.653635
C	7.995277	4.027162	4.666282
H	7.344122	4.816866	5.049384
C	9.424910	4.351933	5.124768
H	10.106849	3.573248	4.769503
H	9.760750	5.287365	4.673447
C	5.650016	4.117630	1.023210
H	5.843513	5.171646	0.816463
H	6.304184	3.555120	0.353814
C	7.534744	2.693291	5.271273
H	6.518956	2.445045	4.957440
H	8.182002	1.884038	4.917373
C	8.623765	2.677053	2.101786
H	8.460197	1.822580	2.760670
H	8.098135	2.465325	1.171464
C	5.021749	4.527541	3.449565
H	5.227423	4.250994	4.484953
H	5.159389	5.606323	3.379757
C	7.606361	2.747974	6.804161
H	6.889286	3.493176	7.167218
H	7.299674	1.785835	7.224683

C	4.187874	3.789160	0.705121
H	3.972826	4.058925	-0.332605
H	4.029551	2.706833	0.789406
C	9.504192	4.418726	6.652743
H	10.530951	4.630928	6.964558
H	8.888198	5.253692	7.006135
C	3.565065	4.185708	3.113834
H	3.389380	3.117705	3.293357
H	2.900107	4.731651	3.789397
C	9.011396	3.116227	7.291859
H	9.023271	3.198950	8.382317
H	9.703748	2.306622	7.031168
C	3.231875	4.512084	1.656305
H	2.195309	4.242885	1.432895
H	3.320176	5.593387	1.501442
P	10.420442	4.618363	1.134561
C	12.250961	4.824140	1.516790
H	12.702993	3.857285	1.263069
C	10.372700	4.327849	-0.724896
H	10.447675	5.339076	-1.136893
C	9.018751	3.746250	-1.167036
H	8.927651	2.721068	-0.790925
H	8.207287	4.337568	-0.748694
C	12.485419	5.077517	3.015561
H	12.007036	6.020207	3.287603
H	12.018861	4.298951	3.621871
C	11.504457	3.461115	-1.305439
H	12.488807	3.828251	-1.017440
H	11.422675	2.441253	-0.912573
C	10.110613	2.904432	1.835322
H	10.510056	2.145772	1.159485
H	10.678459	2.832717	2.762988
C	12.944341	5.918494	0.685690
H	12.795215	5.758282	-0.382878
H	12.487750	6.879891	0.924678
C	11.415270	3.414214	-2.838357
H	11.586219	4.423002	-3.231148
H	12.216274	2.782605	-3.234780
C	13.982165	5.148430	3.340659
H	14.117609	5.363028	4.405104
H	14.438605	4.167922	3.157420
C	8.910362	3.716554	-2.694276
H	7.943360	3.297062	-2.987565
H	8.931406	4.745673	-3.067472
C	14.444388	5.970349	0.998051
H	14.916061	5.027402	0.693547
H	14.915311	6.761604	0.407476
C	10.051855	2.909719	-3.318545
H	9.997608	2.949223	-4.410516
H	9.941950	1.855018	-3.036888
C	14.695428	6.202932	2.490506
H	15.768561	6.199803	2.703505
H	14.320755	7.195748	2.763152
C	7.450131	7.085653	3.009729
C	7.464379	7.349193	4.389328
C	6.347426	7.600953	2.302530
C	6.454383	8.070814	5.024783
H	8.284430	6.983648	4.993963
C	5.338381	8.336953	2.923624
H	6.265718	7.394522	1.242620
C	5.381352	8.574523	4.295602
H	6.511415	8.247128	6.093965
H	4.501034	8.700386	2.335440
H	4.596359	9.137009	4.786991
C	7.950194	6.749005	-0.477673
N	7.718697	7.622380	-1.220113
K	7.871898	9.839102	0.442083

Se	10.162916	7.971517	1.991347
O	8.031781	12.028578	2.113372
C	10.555446	8.384761	3.901180
C	6.956895	12.891331	2.514823
C	8.950241	11.819055	3.204350
H	9.694140	8.890693	4.333556
H	10.665675	7.434531	4.425424
C	11.817910	9.221311	4.065940
H	6.278671	12.975571	1.663466
H	7.356855	13.886717	2.745110
C	6.240820	12.320503	3.725603
C	8.217706	11.259213	4.408007
H	9.433982	12.771109	3.454136
H	9.704743	11.115665	2.851279
H	12.667397	8.685095	3.634437
H	11.725506	10.149934	3.493838
C	12.104049	9.547933	5.533211
H	5.471297	13.011889	4.073249
H	5.766244	13.365528	3.463096
O	7.152039	12.128159	4.805896
H	7.819294	10.265261	4.175730
H	8.892920	11.175223	5.260140
H	11.282386	10.113165	5.982892
H	12.234530	8.634891	6.121132
H	13.014295	10.144290	5.638989

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HTePr

C	9.855122	8.732169	3.663355
H	8.944210	9.328235	3.648066
H	10.558399	9.180332	4.363159
C	10.462714	8.621308	2.270274
H	11.345388	7.975167	2.298024
H	9.748827	8.149849	1.588282
C	10.857985	9.994760	1.723087
H	9.992022	10.659046	1.657673
H	11.601030	10.476903	2.363973
H	11.287641	9.908511	0.721956
H	8.685867	7.402288	5.856651
Te	9.317093	6.766997	4.469222

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I3_Te

Ni	8.884609	5.712983	1.414584
P	8.097265	4.051953	2.668456
C	6.267598	3.667059	2.546021
H	6.169907	2.625625	2.875258
C	8.466617	4.167815	4.493576
H	7.847187	5.009465	4.816488
C	9.933210	4.546653	4.749664
H	10.583661	3.736300	4.403721
H	10.211693	5.439461	4.186760
C	5.809715	3.758542	1.079093
H	5.983912	4.776853	0.722029
H	6.405646	3.098232	0.445817
C	8.068179	2.930759	5.313166
H	7.019586	2.671377	5.151201
H	8.661513	2.069048	4.990233
C	8.873372	2.456000	2.063239
H	8.855336	1.703424	2.852755
H	8.224336	2.091580	1.266084
C	5.385076	4.545857	3.449500
H	5.675597	4.439602	4.495815
H	5.525136	5.595707	3.188072
C	8.322506	3.165918	6.808679
H	7.660747	3.964875	7.162240
H	8.057715	2.266462	7.371973

C	4.324649	3.411767	0.928656	O	9.062427	11.928230	2.997965	P	10.728935	4.528450	1.383198
H	4.026852	3.526676	-0.117427	C	10.074890	8.800832	5.942286	C	12.571615	4.281121	1.662947
H	4.171179	2.356587	1.184884	C	7.967060	12.784920	2.647817	H	12.790191	3.290598	1.245660
C	10.183506	4.777008	6.242548	C	9.605224	12.281946	4.285575	C	10.557076	4.873592	-0.446717
H	11.232628	5.034314	6.401120	H	9.292226	9.295745	5.367938	H	11.119843	5.807247	-0.386670
H	9.602123	5.645432	6.568814	H	9.704773	7.808280	6.199350	C	9.098734	5.166637	-0.832991
C	3.903859	4.181765	3.291809	C	10.369587	9.587107	7.214478	H	8.501015	4.257002	-0.720650
H	3.739117	3.158779	3.651306	H	7.571229	12.428340	1.695024	H	8.654395	5.903065	-0.160571
H	3.300498	4.838131	3.924696	H	8.334263	13.810595	2.515902	C	12.877891	4.250082	3.171386
C	9.778561	3.559121	7.076079	C	6.895606	12.745938	3.722305	H	12.600844	5.214798	3.605650
H	9.925624	3.761597	8.140430	C	8.517602	12.248798	5.341070	H	12.270967	3.494313	3.673953
H	10.431327	2.714112	6.824990	H	10.047091	13.283889	4.225381	C	11.158767	3.818829	-0.386673
C	3.451545	4.284061	1.833455	H	10.393507	11.559869	4.507160	H	12.198589	3.604893	-1.130046
H	2.400914	3.995826	1.739304	H	11.193275	9.110457	7.753208	H	10.607190	2.879295	-1.276913
H	3.524965	5.327754	1.508136	H	10.723992	10.589156	6.953235	C	10.100291	2.786150	1.653053
P	10.428067	4.289716	0.603554	C	9.149102	9.689944	8.135258	H	10.350785	2.156972	0.797688
C	12.233490	4.749647	0.769915	H	6.098937	13.455315	3.492510	H	10.657088	2.395441	2.505596
H	12.798048	3.825882	0.594521	H	6.465017	11.736812	3.774850	C	13.469551	5.306531	0.951490
C	10.152109	3.911660	-1.200604	O	7.434370	13.115677	4.990632	H	13.289398	5.303481	-0.124569
H	10.351668	4.875968	-1.679139	H	8.146000	11.223755	5.457585	H	13.235277	6.311440	1.310767
C	8.679413	3.564767	-1.471660	H	8.905657	12.592311	6.300059	C	11.064589	4.276987	-2.848898
H	8.425283	2.626233	-0.966721	H	8.304628	10.169811	7.632333	H	11.695089	5.163655	-2.985077
H	8.033544	4.339707	-1.051843	H	8.817307	8.698796	8.458850	H	11.469540	3.501780	-3.505749
C	12.503286	5.238020	2.203540	H	9.372164	10.273146	9.033559	C	14.361839	3.974771	3.438164
H	11.850100	6.085771	2.429454	Te	11.811884	8.507937	4.610467	H	14.549714	3.997011	4.515402
H	12.258012	4.461177	2.929456					H	14.611288	2.962853	3.096381
C	11.088994	2.858164	-1.806782	116				C	9.004750	5.636831	-2.286883
H	12.134541	3.124013	-1.637063	l4_Te				H	7.963098	5.838307	-2.539464
H	10.924012	1.892187	-1.317044	Ni	9.418121	5.930171	2.622800	H	9.541071	6.589428	-2.393842
C	10.292765	2.674106	1.535324	P	8.072776	4.211445	3.008431	C	14.952319	5.019489	1.220143
H	10.614690	1.840795	0.908634	C	6.224252	4.229336	2.696449	H	15.221019	4.054526	0.773359
H	11.000137	2.740673	2.362486	H	5.943957	3.168824	2.665209	H	15.565424	5.776633	0.723423
C	12.673024	5.802481	-0.261933	C	8.260259	3.651464	4.782997	C	9.623210	4.613973	-3.243515
H	12.545742	5.423707	-1.278286	H	7.762402	4.453732	5.335704	H	9.589443	4.985561	-4.271298
H	12.035230	6.684133	-0.175408	C	9.732005	3.637169	5.224552	H	9.020917	3.698115	-3.223043
C	10.828038	2.702212	-3.311236	H	10.268060	2.855337	4.677170	C	15.256749	4.987015	2.719585
H	11.094892	3.636451	-3.817798	H	10.212740	4.584563	4.969550	H	16.310974	4.749829	2.888327
H	11.480096	1.925662	-3.720848	C	5.926909	4.847009	1.318656	H	15.083287	5.982814	3.142151
C	13.956927	5.673628	2.403924	H	6.297657	5.870856	1.287031	C	8.188174	7.062837	3.622952
H	14.069511	6.064937	3.417480	H	6.456052	4.308611	0.529959	C	8.269446	7.171924	5.019021
H	14.617976	4.802332	2.316743	C	7.578583	2.321592	5.134250	C	7.196556	7.826360	2.985254
C	8.421120	3.407719	-2.973647	H	6.528366	2.326759	4.836430	C	7.410563	7.995518	5.744454
H	7.377629	3.127669	-3.143469	H	8.059817	1.505301	4.584864	H	9.028911	6.612668	5.554340
H	8.570327	4.376963	-3.462261	C	8.600896	2.766097	1.939710	C	6.333564	8.653301	3.703264
C	14.133538	6.218019	-0.048041	H	8.295690	1.826070	2.402088	H	7.071386	7.764711	1.909891
H	14.789392	5.359726	-0.239681	H	8.036290	2.860735	1.011866	C	6.434273	8.740987	5.089224
H	14.399901	6.985776	-0.780117	C	5.404599	4.905574	3.809177	H	7.505796	8.055881	6.823639
C	9.360299	2.371173	-3.598022	H	5.561636	4.400045	4.764030	H	5.572922	9.223835	3.182996
H	9.191381	2.308633	-4.676459	H	5.737464	5.934707	3.938339	H	5.761732	9.380971	5.648036
H	9.128361	1.381292	-3.186562	C	7.691624	2.038517	6.638872	C	5.642878	7.423880	-1.273717
C	14.369200	6.727076	1.375450	H	7.128333	2.801747	7.187580	N	6.627737	7.813412	-0.778994
H	15.417868	7.004360	1.513394	H	7.225242	1.076829	6.870479	K	8.922680	9.087467	-0.256715
H	13.778249	7.635142	1.540799	C	4.428096	4.855405	1.006817	O	7.507308	11.498908	-0.183579
C	7.596375	6.958425	2.170749	H	4.272802	5.358190	0.049882	C	10.222958	9.595928	3.555287
C	7.737837	7.440570	3.481608	H	4.069476	3.823854	0.897836	C	6.124783	11.269867	-0.533547
C	6.521562	7.462376	1.422217	C	9.849354	3.357902	6.726214	C	7.595179	12.418192	0.915423
C	6.831744	8.350332	4.030474	H	10.903327	3.325895	7.016467	H	9.141201	9.501632	3.512847
H	8.574191	7.115291	4.088014	H	9.395297	4.187685	7.279604	H	10.527305	9.428847	4.586998
C	5.607173	8.363151	1.964858	C	3.908242	4.903370	3.472576	C	10.676565	10.968704	3.075447
H	6.398643	7.153111	0.390530	H	3.537652	3.870549	3.460922	H	6.111903	10.534664	-1.336906
C	5.753583	8.806912	3.277976	H	3.361798	5.424324	4.264147	H	5.688666	12.209817	-0.892735
H	6.969639	8.694533	5.049276	C	9.149970	2.049380	7.107212	C	5.360887	10.746445	0.666003
H	4.780949	8.722283	1.360368	H	9.201101	1.892235	8.188069	C	6.823361	11.890157	2.111751
H	5.040659	9.502313	3.705335	H	9.681965	1.210051	6.643059	H	7.197364	13.393102	0.606858
C	9.395791	7.054842	0.205823	C	3.635903	5.552299	2.113728	H	8.653485	12.534585	1.153955
N	9.683154	7.920737	-0.517336	H	2.565922	5.528377	1.888127	H	11.768860	11.021966	3.047713
K	9.914400	9.613534	1.844958	H	3.928403	6.607285	2.150321	H	10.342170	11.133390	2.044683

C 10.135788 12.087607 3.969717
H 4.301941 10.644125 0.427832
H 5.745080 9.758529 0.939890
O 5.458908 11.650860 1.773523
H 7.287297 10.964879 2.477431
H 6.827471 12.621229 2.921352
H 9.045942 12.049478 4.038070
H 10.528091 11.998143 4.986061
H 10.418028 13.074094 3.591198
Te 11.078458 7.944904 2.389082

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I5_Te

P 7.084035 3.816188 5.420895
C 5.266920 3.980962 4.978983
H 4.832969 2.999495 5.207119
C 7.106494 3.745968 7.290561
H 6.691714 4.719561 7.566948
C 8.541838 3.691789 7.836366
H 8.998655 2.734183 7.566501
H 9.150435 4.471137 7.372442
C 5.108516 4.235502 3.469349
H 5.611869 5.170252 3.215511
H 5.598995 3.449838 2.890929
C 6.242008 2.651701 7.931515
H 5.215844 2.692015 7.560297
H 6.637088 1.666084 7.663401
C 7.436513 2.073885 4.827457
H 6.990514 1.343082 5.504048
H 6.922709 1.972994 3.870778
C 4.511975 5.040877 5.799514
H 4.572500 4.817339 6.865720
H 4.975834 6.016549 5.655333
C 6.247293 2.786552 9.460804
H 5.761905 3.729634 9.736584
H 5.651042 1.984637 9.905520
C 3.633207 4.324622 3.063907
H 3.560833 4.546533 1.995326
H 3.154952 3.349114 3.215354
C 8.551600 3.829961 9.361937
H 9.577564 3.762218 9.734123
H 8.184514 4.826379 9.632736
C 3.038489 5.116184 5.381599
H 2.538384 4.172325 5.631778
H 2.538944 5.899286 5.958574
C 7.671422 2.765825 10.024786
H 7.650368 2.911549 11.108355
H 8.111984 1.776664 9.850471
C 2.890773 5.383500 3.882154
H 1.833813 5.407736 3.601766
H 3.303795 6.371831 3.652461
P 9.802169 3.348589 3.968679
C 11.579696 2.969476 4.452196
H 11.673481 1.880500 4.358500
C 9.753701 3.185673 2.106097
H 10.457231 3.960954 1.783899
C 8.374884 3.575106 1.549192
H 7.627489 2.845521 1.878163
H 8.075674 4.544928 1.952731
C 11.812106 3.352878 5.924878
H 11.656424 4.430163 6.033492
H 11.080417 2.864567 6.571723
C 10.207020 1.835084 1.536432
H 11.190381 1.554808 1.920523
H 9.509701 1.052246 1.853831
C 8.934767 1.834905 4.654003
H 9.131273 0.965833 4.024203

H 9.400812 1.635599 5.619829
C 12.644442 3.619148 3.553715
H 12.511994 3.320702 2.512686
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C 10.235537 1.875798 0.002280
H 10.998191 2.593147 -0.321318
H 10.535650 0.899498 -0.389295
C 13.227867 2.988358 6.384709
H 13.369464 3.308568 7.420871
H 13.344518 1.897733 6.373818
C 8.396110 3.614541 0.018033
H 7.400224 3.861891 -0.360468
H 9.064131 4.420635 -0.304613
C 14.057643 3.243192 4.016559
H 14.205774 2.163425 3.891373
H 14.793214 3.737033 3.375586
C 8.876154 2.285593 -0.573419
H 8.932596 2.353365 -1.663437
H 8.141032 1.503850 -0.345913
C 14.289383 3.620615 5.481591
H 15.290443 3.314994 5.799357
H 14.242474 4.710467 5.582072
Ni 8.649731 5.180926 4.652747
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RETS_Te

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H	-2.703293	16.589932	8.592478	H	12.719167	3.747891	1.169931	H	5.822536	11.295498	3.495774
H	-2.151428	18.170411	9.124284	C	10.344524	4.256054	-0.752740	O	7.143800	12.012023	4.925569
C	0.032327	15.974835	0.519465	H	10.473613	5.253370	-1.183568	H	7.964860	10.280221	4.121248
H	0.523674	15.401060	-0.271759	C	8.940950	3.767222	-1.146866	H	8.952848	11.160264	5.306546
H	-1.040389	15.975865	0.289895	H	8.783389	2.759076	-0.748208	H	10.982214	9.859062	6.600514
C	-0.075574	18.212132	1.677536	H	8.189823	4.428204	-0.720665	H	12.119735	8.511637	6.601046
H	-1.153602	18.312825	1.502080	C	12.604897	5.017858	2.896571	H	12.713781	10.166466	6.432775
H	0.332876	19.226934	1.703743	H	12.153213	5.973964	3.168795	Te	10.412612	8.222257	2.056084
C	0.549803	17.414973	0.530291	H	12.149410	4.257091	3.533999				
H	1.637764	17.399549	0.653875	C	11.399421	3.305909	-1.344695	2			
H	0.344112	17.902716	-0.427103	H	12.413363	3.612896	-1.089006	H2			
C	2.352480	9.682466	1.987300	H	11.262119	2.300728	-0.930455	H	0.000000	0.000000	0.372105
H	3.132845	10.432536	1.812896	C	10.144428	2.890576	1.849835	H	0.000000	0.000000	-0.372105
H	2.487471	8.905180	1.229736	H	10.541122	2.110778	1.196996				
C	3.411103	16.825909	8.581505	H	10.716627	2.846892	2.776482	97			
H	2.560521	16.247709	8.953456	C	13.005675	5.779667	0.520015				

H 4.301172 -1.238906 0.557392
H 5.060394 0.321807 0.880258
H 3.607621 -0.151218 1.764395
C -1.890695 0.246119 -0.431018
H -2.023176 1.292902 -0.706405
H -1.331787 0.199544 0.504671
C -3.236045 -0.460271 -0.293459
H -3.075370 -1.514873 -0.050847
H -3.765022 -0.432594 -1.250624
C -4.099549 0.189709 0.788817
H -4.301181 1.238867 0.557443
H -5.060396 -0.321868 0.880214
H -3.607629 0.151111 1.764385

22

Se2Pr2

C 2.040969 -0.206231 -0.438363
H 2.164265 -1.245278 -0.740844
H 1.459569 -0.171457 0.482409
C 3.384668 0.493919 -0.273472
H 3.225443 1.545795 -0.017535
H 3.928030 0.478462 -1.222953
C 4.232568 -0.173414 0.812053
H 4.433793 -1.219914 0.568592
H 5.193748 0.334025 0.923808
H 3.726671 -0.146944 1.780820
C -2.041897 0.209608 -0.439880
H -2.168195 1.248684 -0.741026
H -1.459691 0.175297 0.480392
C -3.383613 -0.494286 -0.274829
H -3.221389 -1.545961 -0.019983
H -3.927630 -0.479409 -1.223952
C -4.232637 0.169791 0.811813
H -4.436780 1.215982 0.569456
H -5.192401 -0.340296 0.923669

H -3.726080 0.143762 1.780249
Se 0.958350 0.688836 -1.860582
Se -0.957760 -0.680969 -1.863809

11

SePr_radical

C -0.137435 0.556386 0.000005
H -0.055825 1.206761 -0.876107
H -0.055820 1.206769 0.876112
C 0.934036 -0.526815 0.000008
H 0.801569 -1.166996 -0.876267
H 0.801580 -1.166982 0.876295
C 2.341602 0.072302 -0.000006
H 3.101582 -0.712989 -0.000005
H 2.507751 0.695772 -0.883135
H 2.507763 0.695784 0.883113
Se -1.998203 -0.093458 0.000015

11

SPr_radical

S -1.864278 -0.037871 0.000024
C -0.141455 0.553819 0.000004
H -0.044094 1.212479 -0.871432
H -0.044085 1.212490 0.871431
C 0.934291 -0.527733 0.000006
H 0.799947 -1.167165 -0.876482
H 0.799955 -1.167152 0.876506
C 2.340505 0.071976 -0.000005
H 3.100965 -0.712183 -0.000003
H 2.506915 0.695530 -0.882969
H 2.506924 0.695542 0.882949

22

Te2Pr2

C 2.230342 -0.166446 -0.499137

H 2.369909 -1.192126 -0.835897
H 1.597063 -0.169885 0.386539
C 3.561764 0.523361 -0.230337
H 3.391982 1.564660 0.060105
H 4.161933 0.545815 -1.144913
C 4.346485 -0.189181 0.874353
H 4.560373 -1.225710 0.600841
H 5.300186 0.310901 1.060948
H 3.785669 -0.200112 1.812726
C -2.230248 0.166553 -0.498941
H -2.369576 1.192451 -0.835141
H -1.597073 0.169369 0.386810
C -3.561837 -0.523149 -0.230693
H -3.392300 -1.564669 0.059098
H -4.161924 -0.544894 -1.145339
C -4.346511 0.188840 0.874385
H -4.560146 1.225595 0.601534
H -5.300340 -0.311157 1.060554
H -3.785787 0.199031 1.812821
Te -1.100800 -0.856551 -2.077271
Te 1.100833 0.857304 -2.077011

11

TePr_radical

C -0.137033 0.554807 0.000006
H -0.057726 1.200898 -0.877072
H -0.057726 1.200903 0.877080
C 0.935196 -0.527644 0.000009
H 0.808626 -1.170285 -0.875517
H 0.808638 -1.170270 0.875547
C 2.342046 0.074423 -0.000006
H 3.103682 -0.709778 -0.000006
H 2.506723 0.698281 -0.883152
H 2.506736 0.698294 0.883127
Te -2.194299 -0.162086 0.000009