

Supporting Information for
**Reaction Mechanism, Origins of Enantioselectivity, and Reactivity Trends in
Asymmetric Allylic Alkylation: A Comprehensive Quantum Mechanics
Investigation of a C(sp³)–C(sp³) Cross-Coupling.**

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Computational Details

Density functional theory calculations

All quantum mechanical calculations were performed with ORCA version 4.1 and 4.2.¹ Unless otherwise noted, geometry optimizations were carried out with the BP86 generalized gradient approximation (GGA) functional [Becke '88 exchange functional² paired with the Perdew '86 correlation functional³] with Becke–Johnson damped D3 dispersion corrections (henceforth referred to as D3).⁴ A mixed basis set was implemented, in which palladium is described by the small core LANL2TZ(f) basis set with the Hay Wadt effective core potential⁵ (ECP) [28 core electrons on Pd], and the 6-31G(d) basis set was used on all other atoms. Thermal corrections (at 298 K) were calculated from the unscaled vibrational frequencies at this level of theory. The Quasi-RRHO method was applied to correct for the breakdown of the harmonic oscillator approximation for low frequency vibrations.⁶ All stationary points are characterized by the appropriate number of imaginary vibrational modes (zero for optimized geometries and one for transition states). Intrinsic reaction coordinate (IRC) analyses were carried out to ensure all transition states connect the appropriate starting materials and products.

Triple- ζ quality single point calculations were carried out on all stationary points with the BP86-D3, B3LYP-D3,⁷ PBE0-D3,⁸ M06,⁹ and DSD-BLYP-D3¹⁰ functionals with the def2-TZVP basis set¹¹ on all atoms (with the small core def2-ECP¹² on Pd). The Conductor-like Polarizable Continuum Model (CPCM)¹³ was employed in these single point calculations to include effects of solvation. Thermal corrections obtained at the previous level of theory are then applied to these electronic energies to obtain the reported free energies (G_{298}). Calculated free energy changes are for a 1 M standard state at 25 °C, apart from decarboxylation where CO₂ is given a standard state of 1 atm.

These methods encompass a range of functional classes, including GGA (BP86-D3), hybrid GGA (B3LYP-D3), non-empirical hybrid GGA (PBE0-D3), hybrid meta-GGA (M06), and spin-component-scaled double hybrid (DSD-BLYP-D3), where effects from dispersion are accounted for either in parameterization or empirically with *ad-hoc* corrections. As the M06 density functional is parameterized to offer a suitable balance between transition metals and main group elements, we report these energies in the text of the manuscript. However, we encourage comparison of these results to those obtained with the other methods. The values obtained from all quantum mechanical calculations are included in the supporting excel file.

The resolution of identity (RI) and chain-of-spheres¹⁴ (keyword = RIJCOSX) approximations were utilized for coulomb and exchange integrals, respectively, where applicable. Automatic generation of the auxiliary basis sets was employed (keyword = AutoAux).¹⁵ The finest integration grid settings (Grid7, GridX9, NoFinalGrid) were utilized in all calculations.

DLPNO-CCSD(T) Calculations

Additional single point calculations were performed on all optimized structures with the domain based local pair natural orbital coupled-cluster (DLPNO-CCSD(T)) method as described by Neese *et. al.* and as implemented in ORCA.¹⁶ Here, we find the cc-pVTZ basis set (with the corresponding cc-pVTZ/C and def2/J auxiliary basis sets), along with the small core SK-MCDHF-RSC effective core potential¹⁷ on palladium (i.e. the cc-pVTZ-PP main basis set with cc-pVTZ-PP/C and def2/J auxiliary basis sets) with the “NormalPNO” cutoffs to offer an appropriate balance between cost and accuracy for routine use. As before, the CPCM(THF) was employed to account for effects of solvation. Thermal corrections obtained at the BP86-D3/LANL2TZ(f)–6-31G(d) are applied to the DLPNO-CCSD(T)/cc-pVTZ–CPCM(THF) electronic energies to afford the corresponding free energies. The “TightPNO” settings are employed to further refine correlation energy for comparison of select structures.

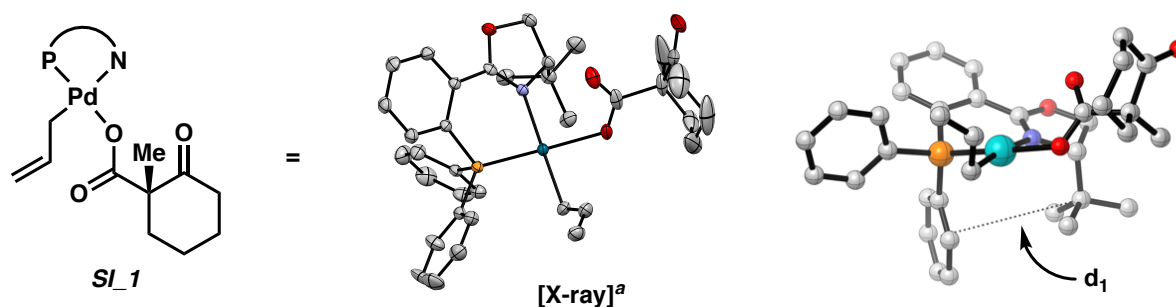
Notes:

- Similar results are obtained with the def2-TZVP basis set in control experiments, although we elected to employ Dunning’s cc-pVnZ family of basis sets for ease of basis set extrapolation with further calculations should the need arise.
- “NormalPNO” – $T_{\text{CutPairs}} = 10^{-3}$, $T_{\text{CutDO}} = 1 \times 10^{-2}$, $T_{\text{CutPNO}} = 3.33 \times 10^{-7}$, $T_{\text{CutMKN}} = 10^{-3}$
- “NormalPNO” – $T_{\text{CutPairs}} = 10^{-5}$, $T_{\text{CutDO}} = 5 \times 10^{-3}$, $T_{\text{CutPNO}} = 1.00 \times 10^{-7}$, $T_{\text{CutMKN}} = 10^{-3}$
- “TightPNO” settings may be employed, however, the computational cost increases dramatically. Thus, we have found an efficient approach is to perform routine single point calculations with “NormalPNO” cutoffs, then refine these values for key intermediates with the “TightPNO” settings.
- When CPCM implicit solvation is employed, the Hartree–Fock reference is optimized self-consistently with respect to the solvent reaction field, but the subsequent optimization of the cluster amplitudes is not. [An alternative is to apply $\Delta G(\text{solv})$ from DFT calculations to a gas phase DLPNO-CCSD(T) energy.]

Initial Benchmarking

We explore density functional and basis set dependence on the geometry optimization of the palladium(II) complex **SI_1**. These calculated geometries are then compared to that of the recently reported crystallographic structure (CCDC 695531) (Table 1).¹⁸ While slight discrepancies between crystallographic and solution phase structure may persist, we utilize this data as a reference point to which we may calibrate our methodology, as well as explore general trends in basis set and functional dependencies.

Table 1. Comparison of geometric parameters obtained from geometry optimization with various functionals and basis sets.



Basis Set	Functional	Pd-P	Pd-N	Pd-O	Pd-C	d ₁	MUE ^a	MSE
Crystal XRD		2.189	2.133	2.136	2.055	4.687	-	-
LANL2DZ [Pd]/6-31G(d)	BP86-D3	2.217	2.201	2.159	2.082	4.610	3.65	3.65
LANL2TZ [Pd]/6-31G(d)	BP86-D3	2.213	2.192	2.151	2.082	4.618	3.12	3.12
LANL2TZ(f) [Pd]/6-31G(d)	BP86-D3	2.206	2.148	2.107	2.067	4.598	1.83	0.38
def2-TZVP [all atoms]	BP86-D3	2.182	2.136	2.111	2.070	4.632	1.25	-0.35
LANL2TZ(f) [Pd]/6-31G(d)	PBE-D3	2.214	2.162	2.117	2.069	4.701	2.17	1.22
LANL2TZ(f) [Pd]/6-31G(d)	TPSS-D3	2.217	2.154	2.101	2.071	4.673	2.50	0.75
LANL2TZ(f) [Pd]/6-31G(d)	BLYP-D3	2.233	2.208	2.152	2.095	4.645	4.38	4.38
LANL2TZ(f) [Pd]/6-31G(d)	B3LYP-D3	2.228	2.209	2.134	2.066	4.683	3.20	3.10
LANL2TZ(f) [Pd]/6-31G(d)	B3PW-D3	2.204	2.145	2.088	2.045	4.586	2.13	-0.78
LANL2TZ(f) [Pd]/6-31G(d)	PBE0-D3	2.211	2.150	2.086	2.040	4.673	2.60	-0.65
LANL2TZ(f) [Pd]/6-31G(d)	TPSSh-D3	2.215	2.153	2.091	2.059	4.653	2.37	0.12
LANL2TZ(f) [Pd]/6-31G(d)	wB97X-D3	2.226	2.179	2.097	2.033	4.612	2.75	-0.80
LANL2DZ [Pd]/6-31G(d)	B3LYP	2.278	2.234	2.133	2.079	5.102	5.43	5.28

Geometric parameters (Pd-X bond lengths, and d₁) given in angstrom (Å). MUE and MSE given in pm. Optimization carried out beginning from the known X-ray crystal structure. ^a CCDC 695531 (reference 18).

From these controls, the following trends are observed:

- (1) Greatly reduced errors in Pd–X bond lengths with minimal increase in computational cost are obtained by employing the larger triple- ζ quality basis set with polarization functions, LANL2TZ(f), on palladium in place of the double- ζ (LANL2DZ) basis set.
- (2) The use of Becke-Johnson D3 damped dispersion corrections (-D3) in the optimization greatly aids in capturing perturbations of the ligand geometry arising from noncovalent interactions (see d_1).
- (3) Density functionals constructed with the Lee–Yang–Parr correlation functional (BLYP, B3LYP) present elongated Pd–X bonds and are among the functionals with the highest MUEs. This trend has been previously described in the literature¹⁹ and has been attributed to the LYP functional underestimating correlation at the uniform electron gas (UEG) limit.²⁰

Thus, for geometry optimization we employ the BP86 density functional with Becke–Johnson damped dispersion corrections (BP86-D3), with a mixed basis set comprised of the LANL2TZ(f) basis set on palladium with 6-31G(d) on all other atoms.

We do not recommend the use of the B3LYP/LANL2DZ–6-31G(d) level of theory as is employed in select literature investigations. We believe more suitable geometries may be obtained with D3BJ dispersion corrections and triple ζ basis sets with polarization functions on the metal center. Apart from B3LYP and BLYP, all other functionals evaluated perform comparably well.

Decarboxylation Control Experiments

In order to obtain accurate barrier heights for the rate determining decarboxylative step, geometry/transition state optimizations were also carried out with CPCM(THF) for comparison to the structures optimized in the gas phase (Table 2).

Table 2. Decarboxylation barrier heights with geometries optimized in gas phase and with CPCM(THF).

Method (for single point calculations)	(boat/ax)-TS5 (gas)	(chair/ax)-TS14 (gas)	(exo/chair/ax)-TS15 (gas)	(boat/ax)-TS5 (THF)	(chair/ax)-TS14 (THF)	(exo/chair/ax)-TS15 (THF)
BP86-D3	16.5	12.5	16.4	15.1	11.5	21.7
B3LYP-D3	18.4 ^a	16.5	21.5	19.2	15.4	27.7
PBE0-D3	21.0 ^a	18.9^b	21.0	23.9	19.0	27.8
M06	22.0	17.1	17.5	21.8	15.2	19.8

DSD-BLYP-D3	20.6 ^a	18.6	19.0	22.5	17.1	24.1
DLPNO-CCSD(T) ^d	26.8	22.0	23.2 ^c	26.8	19.8	28.2

Comparison of barrier heights obtained across a variety of methods with geometries optimized in gas phase and with CPCM(THF). Barrier heights given in kcal/mol from “Method”/def2-TZVP–CPCM(THF)//BP86-D3/LANL2TZ(f)–6-31G(d) (with or without CPCM(THF)). ^a (chair/ax)-TS5. ^b (boat/ax)-TS14. ^c (exo/boat/ax)-TS15. ^d Single point with the cc-pVTZ basis set (with SK-MCDHF-RSC pseudopotential on Pd; i.e. cc-pVTZ-PP), “NormalPNO” settings.

For completeness, intermediates derived from the *S* enantiomer of starting material **1** were also investigated (Table 3). An analogous result was obtained.

Note: Transition state geometries obtained with CPCM(THF) solvation were prone to an additional small imaginary vibrational mode (<5 cm⁻¹) corresponding to a rocking of the ligand backbone. With the point charge CPCM scheme these were unable to be eliminated, however they bear no consequences on the final results.

Table 3. Decarboxylation barrier heights of complexes derived from the *S* enantiomer of **1.**

Method	(chair/ax)-TS14_diast2	(exo/chair/ax)-TS15_diast2
BP86-D3	12.3	18.5
B3LYP-D3	16.7	24.8
PBE0-D3	21.0	25.5
M06	17.4	21.5
DSD-BLYP-D3	18.8	23.1
DLPNO-CCSD(T) ^a	21.6	27.7

Barrier heights reported in kcal/mol from single point calculations with the listed functional/method, the def2-TZVP basis set on all atoms and CPCM(THF) on geometries obtained with BP86-D3/LANL2TZ(f)–6-31G(d). ^a Single point with the cc-pVTZ basis set (with SK-MCDHF-RSC pseudopotential on Pd; i.e. cc-pVTZ-PP) and “NormalPNO” settings.

Prediction of Enantioselectivity

Given the challenge of calculating energies to within the sub-kcal/mol level of accuracy required for accurate prediction of reaction enantioselectivity, we chose to employ a variety of control experiments to assess the fidelity of our results.

With geometries obtained at the BP86-D3/LANL2TZ(f)-6-31G(d) level, we began by evaluating single point energies with a variety of density functional methods (Table 4). These methods include generalized gradient approximation (GGA), meta-GGA, hybrid (meta-)GGA, range-separated hybrid GGA, and double hybrid functionals. Similar trends in relative free energies are obtained across each of the methods tested.

Table 4. Comparison of relative free energies obtained across a variety of density functional methods.

	BP86-D3	BLYP-D3	revPBE-D3	M06-L	B3LYP-D3	B3LYP-D3 ^a
(<i>Si</i> /chair/ax)-TS20	0.0	0.0	0.0	0.0	0.0	0.0
(<i>Si</i> /boat/ax)-TS20	5.4	6.0	5.3	4.2	6.1	5.7
(<i>Si</i> /chair/eq)-TS20	1.6	2.2	1.7	1.4	2.0	1.9
(<i>Si</i> /boat/eq)-TS20	5.5	5.3	5.0	4.3	5.6	5.2
(<i>Re</i> /chair/ax)-TS20	2.0	2.4	1.9	1.8	2.8	2.6
(<i>Re</i> /boat/ax)-TS20	1.0	0.8	0.9	0.3	1.1	1.0
(<i>Re</i> /chair/eq)-TS20	4.2	5.0	4.1	3.7	5.0	4.9
(<i>Re</i> /boat/eq)-TS20	3.2	3.4	2.9	2.6	3.6	3.4

	PBE0-D3	TPSSh-D3	M06	M06-2X	ω B97X-D3	mPW2PLYP-D
(<i>Si</i> /chair/ax)-TS20	0.0	0.0	0.0	0.0	0.0	0.0
(<i>Si</i> /boat/ax)-TS20	5.2	5.9	3.6	4.3	6.1	5.1
(<i>Si</i> /chair/eq)-TS20	1.2	1.7	0.4	1.2	1.6	1.4
(<i>Si</i> /boat/eq)-TS20	5.6	5.8	4.0	4.4	5.8	5.8
(<i>Re</i> /chair/ax)-TS20	2.5	2.2	2.1	2.8	2.8	2.2
(<i>Re</i> /boat/ax)-TS20	1.5	1.0	1.3	1.0	0.9	1.9
(<i>Re</i> /chair/eq)-TS20	4.1	4.2	3.2	4.0	4.3	4.0
(<i>Re</i> /boat/eq)-TS20	3.5	3.3	2.8	2.8	3.0	4.1

	PWPB95-D3	DSD-BLYP-D3	DSD-PBEP86-D3
(<i>Si</i> /chair/ax)-TS20	0.0	0.0	0.0
(<i>Si</i> /boat/ax)-TS20	5.5	5.1	5.0
(<i>Si</i> /chair/eq)-TS20	1.3	1.1	1.0

(<i>Si</i> /boat/eq)-TS20	5.5	5.6	5.6
(<i>Re</i> /chair/ax)-TS20	2.4	2.2	2.1
(<i>Re</i> /boat/ax)-TS20	1.4	2.1	2.1
(<i>Re</i> /chair/eq)-TS20	3.9	3.8	3.6
(<i>Re</i> /boat/eq)-TS20	3.3	3.7	3.7

Relative free energies reported in kcal/mol from single point calculations with the listed functional, the def2-TZVP basis set on all atoms and CPCM(THF) on geometries obtained with BP86-D3/LANL2TZ(f)-6-31G(d). ^a A mixed basis set consisting of LANL2TZ(f) on palladium and 6-311+G(d) on all other atoms utilized.

Given the potentially significant role of noncovalent interactions in differentiating the energy between diastereomeric transition states, we sought to further refine our calculated $\Delta\Delta G^\ddagger$ by employing single point calculations with domain based local pair natural orbital coupled-cluster theory (DLPNO-CCSD(T)) (Table 5). For these calculations, we employ the cc-pVTZ basis set on all atoms, with the SK-MCDHF-RSC relativistic effective core potential on palladium. Calculations are additionally carried out with the “TightPNO” criteria for the two lowest energy diastereomeric transition states found from calculations with the “NormalPNO” settings.

Under standard conditions at 25 °C, an enantiomeric excess of 88% is experimentally observed, corresponding to an apparent $\Delta\Delta G^\ddagger$ of 1.6 kcal/mol. Comparing the relative energies of only the two lowest energy diastereomeric transition states with “NormalPNO” and “TightPNO” cutoffs affords a calculated $\Delta\Delta G^\ddagger$ of 2.3 and 1.9 kcal/mol, respectively, corresponding to 96% ee and 92% ee. From a Boltzmann-weighted average over unique transition states (with “NormalPNO”), 94% ee is calculated. These results are in good agreement with experimentally obtained values, and thus highlight the efficacy of the DLPNO-CCSD(T) in the context of asymmetric catalysis.

Table 5. Comparison of relative free energies obtained at the DLPNO-CCSD(T) level of theory.

	DLNO-CCSD(T) ^a NormalPNO	DLNO-CCSD(T) NormalPNO	DLNO-CCSD(T) TightPNO
(<i>Si</i> /chair/ax)-TS20	0.0	0.0	0.0
(<i>Si</i> /boat/ax)-TS20	6.6	5.9	–
(<i>Si</i> /chair/eq)-TS20	1.4	1.0	–
(<i>Si</i> /boat/eq)-TS20	6.6	6.1	–
(<i>Re</i> /chair/ax)-TS20	3.0	2.8	–
(<i>Re</i> /boat/ax)-TS20	2.2	2.3	1.9

(<i>Re</i> /chair/eq)-TS20	4.5	4.0	–
(<i>Re</i> /boat/eq)-TS20	4.4	4.2	–

Relative free energies reported in kcal/mol with DLPNO-CCSD(T)/cc-pVTZ–CPCM(THF)//BP86-D3/LANL2TZ(f)–6-31G(d). ^aUsing the def2-TZVP basis set on all atoms.

Further controls were carried out in which transition state optimizations were carried out without D3 dispersion correction (Table 6), and with the B3LYP-D3 hybrid functional (Table 7). Both of these trials offer similar overall results to those obtained with BP86-D3 geometries.

Table 6. Optimization without D3 corrections (BP86).

	M06 ^a	DLNO-CCSD(T) ^b
(<i>Si</i> /chair/ax)-TS20	0.0	0.0
(<i>Si</i> /boat/ax)-TS20	4.4	5.9
(<i>Si</i> /chair/eq)-TS20	1.6	2.2
(<i>Si</i> /boat/eq)-TS20	5.3	6.7
(<i>Re</i> /chair/ax)-TS20	2.6	1.8
(<i>Re</i> /boat/ax)-TS20	1.7	2.7
(<i>Re</i> /chair/eq)-TS20	4.2	4.3
(<i>Re</i> /boat/eq)-TS20	3.5	5.0

Relative free energies reported in kcal/mol with geometries obtained with BP86/LANL2DZ–6-31G(d). ^aSingle point calculation with M06/def2-TZVP–CPCM(THF). ^bSingle point calculation with DLPNO-CCSD(T)/cc-pVTZ–CPCM(THF) with “NormalPNO” settings.

Table 7. Optimization with B3LYP-D3.

	M06 ^a	DLNO-CCSD(T) ^b
(<i>Si</i> /chair/ax)-TS20	0.0	0.0
(<i>Si</i> /boat/ax)-TS20	2.8	3.7
(<i>Re</i> /chair/ax)-TS20	1.7	1.9
(<i>Re</i> /boat/ax)-TS20	1.5	2.3

Relative free energies reported in kcal/mol with geometries obtained with B3LYP-D3/LANL2DZ–6-31G(d). The four lowest energy “axial” transition states were considered here. ^aSingle point calculation with M06/def2-TZVP–CPCM(THF). ^bSingle point calculation with DLPNO-CCSD(T)/cc-pVTZ–CPCM(THF) with “NormalPNO” settings.

Additional Notes from Manuscript

Facile interconversion between (*Re*)-13 and (*Si*)-13

A previous computational investigation into the reaction mechanism of a truncated system (beginning from enolate intermediates) highlights internal rearrangements of palladium enolates prior to C–C bond formation as a possible origin of enantioinduction.²¹ This hypothesis is dependent on kinetic quenching (rather than equilibration) of enolates (*Re*)-13 and (*Si*)-13 by their corresponding C–C bond forming events. However, the authors of that study recognize that a transition state leading to the facile equilibration of (*Re/Si*)-13 may exist, but do not explore further, leaving the origins of enantioinduction unresolved.

In this investigation, a low energy transition state connecting (*Re*)-13 and (*Si*)-13 on the PES is found (TS24, $\Delta G^\ddagger \sim 5$ kcal/mol, Figure 1). TS24 is significantly lower in energy than the next lowest transition states, which are those of C–C bond formation (TS20). Thus, enolates (*Re*)-13 and (*Si*)-13 are expected to be in thermal equilibrium. Hence, internal rearrangements of palladium enolates, followed by kinetic quenching via C–C bond formation, is not responsible for enantioinduction.

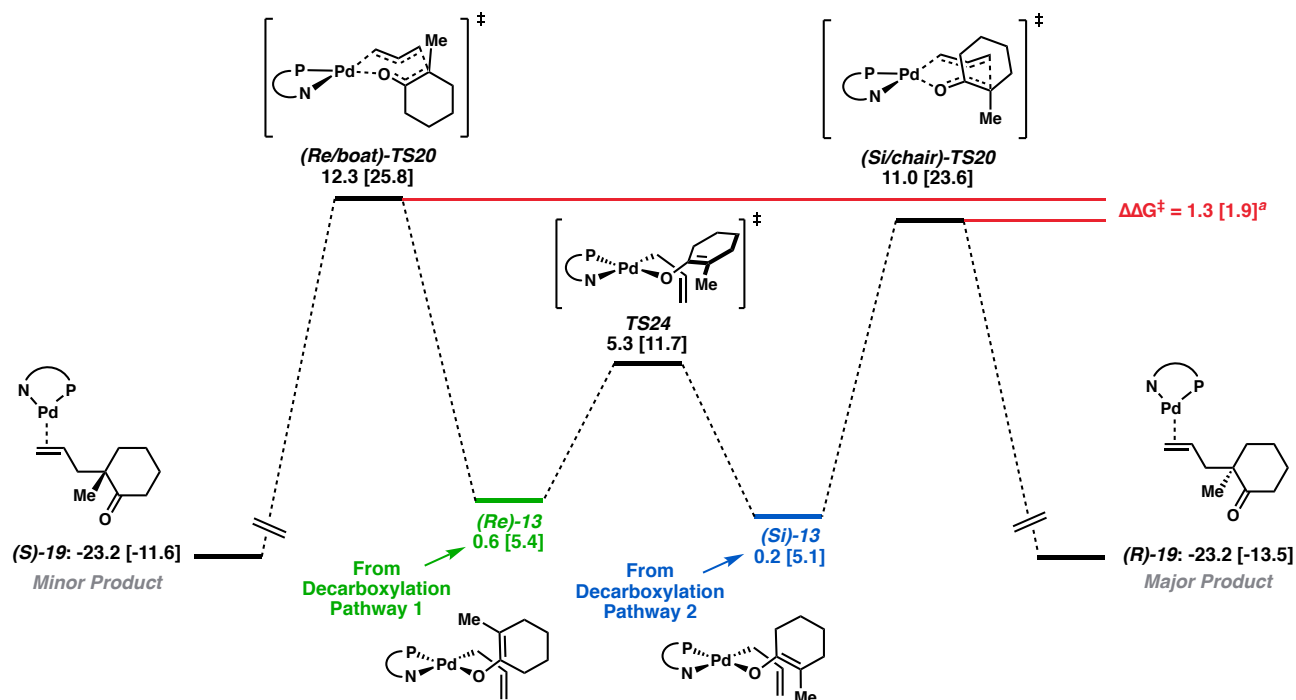


Figure 1. Portion of the free energy surface highlighting facile equilibration between (*Re*)-13 and (*Si*)-13 prior to C–C bond formation. Free energies given in kcal/mol at the M06/def2-TZVP–CPCM(THF) level of theory (see computational details), with those derived from DLPNO-CCSD(T)/cc-pVTZ–CPCM(THF) in brackets. “With ‘TightPNO’ cutoffs.”

Additional potentially lower energy transition states for the interconversion of *(Re)*-13 and *(Si)*-13 likely persist, however are challenging to optimize given the flat nature of the PES and conformational flexibility of the enolate fragment. It is worth noting that highly decorated, sterically encumbered substrates may experience a barrier to enolate equilibration similar or greater in magnitude to that of C–C bond formation. Should this be the case, the mechanism of decarboxylation and/or choice of masked enolate synthon would play a large role in the resultant product enantioselectivity. The pathways, intermediates, and consideration described in this research provide a framework from which this would be evaluated.

Trans Influence in Oxidative Addition

Our investigations into the mechanism of oxidative addition reveal the lowest energy process for C–O bond cleavage to be that of an *anti* displacement-type of mechanism (Figure 2). The lowest energy conformer of four unique transition states are considered, in which displacement of the carboxylate leaving group occurs *trans* to either the nitrogen (*t-N*) or phosphorus (*t-P*) of the PHOX ligand, with either *exo* or *endo* approach of the allylic fragment (Figure 2).

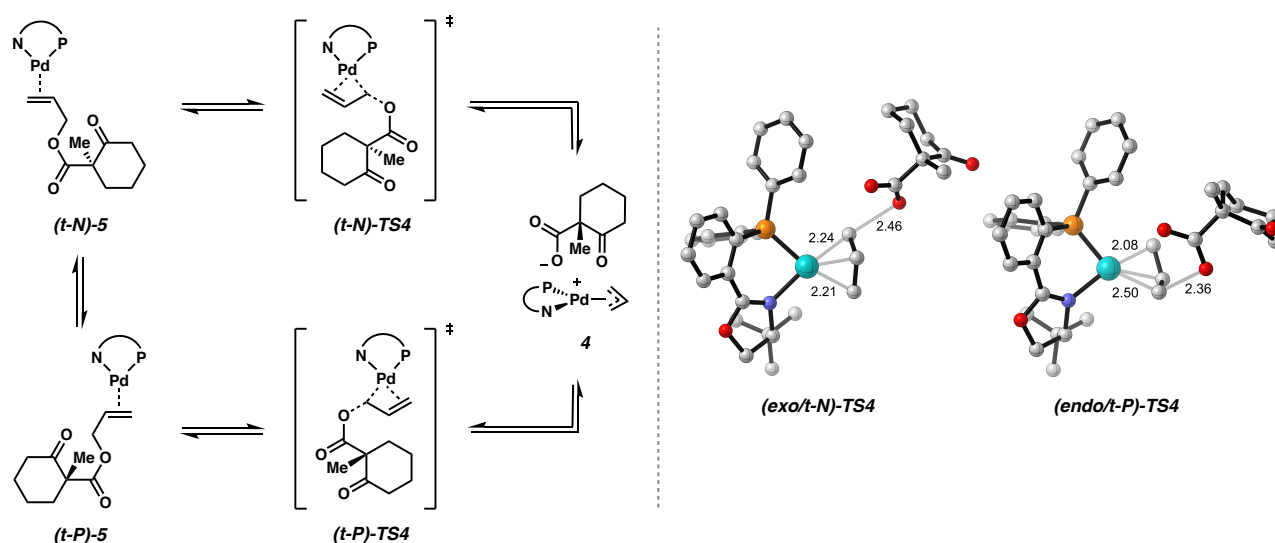


Figure 2. (left) Isomeric Pd(0) olefin-bound complexes (5), their corresponding oxidative addition transition states (TS4), and η^3 -allyl palladium(II) product (4).

Table 8. Relative free energies (in kcal/mol) of isomeric oxidative addition transition states at various levels of theory.

	BP86-D3	B3LYP-D3	PBE0-D3	DSD-BLYP-D3	M06	DLPNO-CCSD(T) ^a
(<i>exo/t-N</i>)-TS4	0.0	0.0	0.0	0.0	0.0	0.0
(<i>endo/t-N</i>)-TS4	1.4	2.0	1.9	2.3	2.3	2.7
(<i>exo/t-P</i>)-TS4	5.9	7.6	7.3	8.0	7.5	9.3
(<i>endo/t-P</i>)-TS4	3.8	4.8	5.5	6.1	6.2	6.5

Relative free energies reported in kcal/mol with geometries obtained with BP86-D3/LANL2TZ(f)-6-31G(d). Single point calculation with def2-TZVP basis set on all atoms (def2-ECP on Pd) and CPCM(THF). ^aSingle point calculation with DLPNO-CCSD(T)/cc-pVTZ-CPCM(THF) with “NormalPNO” settings.

An energetic preference of 3.8–6.5 kcal/mol is found for the *t-N* transition states across the various levels of theory investigated (Table 8). While this may be in part due to steric interactions between the carboxylate leaving group and the phenyl rings of the triaryl phosphine ligand, we also consider electronic effects. In accordance with the anticipated trans influence, elongated Pd–X bond lengths trans to phosphorus are observed (Figure 2). As a hypothesis for the origins of the preference for *t-N* transition states, we consider the research of De Proft and co-workers,²² who provide a ligand-field-based rationale for the trans influence in related square planar Pt(II) complexes. In brief, the authors suggest the repulsion between a strong trans ligand (T) and the ligand trans to T (L) arises from further hybridization (in unsymmetrical d⁸ complexes) between the occupied 2a' and virtual 3a' MOs (figure 3) resulting in a net decrease in Pt–L σ -bonding character, and thus, a longer bond length.

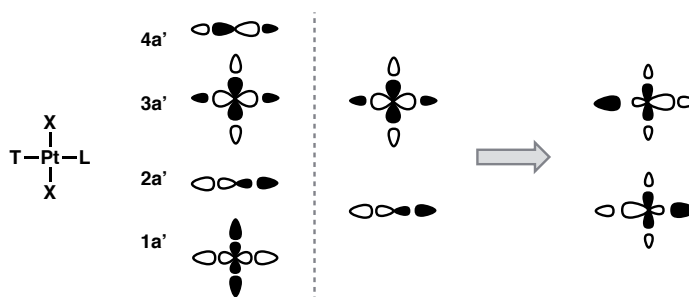


Figure 3. Select frontier MOs of a model Pt(II) complex highlighting potential hybridization of 2a' and 3a'.

In the case of the (PHOX)Pd complexes, we consider this effect may play a role in the calculated preference for displacement *trans* to nitrogen. The reduced Pd–C(OCOR) bond length in the *t-N* transition states should be conducive to enhanced overlap with the $\sigma^*(\text{C–O})$, thus, facilitating displacement of the carboxylate leaving group.

Additional Computations for “Experiment and Discussion” Section of Manuscript

Experimentally, it was determined that for β -ketoester substrate **1**, employing the more electron poor (*S*)-(CF₃)₃-*t*-BuPHOX ligand in place of the standard (*S*)-*t*-BuPHOX ligand, with otherwise identical reaction conditions, did not result in a significant change in reaction rate (Figure 14 in manuscript). Computationally, an identical result was obtained (Figure 4). Henceforth, the suffix “_CF₃” denotes structures that are re-optimized using the (*R*)-(CF₃)₃-*t*-BuPHOX ligand. Note that the experimental portion of this investigation employs the *S* enantiomer of ligand for convenience. The apparent barrier heights of the two lowest energy decarboxylation pathways (Pathways 2 and 3, see text) were then compared with both ligands at the DLPNO-CCSD(T) level of theory (Figure 4). Similar results are obtained with “NormalPNO” and “TightPNO” cutoffs (Table 9).

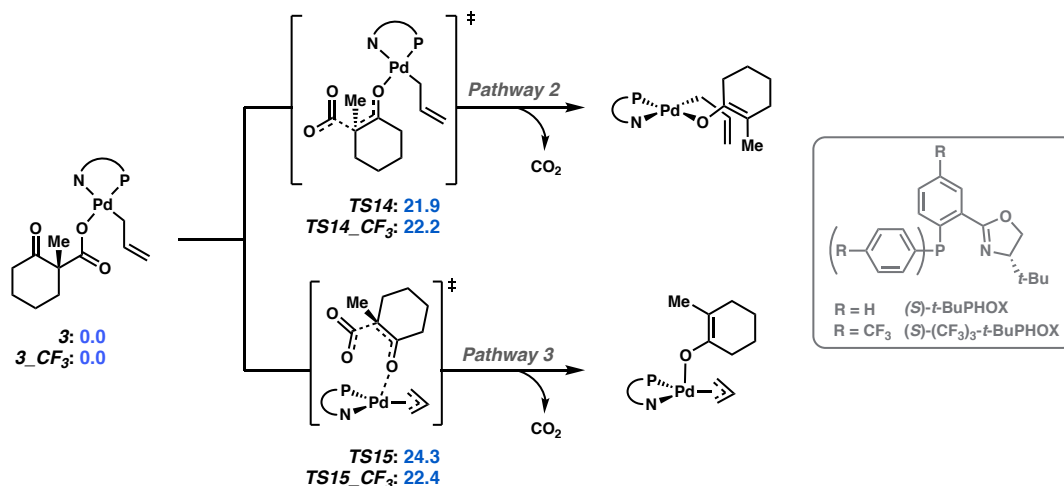


Figure 4. Influence of ligand electronics on decarboxylation barrier heights. Relative free energies given in kcal/mol from “TightPNO” DLPNO-CCSD(T)/cc-pVTZ-CPCM(THF)//BP86-D3/LANL2TZ(f)-6-31G(d) level of theory.

Table 9. Comparison of barrier heights (in kcal/mol) to decarboxylation with the standard (*S*)-*t*-BuPHOX and electron poor (*S*)-(CF₃)₃-*t*-BuPHOX ligands.

	TS14	TS15	TS14_CF ₃	TS15_CF ₃
NormalPNO	22.0	23.5	22.4	21.6
TightPNO	21.9	24.3	22.2	22.4

Free energies reported in kcal/mol with geometries obtained with BP86-D3/LANL2TZ(f)-6-31G(d). Single point calculation with DLPNO-CCSD(T)/cc-pVTZ-CPCM(THF).

In order to experimentally probe the interplay of inner and outer-sphere mechanistic pathways, we prepared α -phenyl β -ketoester **20** as well as the corresponding enol carbonate **21** (Figure 5). Highlighting the role of decarboxylative pathway on subsequent C–C bond formation, compounds **20** and **21** both yield α -phenyl product **22**, however with differing degrees of enantioenrichment. In analogous fashion to intermediates derived from substrate **1** (R = Me), the corresponding set of 7-membered pericyclic inner-sphere C–C bond forming transition states (**TS20_Ph**) are considered. These initial results suggest that inner-sphere C–C bond formation for these α -phenyl enolates may give rise to a similar degree of product enantioenrichment as the α -methyl case.

Table 9. Comparison of barrier heights (in kcal/mol) to decarboxylation with the standard (*S*)-*t*-BuPHOX and electron poor (*S*)-(CF₃)₃-*t*-BuPHOX ligands.

Intermediate	G(rel)
(<i>Re</i> /chair/axial)-TS20_Ph_i	0.0
(<i>Re</i> /chair/axial)-TS20_Ph_ii	1.3
(<i>Re</i> /boat/axial)-TS20_Ph_i	4.9
(<i>Re</i> /boat/axial)-TS20_Ph_ii	3.6
(<i>Si</i> /chair/axial)-TS20_Ph_i	4.1
(<i>Si</i> /chair/axial)-TS20_Ph_ii	4.1
(<i>Si</i> /boat/axial)-TS20_Ph_i	1.3
(<i>Si</i> /boat/axial)-TS20_Ph_ii	1.3

Relative free energies reported in kcal/mol from the M06/def2-TZVP–CPCM(THF)//BP86-D3/LANL2TZ(f)–6-31G(d) level of theory.

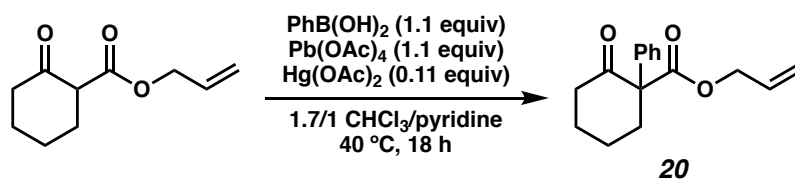
Experimental Section

Materials and Methods

Unless otherwise stated, reactions were performed in flame-dried glassware under an argon or nitrogen atmosphere using dry, deoxygenated solvents. Solvents were dried by passage through an activated alumina column under argon.²³ Reaction progress was monitored by thin-layer chromatography (TLC) or Agilent 1290 UHPLC-MS. TLC was performed using E. Merck silica gel 60 F254 precoated glass plates (0.25 mm) and visualized by UV fluorescence quenching or KMnO₄ staining. Silicycle SiliaFlash® P60 Academic Silica gel (particle size 40–63 μm) was used for flash chromatography. ¹H NMR spectra were recorded on Varian Inova 500 MHz and Bruker 400 MHz spectrometers and are reported relative to residual CHCl₃ (δ 7.26 ppm). ¹³C NMR spectra were recorded on Varian Inova 500 MHz (125 MHz) and Bruker 400 MHz (100 MHz) spectrometers and are reported relative to CHCl₃ (δ 77.16 ppm). Data for ¹H NMR are reported as follows: chemical shift (δ ppm) (multiplicity, coupling constant (Hz), integration). Multiplicities are reported as follows: s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, sept = septuplet, m = multiplet, br s = broad singlet, br d = broad doublet. Data for ¹³C NMR are reported in terms of chemical shifts (δ ppm). High resolution mass spectra (HRMS) were obtained from Agilent 6200 Series TOF with an Agilent G1978A Multimode source in electrospray ionization (ESI+), atmospheric pressure chemical ionization (APCI+), or mixed ionization mode (MM: ESI-APCI+). Absolute stereochemistry is assigned by analogy to previous results by our group.^{24–25}

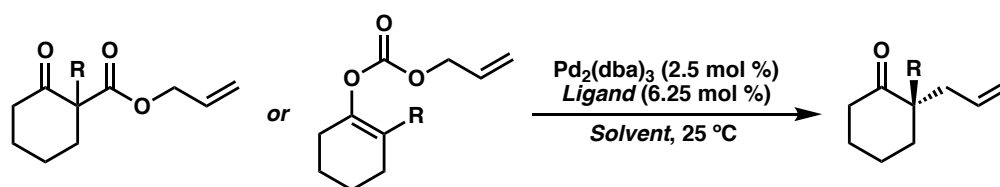
Reagents were purchased from commercial sources and used as received unless otherwise stated. The (*S*)-(CF₃)₃-*t*-BuPHOX ligand was prepared according to literature procedure.²⁶ β-Ketoester **1**,²⁴ ketone (*S*)-**2**,²⁴ enol carbonate **21**,²⁷ and a-phenyl ketone (*S*)-**22**²⁷ are known compounds, and were prepared and assayed for enantioenrichment accordingly.

Note: Experimentally, the (S) enantiomer of the PHOX ligands are employed whereas the data presented in the text depict the (R) enantiomer of ligand.



Allyl 2-oxo-1-phenylcyclohexane-1-carboxylate (**20**).

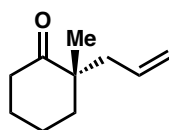
Compound **20** was prepared in following literature precedent.²⁸ To a flame dried flask equipped with a stir bar under a nitrogen atmosphere were added phenylboronic acid (1.46 g, 12.1 mmol, 1.10 equiv), lead(IV) acetate (5.34 g, 12.1 mmol, 1.10 equiv), and mercury(II) acetate (0.38 g, 1.21 mmol). The solids were dissolved in anhydrous chloroform (20 mL) and the solution was heated to 40 °C. After one hour at 40 °C, a solution of allyl 2-oxocyclohexane-1-carboxylate²⁴ (2.00 g, 11.0 mmol, 1.00 equiv) in pyridine (11.0 mL, 1.0 M) was added to the reaction, and stirring at 40 °C was continued for 18 hours. Upon complete consumption of β -ketoester starting material, as determined by TLC (10% EtOAc/hexanes), the reaction mixture was let cool, then filtered through a plug of celite[®] washing with chloroform. The combined organic phase was washed with aqueous H_2SO_4 (3 M, 20 mL). The resulting aqueous layer was extracted twice with chloroform (20 mL). The combined organic layer was once again washed with water (20 mL), dried over anhydrous Na_2SO_4 , filtered, and volatiles were removed in vacuo. The crude oil was purified by flash column chromatography (10% EtOAc/hexanes) to afford β -ketoester **20** (2.00 g, 70% yield) as a colorless oil, which solidifies to an amorphous solid upon refrigeration. ^1H NMR (400 MHz, CDCl_3) δ 7.41 – 7.35 (m, 2H), 7.34 – 7.29 (m, 1H), 7.27 – 7.23 (m, 2H), 5.86 (ddt, $J = 17.2, 10.5, 5.6$ Hz, 1H), 5.25 – 5.17 (m, 2H), 4.65 (dq, $J = 5.6, 1.5$ Hz, 2H), 2.81 – 2.73 (m, 1H), 2.60 – 2.53 (m, 2H), 2.48 – 2.40 (m, 1H), 2.03 – 1.93 (m, 1H), 1.90 – 1.73 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 206.8, 171.1, 136.6, 131.6, 128.6, 128.0, 127.8, 118.6, 66.7, 66.1, 40.8, 35.2, 27.8, 22.1; HRMS (MM: ESI-APCI): m/z calc'd for $\text{C}_{16}\text{H}_{19}\text{O}_3$ $[\text{M}+\text{H}]^+$: , found.



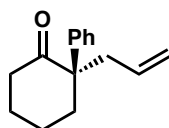
General procedure for asymmetric allylic alkylation screening:^{24–25}

The procedure for the palladium-catalyzed dicarboxylic allylic alkylation is followed as described in our previous reports.^{24–25} In a nitrogen filled glovebox, an oven dried vial is charged with a stir bar,

tris(dibenzylideneacetone)dipalladium(0) (2.28 mg, 2.50 μmol), and *ligand* (6.25 μmol). *Solvent* (1.0 mL) is added, and the catalyst stock solution is pre-stirred for 30 minutes at 25 °C. To a separate vial equipped with a stir bar is added a solution of *substrate* (0.05 mmol) in *solvent* (1.0 mL, 0.05 M). To the solution of substrate is added 0.50 mL of the pre-stirred catalyst stock solution (1.25 μmol Pd₂(dba)₃, 3.13 μmol *ligand*). The reaction vessel is then sealed with electrical tape and removed from the glovebox. Stirring is continued at 25 °C for 12 hours (unless otherwise noted). Volatiles are then removed in vacuo and the product is purified by silica gel flash column chromatography or preparatory-scale TLC.

**(S)-2****(S)-2-allyl-2-methylcyclohexan-1-one ((S)-2)**

Spectral data matches that of prior literature reports.²⁴⁻²⁵ *Note: Compound is moderately volatile, and care should be exercised when removing solvent in vacuo.* ¹H NMR (500 MHz, CDCl₃) δ 5.69 (ddt, $J = 16.2, 10.9, 7.4$ Hz, 1H), 5.07 – 5.01 (m, 2H), 2.42 – 2.33 (m, 3H), 2.23 (dd, $J = 13.8, 7.2$ Hz, 1H), 1.91 – 1.67 (m, 5H), 1.64 – 1.55 (m, 1H), 1.07 (s, 3H).

**(S)-22****(S)-2-allyl-2-phenylcyclohexan-1-one ((S)-22)**

Spectral data matches that of prior literature reports.²⁷ ¹H NMR (500 MHz, CDCl₃) δ 7.35 (t, $J = 7.7$ Hz, 2H), 7.26 – 7.22 (m, 1H), 7.15 (d, $J = 7.5$ Hz, 2H), 5.44 (dddd, $J = 17.0, 10.2, 7.9, 6.7$ Hz, 1H), 4.92 (d, $J = 10.2$ Hz, 1H), 4.88 (d, $J = 17.0$ Hz, 1H), 2.67 (dq, $J = 14.4, 3.0$ Hz, 1H), 2.51 (dd, $J = 14.0, 6.7$ Hz, 2H), 2.44 (dd, $J = 14.0, 8.0$ Hz, 2H), 2.38 – 2.26 (m, 2H), 1.99 – 1.91 (m, 1H), 1.83 – 1.63 (m, 4H).

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Coordinates of Optimized Structures and Spectral Data**3**

Pd	1.93726495957131	5.17249021017598	16.42183767287425
P	1.85122799270712	5.48621297264017	18.60895630042237
O	2.18234776720702	4.91827378174341	14.35291449085261
O	1.14347528034903	6.92921523248409	14.11498304131318
O	4.59886361788811	5.39662230810341	12.21363996420714
N	3.65306669641345	6.45206309329275	16.44963965775423
C	2.11234024082400	7.27020282975972	18.99319134458776
C	1.41769527232526	7.86177958098366	20.06341122476435
H	0.71216134822183	7.25581143538645	20.63818709836010
C	1.61440746244037	9.20844876099915	20.40429544982711
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C	5.15034168404710	4.65561278648892	20.98067819884340
C	4.06051020775765	5.32458835197070	20.40290532628370
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C	1.79594717822454	5.97080109749982	13.67732339989725
C	2.24730989327060	5.94392009429336	12.17395351799376
C	1.03271074837250	5.47178775311761	11.32769355176461
C	0.72838780501729	3.97673583994571	11.48535809009411
C	1.94444158890514	3.14804077530187	11.04649511518275
H	1.73295198647587	2.06510999974715	11.11316944982881

H	2.16199949948277	3.36245448008461	9.98122640444834
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C	2.66315594055942	7.36560237487854	11.76662212745459
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H	1.27486277268871	0.73840544326978	17.42918214415958
O	4.89817746472499	8.31100118334327	16.75797924295998
C	3.83745790971456	7.54328298786237	17.12976657989004
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H	5.56469779570782	2.93043738457903	15.99823766439276

H	4.48727623624883	3.65003701775776	14.75715030372644
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H	6.41212412779749	4.96876408396960	13.78051251490150
H	7.47337462647009	4.16791141025025	14.98208742056961
C	3.50264630447119	3.31066707796711	19.14261027904750
C	4.58541718542765	2.64642693035404	19.73251410546053
C	5.41513056131341	3.31924419060177	20.64492707743199
H	5.79625181012031	5.18289761010584	21.69028095714962
H	6.27051239766171	2.80225842590539	21.09200903095728
H	2.85722744921696	2.79622797964345	18.41979602576113
H	4.79021664533081	1.60413965990115	19.46733807251239
C	-0.80348500403748	3.76484201362245	21.27727456698002
C	-2.03085460329267	4.28476732033118	20.84066543477756
C	-2.07000556381215	5.17869981594608	19.75666945382742
H	-0.91127176501003	6.22041784339342	18.24456405223381
H	-2.95944941295832	3.98983020858622	21.33993381581916
H	-3.02700866007654	5.58006938721129	19.40837787660828
H	1.34746875237663	3.73617326136338	20.97984433618469
H	-0.77085809948630	3.06611761594936	22.11956828011592
H	0.16322891769716	6.09208738959046	11.61068611284104
H	1.24720578560303	5.68623814462357	10.26111137562445
H	0.48567749371199	3.75177732353050	12.54126827473037
H	-0.15875093380075	3.70818378991236	10.88307904814359

3_THF

Pd	1.98128392158691	5.20401831592693	16.43487328678723
P	1.87386308700032	5.50399660692367	18.63077949561165
O	2.27647663657365	4.98133017787613	14.37054777894198
O	0.82300572385838	6.67449453643036	13.91676486413066

O	4.54695374736568	5.04931734163205	12.06776200400951
N	3.67364591871346	6.50249122997806	16.47664443878268
C	2.10690762096832	7.28937953530554	19.01612709907742
C	1.38934033536178	7.87099573312258	20.07632760470015
H	0.67797103498181	7.26124638663723	20.63930507209694
C	1.57354662970648	9.21791683053386	20.42714761902520
H	0.99731986890681	9.64555292387840	21.25315937732307
C	2.49682837693145	10.00247898526978	19.72334176334780
H	2.65025985692934	11.05242344881061	19.98895898320724
C	3.22945091493576	9.43794390434543	18.67177946706938
H	3.95104645020192	10.04312316033258	18.11877019568825
C	3.04483692387812	8.08921072319103	18.29942657703671
C	0.37512983834101	5.00796416781239	19.54800796084243
C	0.41996288343744	4.06928231900902	20.59579998656867
C	-0.86770929149947	5.52657765917579	19.12177575735718
C	3.27384649210180	4.69016703510339	19.48988910876600
C	5.17893965115707	4.71970807129801	21.00272162953569
C	4.08117339161051	5.37255243398672	20.42013621716084
H	3.86237792874633	6.41192182936611	20.68185276514527
C	1.70442388865862	5.85385902877953	13.59526031363042
C	2.26130039691665	5.84821534090441	12.13327467881430
C	1.08921517817792	5.55862167162007	11.15869725410630
C	0.57169701391083	4.11769280107155	11.26234278982662
C	1.70016789322219	3.12110952580114	10.95989566392972
H	1.33748228401832	2.07944017611936	11.02405527609083
H	2.05091819184247	3.27552640418938	9.92081183284266
C	2.88061559402923	3.31418811335210	11.93457984289404
H	3.75127308714809	2.69198640409186	11.66649833603502
H	2.55722576035484	3.02526033237585	12.95225946546692
C	3.34420496100253	4.76129218985853	12.04293808690369
C	2.85604432530018	7.24176012547070	11.86109872945874

H	3.68113891461779	7.46849256655115	12.55616290347517
H	2.07024497113946	8.00390097434720	11.98394702520547
H	3.25465770806000	7.29638486051361	10.83347998357519
C	0.36563357971847	3.92641439010279	16.28416330362012
H	-0.39778176253635	4.13274251536204	17.05027424875313
H	-0.01995197085169	4.14578493690637	15.27480401501002
C	0.95394703226940	2.57626120028528	16.40373593584428
H	1.56720804589860	2.24230049767792	15.55326441941183
C	0.82460736897665	1.75214585345510	17.47309095641147
H	0.22863471784286	2.04595661479768	18.34624902885576
H	1.31356093636266	0.77270047293356	17.51088083499952
O	4.93376611793538	8.33836480467563	16.83838528817263
C	3.86066861332367	7.57968964234999	17.18248165026204
C	4.80621576864709	6.35337830048893	15.52401902463094
C	5.47011570793885	7.74695550469495	15.60484860937218
H	5.17957250896988	8.40928961577310	14.77325991827101
H	6.56354125336593	7.73319012220805	15.70554419428534
C	5.73388498537604	5.15073132030331	15.88456251313295
H	4.38993119960374	6.16287192566452	14.52297488790320
C	6.31570159812344	5.30510677822272	17.30154994829178
H	6.97130073733758	4.44858382604716	17.53589429398563
H	5.51591568554740	5.32640236589824	18.05953541832901
H	6.91964518420236	6.22475490408848	17.40493244268246
C	4.93455183152838	3.83651664956685	15.78885833281760
H	5.59546775493182	2.97782165141515	16.00480353298097
H	4.50306747516178	3.71253108130660	14.78214473480813
H	4.10220073096573	3.81803249969479	16.51509461749609
C	6.86254767506622	5.10518044493409	14.83178037573544
H	7.50640598087322	6.00226215107499	14.86513423330318
H	6.44072681526788	5.01533095939416	13.81509464041902
H	7.50910695686493	4.22908056596796	15.01667819850087

C	3.56164038627971	3.34985302546400	19.15569846503027
C	4.65305291894923	2.70162859443613	19.74853688670877
C	5.46749686613387	3.38758302254811	20.66599539087367
H	5.81030041867663	5.25598967315235	21.71829926888469
H	6.32808305354370	2.88361215213105	21.11743858568641
H	2.92601663689480	2.82353894497030	18.43378976858349
H	4.87508837002254	1.66266959702290	19.48471709646891
C	-0.77043579185360	3.65599497723029	21.21588604223455
C	-2.00314174166297	4.18151412072948	20.79869112166761
C	-2.05010614588749	5.12213167949877	19.75403596485848
H	-0.90340837937821	6.24571105576106	18.29576260476340
H	-2.92919138589083	3.85714146222432	21.28387887804281
H	-3.00991668015695	5.53185449540713	19.42420997284473
H	1.37991124848628	3.66153629065098	20.92498172994639
H	-0.73099671176745	2.92363841863745	22.02845955022158
H	0.28863390620170	6.28696187587264	11.37909760469305
H	1.43523662470492	5.75061002096538	10.12391922465634
H	0.17464602610258	3.93478867114390	12.28069413180336
H	-0.26920025830429	3.97013645587092	10.56072687927745

3_diast2

Pd	1.79120909723773	4.77199683596626	16.40315163250144
P	1.75114375326550	5.29317844461218	18.55582028146780
O	1.86793799818326	4.30727503854247	14.35167530370562
O	1.53420802431979	6.51825552124229	13.90245253289956
O	1.69523244531044	2.54893054687976	11.52251018494749
N	3.40697105297827	6.17292479018062	16.28115103040377
C	1.86007702022914	7.12265532254060	18.75751866819605
C	1.15115702714273	7.75449335489326	19.79470539517148
H	0.52722808437591	7.14889573620280	20.45742479573997
C	1.23031069935436	9.14142922641755	19.99182584748449

H	0.66185772804199	9.60689296586525	20.80326013076235
C	2.03759871432441	9.92016820430470	19.15286317471856
H	2.10624536301637	11.00275252757183	19.29643196043304
C	2.76090147107274	9.30860619356439	18.12256728657869
H	3.39486574588913	9.90379198598488	17.46192994870663
C	2.68174161277224	7.91693432470155	17.90583819539241
C	0.33787318506707	4.80264302029623	19.60620011901925
C	0.49447062493327	4.00277796758142	20.75298581725752
C	-0.95711958270455	5.17582596036917	19.18424499266196
C	3.23984511757309	4.67782092222646	19.43588681426425
C	5.21048549017475	4.99991214627777	20.82576127963344
C	4.04508087764641	5.51142513909768	20.23447079598503
H	3.76877928822891	6.55950486746054	20.38363716789144
C	1.64286645063517	5.32671862232066	13.56282400513013
C	1.45752595248294	4.90708971312391	12.06973908907496
C	1.98947166120613	6.03668691512849	11.15164801023433
C	3.51158085001810	6.21356963034016	11.25334483470188
C	4.25174713101155	4.90656342589025	10.93112386786585
H	4.07140401762754	4.63607364686305	9.87239120152483
H	5.34532957590062	5.03373743141262	11.04201338521636
C	3.76340524637874	3.75292012536380	11.83502628878141
H	4.05008207362819	3.96504392598557	12.88220778744936
H	4.20815136524006	2.78506072424954	11.55079087970133
C	2.24186979131991	3.61387084428115	11.79863983838549
C	-0.04953881264191	4.68023046561070	11.85524608860782
H	-0.41724257893953	3.88337477416235	12.52081364943047
H	-0.60184053247458	5.61144109703466	12.06539182736211
H	-0.24716641375243	4.36751211036916	10.81600286090576
C	0.25031122350907	3.39868466235926	16.45079725526722
H	-0.49617285296791	3.63466622079841	17.22458392615872
H	-0.17422266362845	3.48895907984660	15.43864916784563

C	0.94390297948050	2.11678982508756	16.68360978607268
H	1.53809675890252	1.73489719878597	15.84110649137774
C	0.91787297998949	1.40987685223883	17.84112769716216
H	0.32754560689217	1.74905988318433	18.70123988322175
H	1.46639443459870	0.46876219037492	17.95499869343281
O	4.42950871248260	8.18588300337836	16.27996518124136
C	3.48606537463739	7.35684002125233	16.80708546876194
C	4.47954605126444	6.02819909336381	15.27271852625251
C	4.96800731913793	7.48650898138720	15.11170550523780
H	4.54862417453798	7.97162251423915	14.21522489739316
H	6.05970626446153	7.61384372458167	15.13471462025104
C	5.55682058025639	4.98989055687516	15.71135171562535
H	4.01481713807897	5.66932082700307	14.34284264478839
C	6.19865266883569	5.39371184980907	17.05181813688512
H	6.96646099966848	4.65626392322790	17.34322760927465
H	5.44690740091409	5.42502005322806	17.85694299005475
H	6.69081843400543	6.38195266900239	16.99824599884357
C	4.89733768362678	3.60366032556185	15.85328502188459
H	5.65561256768459	2.84935245980228	16.12985960731509
H	4.41342402971179	3.28594271057557	14.91443589185402
H	4.11867465011831	3.61083611003826	16.63476706633875
C	6.62600453783627	4.91935689000617	14.60087479575188
H	7.17475149581938	5.87094855398720	14.48162502826603
H	6.17256636268356	4.66175426582021	13.62656829030269
H	7.36974696068466	4.13987707119297	14.84166976936848
C	3.59957068648657	3.32740635896949	19.24166467708950
C	4.75837414012925	2.82144935924206	19.84441325604274
C	5.56921727335937	3.65763545458518	20.62985846918980
H	5.84076957384265	5.65422129433431	21.43683410682036
H	6.48212680050845	3.26299422731686	21.08777327595729
H	2.96587221773574	2.68361680838699	18.61857602619512

H	5.03540985312904	1.77368016402666	19.68924374459545
C	-0.63483811744438	3.58352160983112	21.47366383320850
C	-1.91900963033071	3.96556672624374	21.05884362504865
C	-2.07857065315301	4.76763406842978	19.91567853645121
H	-1.07661454779377	5.78253703938680	18.27956057914205
H	-2.79776544031867	3.63465509108475	21.62162906464434
H	-3.07969465110069	5.06196043758890	19.58502697272674
H	1.49616065781209	3.70652802007808	21.07723863201173
H	-0.50798068083116	2.95689797311923	22.36242756430978
H	1.47563296898209	6.96903767700509	11.44239951049091
H	1.71054382024478	5.80518247885553	10.10454380464501
H	3.84590267614346	7.02006053901009	10.57478785950429
H	3.75906456330308	6.54254866058105	12.28139782550230

(exo)-4

Pd	3.76982554734718	8.51349208308285	20.38189600960167
P	4.88793178646043	9.58035117913127	22.03644334179565
O	3.10272527483990	11.99220679837320	18.37409952777174
O	2.34438629147395	10.02479514875439	17.52364728253471
O	0.93475915454870	10.23701519508732	21.14022251449127
N	4.91751764069395	9.63053308007621	19.04777674020380
C	5.05802897637301	11.36080189167074	21.62579299092888
C	5.01393324112006	12.31574556441978	22.65926191892455
H	4.88424420077682	11.97905736414261	23.69152701318672
C	5.11106730990096	13.68506576488564	22.37854388154380
H	5.05927311459698	14.41200561638174	23.19520216718265
C	5.25709455458759	14.11488201594671	21.05147516054481
H	5.31402396235634	15.18268766027001	20.81920813859280
C	5.31226271736720	13.17766528878587	20.01524567190931
H	5.38428133678044	13.49360037970991	18.97390915875837
C	5.21273782408580	11.79692607312468	20.28360512185455

C	4.16767173822351	9.57025563146250	23.71420885374294
C	4.94758108679664	9.35622081825176	24.86623433770591
C	2.77761055849694	9.79750684913735	23.82331680750381
C	6.61319802264267	8.98905676833746	22.20857820357480
C	9.01551520896308	9.36302166982945	22.31598162981155
C	7.70875552958976	9.87143619232515	22.26335484644532
H	7.53761096230115	10.95201471435077	22.25004165888573
C	2.23756134720393	11.07758398217951	18.20834870129390
C	0.82455577686341	11.30003947816907	18.96597810809990
C	0.24547359675562	12.69145638125018	18.55242994534310
C	0.95339693434099	13.91080734201674	19.15830974719434
C	1.03427181880288	13.78668170613659	20.68529939251564
H	1.56699782865845	14.65023443089356	21.12537457215270
H	0.01535435355430	13.78300404613064	21.12230497124148
C	1.77004479618847	12.48631819177791	21.06695059053876
H	1.84319907060643	12.34285350290082	22.15788741703942
H	2.78633175177434	12.54359569976549	20.64035431322963
C	1.13667633030517	11.25535825250654	20.45035843785131
C	-0.16902235990176	10.20344198974194	18.56853385855283
H	-1.11188288691408	10.30782962775486	19.13563639547993
H	0.24008073705272	9.20174858040634	18.75059922958773
H	-0.39051827208632	10.27660652196889	17.49120949363128
C	2.59932907397293	7.09821289362193	21.46752337037930
H	3.22967156822267	6.19730257206008	21.46793137936252
H	2.21393734385700	7.40277481149629	22.44568687662671
C	1.88368013086813	7.47249594346061	20.28819765144458
H	1.07068387021519	8.20240831047548	20.39252382440341
C	2.49103803076810	7.28493802541232	19.02756126256154
H	3.15242267923410	6.42747486783563	18.85138644959915
H	2.11499839500371	7.83604931336335	18.15947600743538
O	5.86540542474449	11.39345954069623	18.02070734983528

C	5.26809339670485	10.88823228077444	19.12185393896913
C	5.29749091184243	9.12096343828052	17.70341852884504
C	5.54799395441247	10.44251845871308	16.95306775285063
H	4.61554180215376	10.79919425390643	16.48752948463192
H	6.39549913403728	10.44731871524032	16.25469458643613
C	6.50328372708894	8.13290635763175	17.77553783591063
H	4.41518199178876	8.61787837389127	17.27803420433241
C	7.72140360571273	8.79011412961967	18.45439853692127
H	8.57437989954633	8.08890633760578	18.46811990745953
H	7.49531010114641	9.05940477799167	19.49933665602319
H	8.04433960157677	9.70405836703440	17.92628741917604
C	6.10066313180018	6.87653995123212	18.57195218027684
H	6.96111775509863	6.18961886862614	18.66488264260970
H	5.28153013663315	6.33220779102633	18.06952526055357
H	5.76189098706122	7.13822354896727	19.59168367963681
C	6.86249981024220	7.70153371764510	16.33816480987714
H	7.24896858389428	8.54071580796765	15.73378826087026
H	5.98304295461139	7.28227255020063	15.81616638605840
H	7.64619146358707	6.92363212479141	16.35893739414753
C	6.83729784992526	7.59625044750312	22.21310627477624
C	8.14245395776209	7.09363209961217	22.27625096165537
C	9.23385771428275	7.97714365017492	22.32129860147143
H	9.86470839118178	10.05323468748876	22.34693756593753
H	10.25498381351233	7.58387978532035	22.35452826767284
H	5.98254932831790	6.91409548254677	22.15037997432341
H	8.30980477266296	6.01180049351735	22.27522034361277
C	4.33870587227593	9.36999947171840	26.13072068485248
C	2.95982333392412	9.60445070451011	26.24474295768209
C	2.18444994578285	9.82087599833125	25.09261306581715
H	2.16597899551091	9.96016470345127	22.92279340495374
H	2.48770740311386	9.61517098684938	27.23272042768634

H	1.10810229312214	10.00172399256589	25.17911763416363
H	6.02391403792092	9.18004836747775	24.77252411160087
H	4.94410480778794	9.19865132165873	27.02690705405988
H	0.25111518838332	12.75312131520896	17.44837567064398
H	-0.82073605489871	12.70749268761774	18.85955166257797
H	1.97299379625525	13.96816008502209	18.74395968781352
H	0.40922822382379	14.83166410871979	18.87428986021695

(exo)-4_THF

Pd	3.77672104312883	8.53392133139901	20.39522764687012
P	4.91007599204133	9.57909365764347	22.05841009932505
O	3.00411817859407	11.99902632415078	18.14907102650644
O	2.19124370382016	10.03186664664707	17.35425272151909
O	0.85982451061810	10.26794386537656	21.11220016450327
N	4.90637566906197	9.65979595131289	19.05675018542189
C	5.07840820797574	11.36265551338301	21.65179780733536
C	5.02822814312601	12.31421613020987	22.68613036597177
H	4.89952966928522	11.97817353611230	23.71851153599051
C	5.12397222441532	13.68666896107754	22.41070581541451
H	5.06848055868963	14.40902951331019	23.23068155805334
C	5.28082528571939	14.12312194327196	21.08773424786759
H	5.34488573715601	15.19120741541520	20.86050872705636
C	5.34652183758980	13.18733783508378	20.04871318702503
H	5.44244410120752	13.51454093970695	19.01253224170121
C	5.24261869214716	11.80571560779869	20.31149251574627
C	4.18206138416614	9.56480320208051	23.73191623480388
C	4.95930829574769	9.34661575847835	24.88522525134127
C	2.79197702509932	9.79327459132594	23.83985194626655
C	6.63048650753972	8.98022127413348	22.22032897722199
C	9.03263698386018	9.34663416632733	22.34700300732516
C	7.72731817121255	9.86036161672233	22.29812918208597

H	7.56315417347234	10.94193294074297	22.30954193556267
C	2.13627177318342	11.07931685793080	18.06100562972776
C	0.77820862638952	11.28527827815596	18.91340325856417
C	0.16941624710794	12.68290697264338	18.55234671721572
C	0.91200091058131	13.89828552997515	19.12546377055208
C	1.09994759800433	13.75979625381698	20.64169640928833
H	1.67112093503253	14.61388104602463	21.04964807762189
H	0.11557034145687	13.75627724413359	21.15098508596402
C	1.85399513600245	12.44893640023332	20.95526913991417
H	2.01502036078560	12.30129576762425	22.03549427651665
H	2.82928066188502	12.49796829571646	20.44182349267880
C	1.13713564911151	11.24502448271208	20.38906279154357
C	-0.23896227703204	10.19271431941956	18.56732751747042
H	-1.15177325345992	10.30329537013031	19.18077066366494
H	0.17511659135790	9.18917600703109	18.73389862943923
H	-0.51873358716259	10.26680125855550	17.50322014669838
C	2.62259156301423	7.10184691079331	21.47696550433694
H	3.26557485128544	6.21060177886359	21.45864948000469
H	2.24375051682118	7.39041034483426	22.46258196155063
C	1.89322283619861	7.48628897597064	20.30898297778855
H	1.06909069522363	8.20102074970510	20.42543733748950
C	2.48823980766444	7.31997373354856	19.03907979672842
H	3.15634769574612	6.47290019407515	18.84224823500697
H	2.09446752737520	7.87590869168456	18.18201365217264
O	5.87964378784907	11.41403921591168	18.04308464582688
C	5.29956296709217	10.90082590947679	19.14935898151774
C	5.29876220173305	9.14448919996752	17.71625717472349
C	5.57193452546907	10.46150573820679	16.96855330256589
H	4.65305440120836	10.83172820088089	16.48846924949079
H	6.42901356828970	10.45847083553531	16.28343902600130
C	6.49719578126322	8.14753296740931	17.80101593950224

H	4.42144609321976	8.64096539516976	17.28171494053515
C	7.71510617258034	8.79684297350521	18.48817795333331
H	8.55974433838859	8.08615445638328	18.50745503245033
H	7.48622583062762	9.06761721956778	19.53249782449217
H	8.05092427441716	9.70530592592569	17.95816764521020
C	6.08056725538179	6.89224229659057	18.59146580349156
H	6.93698144949385	6.20096896381135	18.68564161850345
H	5.26044281241591	6.35545044551111	18.08289583523538
H	5.74146190298941	7.15057083567260	19.61217485793182
C	6.86329044049164	7.71707087705898	16.36454705932665
H	7.25627491305996	8.55612691272097	15.76441554644776
H	5.98451691796092	7.30080024351063	15.83904904891272
H	7.64407673913003	6.93664795811961	16.39363203313109
C	6.84826462943639	7.58603263433857	22.19883735876678
C	8.15252425020374	7.07878828768114	22.25716146513471
C	9.24629762093956	7.95917851654525	22.32448755175473
H	9.88318860020654	10.03361922134267	22.39906682151834
H	10.26597705203689	7.56238730383580	22.35535500175801
H	5.99419002914502	6.90439191629507	22.12329361804303
H	8.31645747406432	5.99688278960198	22.23610086823436
C	4.34665355612420	9.35683595027890	26.14886121410336
C	2.96695011604689	9.59232073717027	26.26068129493926
C	2.19330445146314	9.81388481203100	25.10704129774100
H	2.18601967617614	9.95800675409210	22.93768389622117
H	2.49231851979916	9.60040063753922	27.24717580191512
H	1.11710765426922	9.99538102535188	25.19407516560328
H	6.03603455169117	9.17164774229587	24.79616596771037
H	4.95011467453026	9.18230518852528	27.04535121304040
H	0.10078076997860	12.75646349219625	17.45058728301366
H	-0.87327371779907	12.69154808735303	18.93072836378006
H	1.90265151154340	13.96361759320150	18.64707897525214

H 0.34728490483607 14.81970655409899 18.88772238998601

(exo)-4_diast2

Pd 3.50737802494671 8.75213013966101 20.54213165485143
P 4.75218071113010 9.69633958458875 22.17835669701773
O 2.04718239154017 9.96710694441091 17.41784566819870
O 0.10995944077679 9.42861160057925 18.49045703828610
O 2.82502727952429 12.86989879490895 18.68691334066203
N 4.63497581034527 9.89750871130418 19.19707561142072
C 5.06438205211968 11.47236135505303 21.84839039744676
C 5.17360940298272 12.36624938614388 22.92986252207011
H 5.09109229357695 11.98330009821903 23.95082207421001
C 5.36952989766761 13.73747872828343 22.71299095219888
H 5.44303058387490 14.41709170074459 23.56794421129037
C 5.45377017235132 14.22994459150143 21.40335054604481
H 5.58570991280359 15.30089645593701 21.22245810076999
C 5.34584645595561 13.35376466075264 20.31854396618915
H 5.36761891117672 13.72586045085573 19.29439359330270
C 5.15682401929563 11.97115141877900 20.52206064227418
C 4.11124065924870 9.66760729760418 23.88875395008867
C 4.90089894329521 9.28863383618473 24.98974819591665
C 2.76511382752570 10.04547575595445 24.08240528492678
C 6.41932159118848 8.94112689118233 22.24131362782479
C 8.84802981022054 9.08969143835029 22.23771751050351
C 7.59346733091711 9.71762424176626 22.26304755554213
H 7.52399573175751 10.80919953356389 22.28730367152153
C 0.97363082663646 10.22828314996363 18.03886254827341
C 0.69158294133295 11.80796730676946 18.26808629299463
C -0.67870965628060 12.03098034846646 18.95668987590873
C -0.73810135243673 11.58047953916197 20.42353169010606
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H	0.24940191026562	13.31842073147424	21.28412903103593
H	0.36144160901711	11.86715741361970	22.29701911653733
C	1.76013968736786	11.91249961722394	20.62265396711770
H	1.96559170457994	10.81870630680264	20.69650115268538
H	2.57413378877310	12.43496777994839	21.14949386872185
C	1.83648363455567	12.27464654741324	19.13858071717814
C	0.73086754658243	12.49501859858117	16.89502549728311
H	0.65015731092965	13.59231414355402	16.99742368200699
H	1.67352617754854	12.25969086700161	16.38198091861755
H	-0.10838409853194	12.13897114787059	16.27174397882218
C	2.25137296756730	7.42522892706631	21.62270254694215
H	2.86673786580352	6.52296044921210	21.75206160547166
H	1.79030679918639	7.79819809164644	22.54382105125271
C	1.61923483574967	7.67598443718961	20.36058957625680
H	0.76206514077353	8.35617778025459	20.26042356026931
C	2.32305796992137	7.39186669768066	19.17862352899140
H	3.05182341682104	6.57174983165688	19.14505016787010
H	1.97163325118457	7.84443158316147	18.24322104709838
O	5.49033645463191	11.70810657287911	18.17668164171611
C	5.05643111093831	11.12948724319195	19.31422718732536
C	4.89583940269605	9.45376777875415	17.79666328383620
C	5.04810094101120	10.81163671410060	17.09588994502702
H	4.06361672164545	11.17504730024898	16.76304143284744
H	5.80796505642425	10.86796612376473	16.30542889955538
C	6.12663836093544	8.49718161886821	17.72271921547211
H	3.98379762878936	8.95832049534787	17.43286286811302
C	7.39147974674183	9.15189297147102	18.31384346314403
H	8.25553878317045	8.47272281535285	18.20566351097770
H	7.26730769532959	9.35865966110805	19.39058123410680
H	7.64289122877252	10.09956138646087	17.80681907427598
C	5.82614342221694	7.20013328413076	18.49848700135842

H	6.70870838570799	6.53545959339871	18.48843048359916
H	4.98188818209166	6.65358230353737	18.04392708372269
H	5.57354402745840	7.41156560357424	19.55309263837883
C	6.35959091914273	8.13486029744042	16.24066177557222
H	6.67436173271168	9.00689421675254	15.64129820966692
H	5.44275974338557	7.72071989787075	15.78394479951347
H	7.15550782457315	7.37378336316556	16.15651036766849
C	6.51191781045945	7.53390611986619	22.19933780139408
C	7.76628904648340	6.91213121037215	22.18580341436247
C	8.93604245199473	7.69007423498046	22.19847249867517
H	9.75831468192807	9.69771014963717	22.24341720990924
H	9.91644584282073	7.20385510654629	22.17173708475000
H	5.59560990639043	6.93494646808718	22.16108527814981
H	7.83170042057347	5.82008634275277	22.14950513460142
C	4.34464925675765	9.28714807987956	26.27873267753247
C	3.00907083145246	9.67114198563808	26.47098968927955
C	2.22076886503161	10.05451587078883	25.37189007326920
H	2.15440773294439	10.33402220121306	23.21944493432395
H	2.57880584388783	9.66897966053686	27.47757355634188
H	1.17805591302546	10.35313937913838	25.51922320530855
H	5.94447874516547	8.99646150019327	24.83665385600069
H	4.95857000932931	8.98659109323995	27.13394312641083
H	-0.92668077012542	13.11129411073754	18.89632219243772
H	-1.43937325380511	11.48381854646633	18.37377004592899
H	-1.72300772748852	11.83833357871428	20.85684894826031
H	-0.64190869092276	10.48165338485558	20.43928747929073

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Pd	3.82544092794428	8.47749709638623	20.36464342618176
P	4.83976514622663	9.58686678435991	22.05059018267148
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O	2.38850932832113	9.85912523172671	17.69268389096192
O	1.07264353610788	10.30196986453283	21.29720279526354
N	5.04227724349224	9.59821508476140	19.08354728274141
C	5.02029815603140	11.36449498651045	21.64945268108584
C	4.93485246980127	12.32616705758888	22.67327519605002
H	4.76274400627101	11.99571090135714	23.70122059499614
C	5.05003898763167	13.69290154815382	22.38740499688464
H	4.96935819420021	14.42624319664866	23.19595746010144
C	5.25261485417788	14.11168445570394	21.06431263425114
H	5.32436282188672	15.17743171641971	20.82664057381099
C	5.34763978042466	13.16679695877206	20.03785108640893
H	5.46803306932487	13.47716482027745	18.99935499752456
C	5.23468562270600	11.78735371601582	20.31065970673176
C	4.17997288208691	9.55289699659001	23.75344803226740
C	5.00279494768662	9.28761664085701	24.86541782014512
C	2.80257882601731	9.80915480396737	23.92936739767587
C	6.57043202228780	8.99051139416449	22.17892074551061
C	8.97434811649642	9.36560121459379	22.24816038175749
C	7.66628517238439	9.87294274882523	22.21729182604908
H	7.49513912399116	10.95348375166429	22.20936445535329
C	2.26316171018618	10.95765300157941	18.30210485468398
C	0.85292397106594	11.18923556912837	19.06083587415473
C	0.21472904223142	12.51390782222085	18.53526628353023
C	0.88408904012178	13.80506893426431	19.02508117308373
C	0.97455081379632	13.81721422429933	20.55679760849970
H	1.47037387655263	14.73771750101498	20.91730099259687
H	-0.04245156927524	13.80881222372307	20.99818528056939
C	1.76593278317678	12.58754355780059	21.04543588276531
H	1.84583498493631	12.53785230611565	22.14413629894220
H	2.78045157778660	12.65336833170837	20.61400673900357
C	1.19486404430873	11.28024382109182	20.53559824629836

C	-0.09883249921807	10.01830335585105	18.79416717350460
H	-1.08120326321894	10.20591831790099	19.26578178017069
H	0.29687668219224	9.08040268474375	19.20770326589716
H	-0.23914937335636	9.88508465497883	17.71013645637976
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H	2.49726093170207	7.02891102138225	22.38578595313834
H	1.49307193318620	8.14347919108311	21.28635669061365
C	2.68921279315929	6.60842263309608	20.25110463904948
C	2.65683676970226	7.16364360138832	18.95882376902160
O	5.91335268937095	11.40145890436075	18.05555582820985
C	5.34054722468826	10.87015123442658	19.15917728632948
C	5.41958314458371	9.11375633706430	17.72788831793170
C	5.62697366378951	10.44763199394596	16.98477315550787
H	4.68623728768779	10.78012766808483	16.51842273344269
H	6.47342243388296	10.48231827386836	16.28568587057715
C	6.64761242636221	8.15358586160593	17.77411182740279
H	4.54362687121462	8.59502907010186	17.30938387849653
C	7.85918891218850	8.83657241306519	18.43867253075497
H	8.72832731925090	8.15532315582304	18.43915163239858
H	7.63896192292170	9.09745857774578	19.48695001713446
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C	6.28820804065613	6.88356118420907	18.57030883648556
H	7.16247278539520	6.21011923510472	18.62823703864494
H	5.46245363747719	6.32990103972154	18.08924803115262
H	5.97702732877425	7.13195020955190	19.59947707447866
C	6.99324625087621	7.74072103242168	16.32807716972500
H	7.34439243608427	8.59354833029101	15.72109075381340
H	6.11696737031268	7.29879502053740	15.81942668367549
H	7.79910082362052	6.98551974276863	16.33065114785263
C	6.79607064083972	7.59828827245820	22.18170557409768
C	8.10251448025855	7.09624442117853	22.22239412194994

C	9.19413688509221	7.98006318932391	22.24875145322640
H	9.82319139773107	10.05676301381256	22.26565214404728
H	10.21597244558278	7.58753920853113	22.26460030968242
H	5.94022656250076	6.91610998869765	22.13391035118192
H	8.27004064624479	6.01445045186526	22.21845463099548
C	4.44870351448470	9.27739145274789	26.15434635767367
C	3.08154705463215	9.53819777489628	26.33445236891064
C	2.26447797017572	9.80696232811464	25.22333801895687
H	2.16256012592949	10.01836270402187	23.05954961082928
H	2.65193156709146	9.52978683154670	27.34173667546202
H	1.19742214863324	10.01004397984454	25.36152716143999
H	6.06978295518124	9.09106784402769	24.72223557637318
H	5.08790399033741	9.06692793698765	27.01816210095537
H	0.20465824588919	12.48002857531476	17.43002279744976
H	-0.84743615864717	12.51833501342119	18.85596970599814
H	1.89964740890939	13.85993534859574	18.60006352493384
H	0.30800987862161	14.67870886803678	18.66535143721804
H	3.17084906395342	6.64537733841968	18.14324234438877
H	1.97958417732903	7.97198066608779	18.65418830448840
H	3.27291947086861	5.69325200179439	20.42235889380808

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P	4.34758191211781	10.17536989900751	22.30817083158331
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C	5.52781938585148	11.60360606101774	22.24415969384172
C	6.06899595012110	12.13377672821824	23.42930078059057
H	5.78367278360046	11.68830460899507	24.38601535898452
C	6.96771108842054	13.21120644194800	23.41019944298812
H	7.36549760953579	13.60190189188200	24.35255441372188
C	7.35678115952664	13.77424242756236	22.18835037400271

H	8.06230477405162	14.61029332123054	22.15919296612043
C	6.83261315057877	13.26362828954262	20.99568644070336
H	7.12424154570987	13.69581652515817	20.03592401503663
C	5.91070143392224	12.19414194034016	21.00150961306569
C	4.07439261067216	9.93768054139228	24.11103723141505
C	4.94265757150007	9.19465029113778	24.93609526073748
C	2.92225390093547	10.52890856080884	24.66682302644740
C	5.44891995112128	8.76164219874000	21.87759913645188
C	7.62394118173887	7.74885623932612	21.44523198170545
C	6.85362464658042	8.85628688899137	21.83388290123590
H	7.34409035459540	9.79943844609303	22.09401912608674
O	-1.21111086076597	10.05371802789736	18.81286508039911
C	0.66797692937326	10.52111910267884	21.45426840348694
H	0.36236924309014	9.49328791813504	21.68926376145544
H	0.46251662121825	11.25104704702142	22.24910454229815
C	0.67874846269869	10.95354327308525	20.08674585109233
C	0.26805510401830	10.02884818104572	18.98093102627332
H	0.55806188443593	8.98687492543555	19.17830339805995
H	0.64050072992636	10.35013624254487	17.99584230746494
O	6.13020674523120	12.16598897973489	18.60982051985517
C	5.39710190784427	11.75282675940263	19.69110140594242
C	4.29884028544209	10.79149055021350	17.97133650338005
C	5.36138798581503	11.78209867508108	17.43158567143399
H	4.91640734250180	12.69864345144510	17.00724107270074
H	6.06831536586800	11.34964258761702	16.70893425612796
C	4.56966130148236	9.28973795045042	17.63591850676358
H	3.28944665826692	11.04859515276993	17.60579423685754
C	5.94281036799877	8.85054557904079	18.17727777195248
H	6.12826819182746	7.79247184154855	17.92510780526680
H	5.98499587456242	8.94183535138264	19.27315980508536
H	6.77007300279106	9.44393757979805	17.74761257406277

C	3.46223278718862	8.42151271717835	18.26234544997626
H	3.67969306150757	7.35058335494913	18.10276896000838
H	2.48147467708912	8.64104302397129	17.80627573326410
H	3.37519122981846	8.60281927526474	19.34909259824138
C	4.52099560429872	9.11931441905240	16.10297249558274
H	5.33388838148958	9.66388739775877	15.58956730187947
H	3.55783231212482	9.47236896418953	15.69073285700062
H	4.62670756716066	8.05222387581868	15.84032323119191
C	4.82781597360372	7.54159148996956	21.53640936227819
C	5.59934623676040	6.43526577855718	21.15965371910754
C	6.99945616227027	6.53887895415288	21.10706822092540
H	8.71503956677420	7.83409841349376	21.40459674934027
H	7.60201243456371	5.67822519068021	20.79874304640606
H	3.73439980913281	7.47541996591867	21.55460346391953
H	5.10676141976266	5.49433511820787	20.89359219941751
C	4.66417294372878	9.05621539269185	26.30356769893126
C	3.52289777153133	9.66065806230615	26.85540162836432
C	2.65290624904913	10.39820889346058	26.03607962682273
H	2.23993016241370	11.07561421477071	24.00647131596170
H	3.30659960117943	9.54828432701880	27.92297588773312
H	1.75620117092015	10.86020184764983	26.46218958604156
H	5.83138019432920	8.72340384934425	24.50381469488170
H	5.33837000794147	8.47308892679706	26.93990951524437
C	-1.89316366416832	9.11167365759135	19.50528612764787
O	-1.37802375755212	8.17459865962374	20.10961648418649
C	-3.41062007702694	9.33936921852709	19.40943038049271
C	-3.75430082905768	10.84377993847782	19.61276242862757
C	-4.08424777224103	8.54169110042063	20.55534770720893
C	-3.75816222572157	9.02456196873020	21.96280056340787
C	-3.34701295701785	11.34894221053080	21.00542141640094
H	-4.84723412675043	10.96454475455574	19.47555503518232

H	-3.25677193951431	11.42767135979931	18.82037849701904
C	-4.04275196522652	10.53884973158504	22.11059888531544
H	-3.60051743877769	12.42061595083599	21.10247025566120
H	-2.24771491829293	11.27243583593897	21.11587307144197
H	-5.13604802564627	10.70794861963033	22.05538171635758
H	-3.71830494493858	10.87961728963044	23.11059309241428
H	-2.68363840398176	8.83575681778914	22.14138145954069
H	-4.34180470935048	8.42394000048068	22.67919821129912
O	-4.88034909729664	7.63716730642187	20.32938092145363
C	-3.89432777128691	8.83609290083919	18.03702664468842
H	-4.98870613461384	8.94483589994039	17.96280911690406
H	-3.65606165829858	7.76868607057119	17.90602771413209
H	-3.41633346297205	9.41622014779227	17.23063806837667
H	0.52632673417816	12.02168140898884	19.87532293524547

(endo/t-P)-5

Pd	3.36621561892868	9.35464153710594	19.07209178253903
P	3.87560443787314	9.81937095716794	21.23774029741000
N	5.46752570682421	10.00442834016532	18.66238236271576
C	4.82365401241862	11.40176993270764	21.38552204581813
C	4.60779851830644	12.25847177162333	22.48101253601333
H	3.87505436280280	11.96882920056900	23.23925859660444
C	5.30693171033245	13.46626539756409	22.62037741896019
H	5.10989332036202	14.11170637181907	23.48260923672294
C	6.25776035965851	13.83436139669783	21.65993484880168
H	6.81264899207764	14.77267907823320	21.75628805337285
C	6.49965111574210	12.99237745430287	20.56916350372738
H	7.24309764921217	13.26658116262263	19.81774022084990
C	5.79168665607774	11.78058641237684	20.40713603799439
C	2.54748997295631	9.99794432950210	22.49531323202029
C	2.43701006963708	9.15611334081600	23.61922928672431

C	1.52472945338243	10.93821308853586	22.23614451641027
C	5.03954763204930	8.60331486272518	21.98552800159518
C	7.06873439360244	7.99611073461129	23.19116379413498
C	6.17679856365440	8.97566864282229	22.72822754031290
H	6.37035135414776	10.03290142116015	22.93363647534981
O	-0.89104574795072	9.03027308793047	19.19319520097689
C	0.40449718124954	9.71959283072089	19.05816201956412
H	0.60615320769048	10.17438882442251	20.03891794400721
H	0.31003805173715	10.52665347805511	18.31101224380081
C	1.42826462949288	8.68885060602693	18.65958751465170
H	1.28449435057415	7.72015826863222	19.16127463760343
C	2.12714437518703	8.72693679294029	17.41524416092711
H	2.50045417030719	7.79666640035614	16.97089015846696
H	1.92546447476863	9.53619390874262	16.70083599169667
O	7.33089748360536	11.29551910558646	18.63465016688387
C	6.13544024337947	10.96883798171806	19.22129750109449
C	6.30072391447381	9.43255581071825	17.57838931944257
C	7.41633832289121	10.49627126513566	17.41863330504145
H	7.24690336942271	11.16923687041043	16.56040971548655
H	8.43700141849449	10.09023601137876	17.36935525175581
C	6.80756964450664	7.99575683226418	17.93082479262277
H	5.67813896663279	9.36299897694349	16.66980982440717
C	7.60455509533126	8.00751115864341	19.24932999054146
H	7.97324670813695	6.99286548935153	19.47841152780984
H	6.97257584977077	8.32801659045940	20.09240172671109
H	8.48268456571386	8.67661186613537	19.19993255308669
C	5.60306641590082	7.04505885650790	18.06476178677774
H	5.94834654352888	6.02951912514661	18.32958637869596
H	5.03723231121985	6.98192917350439	17.11819656373759
H	4.90212663832942	7.39300600173625	18.84582264039931
C	7.69698300226036	7.49866059952676	16.77148023853062

H	8.62144198404031	8.09310622389091	16.65902892411079
H	7.15290553602855	7.52559111075566	15.80948433995401
H	8.00234052214247	6.45361399940733	16.95463685375783
C	4.80251664537237	7.23635989252145	21.72426810024840
C	5.68477379700992	6.25961321416611	22.20312827543222
C	6.82520835962180	6.63897316917138	22.93038725756924
H	7.95751514402106	8.29544472897758	23.75672201763589
H	7.52538182763136	5.87744491736745	23.28920718329696
H	3.93005118597690	6.95341780011631	21.12496799763290
H	5.49171032565852	5.20242442286188	21.99354986951122
C	1.32273974232353	9.25545696649349	24.46753411360068
C	0.31588670965947	10.19802006477400	24.20804442792699
C	0.41921661853730	11.04174969938726	23.08855673569735
H	1.60119528390074	11.59246539533933	21.36067077221228
H	-0.55154165963700	10.27321523201601	24.87146044166594
H	-0.36975108711049	11.76439885258853	22.86210611905697
H	3.22185592034616	8.42268054353726	23.82764014664963
H	1.24555320624345	8.59580455633298	25.33843591470180
C	-1.78690048273177	9.62418677101045	20.01896879343171
O	-1.67888793903292	10.76743361500483	20.44993264658553
C	-2.91567402530486	8.63498365888999	20.35346199711673
C	-3.76267578195923	9.17908287453920	21.53661873439600
C	-2.24625234143995	7.31018742916915	20.80695784371751
C	-1.41691095138674	7.42647916716755	22.07835414835938
C	-2.98427873335729	9.26447842623332	22.86051898133836
H	-4.63437540595923	8.50691285497179	21.65600462985754
H	-4.14961911535570	10.17508330721605	21.25755384834346
C	-2.32279979034137	7.92830533901563	23.22962868722723
H	-3.66699787729536	9.58788456616597	23.66799176896584
H	-2.20697819151303	10.04095390985626	22.76148230908458
H	-3.09750485672371	7.16456188017572	23.43685223543443

H	-1.71892768420102	8.03358431097464	24.14876338274973
H	-0.59694011644735	8.15567233700033	21.92786133871590
H	-0.97203928059578	6.44350850067414	22.30206194429910
O	-2.44850570407260	6.24537044235122	20.23491514360454
C	-3.77837617185182	8.40015690579107	19.10133700255074
H	-4.55105854883805	7.64476660966479	19.31852006043223
H	-3.16327781400299	8.02533288001728	18.26969367548084
H	-4.27062100237945	9.33860422067877	18.79325659693138

(exo/t-N)-5

Pd	3.09928839251058	9.61000075673209	21.28013025367354
P	4.71044110873229	9.79686351444528	22.87400475870652
N	4.55319737264266	10.77109053236277	20.03374073344426
C	5.37065805820842	11.52121047808155	22.94596310644381
C	5.62073707549157	12.14325880981463	24.18286616291806
H	5.44083605910065	11.58308069412660	25.10427881003458
C	6.09736801887263	13.46047140445656	24.25555508281613
H	6.27729678030233	13.91850189797824	25.23394976248555
C	6.34233012770464	14.17984196330692	23.07872252987418
H	6.71097217537524	15.20942682485082	23.12238974879980
C	6.09955387995485	13.58179312889724	21.83774892037913
H	6.25112641213406	14.13953840741781	20.91307708826962
C	5.60726377287910	12.26227155167839	21.75046540256781
C	4.41622608606956	9.38550489586788	24.64167568832627
C	5.42144754515896	8.91316819310173	25.50903534145762
C	3.10254356350161	9.55219007309611	25.12403633485646
C	6.22680066386584	8.82948865705268	22.47096508204206
C	8.63082306544056	8.59355509811719	22.14173240930900
C	7.52599253017292	9.37054048320172	22.52439093249773
H	7.67100680408918	10.40424335284956	22.85304514065031
O	0.51691938170708	11.29314791605027	20.33358618538846

C	1.32780306245657	8.61502039018278	21.75073248495940
H	1.54808991651170	7.58874650639420	22.07442077685950
H	0.70467836319438	9.18270104583356	22.45718423031390
C	1.26528514238292	8.92529490775437	20.35396059165949
H	1.51620501544267	8.12886999643711	19.63882705948892
C	0.31022367674124	9.94413592044542	19.77915085528885
H	-0.74300083071409	9.73728919012772	20.04004895738918
H	0.41223350898562	10.01179591017201	18.68547327195394
O	5.96709138498179	12.41655660292288	19.38673925823304
C	5.33479992459807	11.74776643887738	20.39387712424783
C	4.65587739995545	10.61953575087882	18.56012873709658
C	5.35876767621961	11.93428881174342	18.15096594139312
H	4.64089029428110	12.70178502632765	17.81839417566567
H	6.16674846946406	11.82540773613165	17.41358739795359
C	5.40161436537735	9.31014600150625	18.15349773964975
H	3.63031215382107	10.58552355836598	18.16013182332687
C	6.81858423517582	9.27167597105154	18.75557610764088
H	7.33755393541323	8.34548770195871	18.45286826316890
H	6.78111736899045	9.28683753967363	19.85587090062096
H	7.43468796970372	10.12487585894039	18.41907208094000
C	4.59751335975705	8.09156199102767	18.64479880922529
H	5.11881775778132	7.15519309908598	18.37465777300023
H	3.59128834911778	8.07204662224253	18.18912203626572
H	4.46289660036948	8.11621862522627	19.74133685970746
C	5.47455283583441	9.25757648962299	16.61269790422138
H	6.09602408906640	10.06789368496268	16.19119665459656
H	4.46723074521452	9.33048809588584	16.16326115025609
H	5.92086602362283	8.30088345198161	16.28819349834605
C	6.05116977620668	7.49812018282745	22.03826181659729
C	7.15596165680283	6.72150155744696	21.66798611277159
C	8.44845259669138	7.27033424483267	21.71289494121092

H	9.63626541448579	9.02648841247015	22.17544678897614
H	9.31106655660817	6.66865050075718	21.40811429435007
H	5.03679382816211	7.08898697722887	21.97583986203370
H	7.00750378453883	5.69118670282461	21.32816416186115
C	5.11523771307153	8.62263474496407	26.84652662782049
C	3.80824543552546	8.80671607492521	27.32655645150393
C	2.80238466526167	9.27311305656955	26.46441014340623
H	2.32542572154056	9.88836761663593	24.42803818015721
H	3.57188694962432	8.57758025809326	28.37105498853381
H	1.78025382650769	9.40671852904563	26.83426292182146
H	6.43991307024967	8.77228433071848	25.13239922573543
H	5.89836089275995	8.25102315544589	27.51610667684395
C	1.33669776071238	12.10102298606021	19.63044726657958
O	1.79261562569416	11.83621945011467	18.51843601849916
C	1.59839215369570	13.40910587485685	20.39867409879278
C	0.26448276981711	14.21144147536907	20.51106087096311
C	2.61781938068969	14.23380479453268	19.57568017437933
C	2.11271647653007	14.85259861617687	18.27968821473945
C	-0.26455904141160	14.69769484570922	19.15513229153493
H	0.45240471793796	15.08271203640178	21.16916300058264
H	-0.47486200247851	13.57221843228531	21.02348532399970
C	0.77034167232213	15.59505182099169	18.46104681391851
H	-1.21290120240647	15.24638647875876	19.30008586196602
H	-0.49622080891560	13.82774069491757	18.51002955608494
H	0.93346231129929	16.50371218631925	19.07310096269265
H	0.40124624669600	15.93683739621554	17.47731811224822
H	1.96885896196297	14.01433653290952	17.57259328857581
H	2.90390613364119	15.51172130622109	17.88568041423755
O	3.77188759516299	14.39737540417371	19.96319826181001
C	2.14550767791709	13.08197439188883	21.80056537213272
H	2.57517101406561	13.98613781918245	22.26060043975436

H	2.92920041655560	12.31063869424727	21.75330502266041
H	1.33532858481436	12.69129085863469	22.43565350181455

(exo/t-P)-5

Pd	4.04537252694370	9.64613856831264	18.43647835369882
P	4.14942573055338	9.91581704861252	20.69521261063024
N	6.22645377464897	10.15155000735279	18.53031373980191
C	5.01746215004576	11.50757651223709	21.05802206086783
C	4.52749577285320	12.38184553670515	22.04438686992263
H	3.62585920982870	12.10189398093502	22.59625898642060
C	5.17169867335121	13.59347171096355	22.33704739762917
H	4.76084147005037	14.25401448934768	23.10764738415483
C	6.33996352168187	13.94634800054274	21.64972346033419
H	6.85690848811123	14.88434556927457	21.87462160092742
C	6.84479626466220	13.09337631356801	20.66156897599186
H	7.75067307033645	13.36107240002500	20.11315396210649
C	6.19343784286570	11.88295578586426	20.33909092594977
C	2.64799729129482	9.94772561951127	21.75538004465885
C	2.67120316771499	9.68382815656876	23.14098504181778
C	1.41617254374686	10.17866169532762	21.11181510750193
C	5.22473662421010	8.70073156408878	21.57202373460841
C	7.07101800066074	8.08342040786613	23.04025219695511
C	6.25808762108111	9.06773013021473	22.45565088772682
H	6.43401668725842	10.12461295543373	22.67850118068396
O	0.21723592571838	7.87221870225254	17.36297111823931
C	1.52267708847181	8.11564667325775	18.03406244820728
C	2.19935429674766	9.34902530274650	17.50436123408845
C	3.20156944624011	9.30771574058353	16.48564410798089
O	8.08061067600540	11.39153141536599	18.93637995132541
C	6.78326364224525	11.08033242974177	19.24869545982248
C	7.23931596744792	9.61366252570825	17.59445012393750

C	8.40538414041135	10.62713665812040	17.73769917805808
H	8.46503583635005	11.33538388376805	16.89378083884643
H	9.39251597342429	10.17025254119656	17.90111406435010
C	7.60800728083111	8.13115907546826	17.91797030580024
H	6.80709991360546	9.64233134760507	16.57885705471329
C	8.16404284916673	8.00890630474577	19.34872326255758
H	8.41427761408404	6.95730886334282	19.57069945863973
H	7.42117167670528	8.33749774006814	20.09137365825000
H	9.08381119747766	8.60475483671404	19.49126749412726
C	6.35059492444669	7.25227251160452	17.77417776862670
H	6.59400862448518	6.19943333369853	18.00451541523919
H	5.94849962788444	7.29725730839596	16.74626282626768
H	5.54827747377655	7.58607616039692	18.45740441551436
C	8.66019703038994	7.66140311786068	16.89176583752035
H	9.60899472891389	8.22218825331298	16.97239487918951
H	8.28608837001099	7.76834040890490	15.85700399605056
H	8.89642902873790	6.59531744078611	17.05510459132118
C	5.01289783438729	7.33442978475046	21.28981849210170
C	5.81667139123775	6.35386665913255	21.88357497225155
C	6.85283886058426	6.72718992948678	22.75608944141692
H	7.87834814762035	8.37940671074139	23.71858260965055
H	7.49136062928456	5.96181978904873	23.20925460156351
H	4.22128801842578	7.05218690061496	20.58686161130215
H	5.64470905573331	5.29695242537262	21.65460276450167
C	1.47430589065158	9.66684917864048	23.87075737141860
C	0.24891256898365	9.90098010369470	23.22259785366083
C	0.21961095181577	10.15349032542497	21.84240935137677
H	1.39405838311891	10.34887523275610	20.03135325255851
H	-0.68436786652384	9.87241325454320	23.79525975645153
H	-0.72713264619361	10.30866147167194	21.31694088173454
H	3.62451663939327	9.47943325470762	23.64004317443701

H	1.49558394704820	9.45934107733235	24.94610482569049
C	-0.80416580353055	8.64169753876188	17.79901703706406
O	-0.71873336999975	9.48061777321420	18.69227664197210
C	-2.08083892331737	8.35913449795387	16.98815085156912
C	-3.31766145422262	8.78309506367748	17.82639765757245
C	-2.19127486158252	6.84558460252263	16.68650920853822
C	-2.37958694109997	5.96133349351014	17.91324422317943
C	-3.51740975513246	7.91325715811105	19.07793809202188
H	-4.20949956737890	8.71371222091425	17.17412255916855
H	-3.19169159342482	9.84256718945782	18.10902547747943
C	-3.61916802663371	6.42311669614415	18.71750722277389
H	-4.42752622654865	8.23848157925756	19.61435475952304
H	-2.66707997369464	8.07496072661607	19.76619918234988
H	-4.52663879487271	6.24893566027755	18.10717973169424
H	-3.72355641862685	5.80431500336351	19.62720509021973
H	-1.47967926898599	6.04766304337509	18.55254828508026
H	-2.46858019768176	4.91461606727343	17.58038996980910
O	-2.21055932571873	6.40695100757867	15.54189161118695
C	-1.98452126670986	9.16455659548964	15.67807690357725
H	-2.87226435586663	8.96878149387431	15.05496646193717
H	-1.09463875266188	8.86632301951265	15.10307562748388
H	-1.92808123214895	10.24395733393947	15.89867879352503
H	1.59697462329783	10.26214685359196	17.61127657240932
H	3.33147317797144	10.16304726326743	15.81151383420235
H	3.51526943453007	8.33959420906077	16.07145966520501
H	1.31482627150375	8.18625666334557	19.11307630267007
H	2.09808703149110	7.20401211959196	17.81541326660913

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Pd	1.95301251474945	5.18690105184296	16.40101348756917
P	1.85434575751609	5.48084576029848	18.59416626187016

O	2.13734481085593	4.90588318129688	14.32555073161176
O	1.82973719837792	7.15898871339354	14.16931267977900
N	3.67999726737768	6.45422480156953	16.48825658970734
C	2.10546775364878	7.26093176815599	19.00392386711035
C	1.40160004424171	7.84029568511699	20.07459272489182
H	0.69475653428422	7.22659437063287	20.63937031563970
C	1.58998537080158	9.18503016679776	20.42789723056691
H	1.02277345036379	9.61125866832374	21.26152300701481
C	2.50427009155262	9.97144271880913	19.71544775023852
H	2.65930423972963	11.02152279894544	19.98138865431565
C	3.22392497934867	9.40985824296573	18.65458949804660
H	3.94021177188485	10.01169436318119	18.09133073637425
C	3.03508071073250	8.06276953492532	18.28057377447402
C	0.35839058892500	5.00802355491025	19.53275311147671
C	0.39407356649907	4.08172393406282	20.59101362939900
C	-0.88045562630177	5.53241215448736	19.10323728851318
C	3.24461192048820	4.65065044945908	19.46100736835466
C	5.17072117380408	4.65565061930856	20.94798392958480
C	4.07795290110957	5.32361482301899	20.37407817079915
H	3.88124206949375	6.37000278797290	20.62580107083022
C	1.99548244675813	6.03302330970693	13.66399045231338
C	0.30743548658971	3.94911560522494	16.24556486293099
H	-0.48106059032012	4.21478386879739	16.96677575852963
H	-0.01735953852184	4.13174617021753	15.20930675898356
C	0.85112229390219	2.59305946807801	16.45768953898481
H	1.49771985534429	2.20728479186582	15.65587651831745
C	0.63816310757220	1.81838279826249	17.55058015111802
H	-0.00529631871697	2.15627874547413	18.37160082410766
H	1.08793756683733	0.82444650419132	17.64926961053037
O	4.88610021296066	8.34201815255454	16.77748262208020
C	3.84178290432728	7.55358842977565	17.15840242600187

C	4.78434219051824	6.32586465734035	15.51076366368605
C	5.41894811199033	7.73616807618569	15.55621604906766
H	5.10066775873653	8.36715865446997	14.71068873404735
H	6.51493607273072	7.74667388963475	15.64369589941641
C	5.73497310922789	5.13879794742931	15.85799185801140
H	4.33655664008811	6.12629149379907	14.52603920035690
C	6.33495302575976	5.30401926145842	17.26645625477943
H	7.00998341742158	4.46079816759934	17.49396181761277
H	5.54502917315574	5.31239642195590	18.03447178558082
H	6.92254304855261	6.23533067374255	17.36355825093998
C	4.94271194461496	3.81861349967342	15.78083842858689
H	5.61587068500046	2.96102151939613	15.96101444059487
H	4.46268209086023	3.69793923363896	14.79506201928616
H	4.13983929145854	3.79119056058185	16.53786946536037
C	6.85455527165621	5.10275950005100	14.79659973285147
H	7.49307366240908	6.00429606242804	14.82326028497170
H	6.43442580285252	5.01006680755350	13.77857625767343
H	7.51091349439114	4.23214242386187	14.97047310865535
C	3.50272571805191	3.30224614810092	19.13521857598540
C	4.58830179079110	2.63884980274167	19.72118105535840
C	5.42842608689536	3.31582611311229	20.62099383341858
H	5.82388583965597	5.18640011449041	21.64839815731790
H	6.28526899951408	2.79910739558750	21.06569537881260
H	2.84537614264555	2.78443968315519	18.42597505010650
H	4.78628761252288	1.59318560547077	19.46395162689686
C	-0.79876246290943	3.68658733946024	21.21667948603057
C	-2.02660776545958	4.21738485021970	20.79488621317514
C	-2.06538624382659	5.14603312593714	19.74049924351883
H	-0.90643318497415	6.23959844692031	18.26655815778834
H	-2.95545418872353	3.90487787736117	21.28289577987880
H	-3.02240420601145	5.55773356958283	19.40445649673224

H	1.35175219065761	3.66794858316640	20.91944236188599
H	-0.76590166874985	2.96129560724355	22.03621688104036
C	2.05311045565480	5.84251153551776	12.14341646713698
H	2.12433091660446	6.81697691894549	11.63754726552907
H	1.13806991937284	5.32665463473839	11.80289705442978
H	2.90742274064720	5.20398580382380	11.86154226141292

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Pd	3.62576946115543	8.52091244337630	20.17726813243701
P	4.61873511764579	9.61620145496597	21.89697203219909
O	2.02276025973152	10.84405908599532	21.51735406160215
O	2.25946619866847	10.35454374715676	19.30755323733428
N	5.03383644454904	9.54818509863936	18.94396002953300
C	4.74571167491207	11.38985108061292	21.44051351278174
C	4.54950629520853	12.38218430053012	22.41431659408338
H	4.30489509398441	12.07664150771061	23.43501971648648
C	4.63251318797196	13.74162046266000	22.08853015472728
H	4.46249015728502	14.49697661773186	22.86245685519782
C	4.92028267912007	14.12812890348978	20.77093029429055
H	4.98098740158595	15.18766383611660	20.50382148818669
C	5.12618095874477	13.15318499579823	19.79087887522683
H	5.34656288351370	13.44356618127514	18.76165267907218
C	5.04159192035060	11.77695255205033	20.10317772671387
C	4.07234053274100	9.52877798765519	23.64799794244737
C	5.01607471441071	9.47179495987182	24.69559936395463
C	2.69447567946748	9.45785056545394	23.94492606149390
C	6.39930923470986	9.13848417912007	22.02884757171011
C	8.78199015457244	9.64906041146899	22.12373772899223
C	7.44665536662112	10.07928118456900	22.05925776155008
H	7.21721815505524	11.14866318558363	22.02687279104669
C	1.83308321704313	11.06633687911616	20.28188335176964

C	2.21615570649422	7.31405398827779	21.18154302915800
H	2.46025122848342	6.97458348138044	22.19387259169572
H	1.29297010319242	7.89990369617788	21.09498812984685
C	2.70208689580326	6.57377953183928	20.05223335877925
C	2.54573223116802	7.17193837053062	18.77939715156180
O	5.87106773643625	11.36470341487719	17.89696221022152
C	5.28835765475965	10.82478938014969	19.00700608219295
C	5.52923494618349	9.02475450604736	17.64963998798359
C	5.85462259844287	10.32612976503360	16.87541170042531
H	5.07532586156717	10.59126798272877	16.14151787535461
H	6.84025502714600	10.33558603986894	16.38797601724855
C	6.72589134009337	8.03802192032826	17.82057098405178
H	4.69861322312447	8.48135066347130	17.16758331155806
C	7.88674764824395	8.72043187843586	18.56693600293792
H	8.73240593004870	8.02029828097116	18.67887682098852
H	7.57642996812162	9.03390507506228	19.57534688376788
H	8.26108346823320	9.60995387074476	18.02857975046058
C	6.25758045554977	6.80276953401320	18.61371625017230
H	7.10407759650285	6.11230040172951	18.77786405405397
H	5.47115575829264	6.25358547065797	18.06451436434629
H	5.84469885547807	7.09488404167232	19.59345732454352
C	7.18182661329487	7.57976025563546	16.41942866288903
H	7.59550971744030	8.40777039377200	15.81641018276775
H	6.34587415744816	7.12904401370354	15.85317172261004
H	7.97419733538628	6.81649307597800	16.51231526362017
C	6.70834428402150	7.76354973855720	22.07413436122481
C	8.03937476679369	7.33591662240913	22.14942534652767
C	9.08070321821706	8.27938071588067	22.16829269262127
H	9.58993955292493	10.38824531363252	22.13607002806850
H	10.12265413989867	7.94591167443518	22.21313960653529
H	5.89147872564309	7.03404178963456	22.03490784516815

H	8.26683993312938	6.26526541728269	22.18154169730433
C	4.58586916274052	9.34636848139259	26.02452182575474
C	3.21587872584349	9.26998362788569	26.31696770280709
C	2.27543834405740	9.32828036687640	25.27555768093360
H	1.98079855595535	9.55528882975914	23.12326892679398
H	2.88177861981090	9.16743001894069	27.35504284079233
H	1.20470046901160	9.27712956592490	25.49988185381392
H	6.08575002064116	9.52132764768425	24.47330661632534
H	5.32545733443369	9.30497034692258	26.83121389647885
H	3.06456450485159	6.75041183844666	17.91192663455826
H	1.69721983119636	7.83206204096922	18.56961814188630
H	3.38065744339124	5.72353766048908	20.18973019163004
C	1.08535689180585	12.35904485036584	19.91659654074401
H	1.79693319988496	13.20160088749783	19.99248127969601
H	0.26936826664378	12.55193944237403	20.63202797464253
H	0.69235516312044	12.32508246860383	18.88841863961959

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Pd	3.62799603197888	8.46379289791822	20.75579887820054
P	4.72653947795826	9.57326347378583	22.39167697955028
O	1.10239524300729	10.21975234940778	21.75574996835816
O	2.35204957861575	10.55523198824775	19.88700184494911
N	4.92785929741976	9.50773409655552	19.43242873445815
C	4.77540789589921	11.34975603807011	21.92000200918229
C	4.65525859095977	12.33577001100713	22.91291821017768
H	4.52970662851021	12.02655428224555	23.95419933395770
C	4.68096281318395	13.70117889670813	22.58862095879900
H	4.57718794445827	14.45012032260686	23.38000391134454
C	4.83625603852190	14.09337572557364	21.25293407891049
H	4.85292045247022	15.15421888098469	20.98486509331975
C	4.95950212549487	13.12442410360997	20.25152554193954

H	5.06978916658334	13.42249854861702	19.20708586586168
C	4.91885420226645	11.74858621549106	20.56028443456249
C	4.11025790574511	9.56391719139407	24.11219742207596
C	4.96360086637437	9.32949130271816	25.20800954298390
C	2.73071073820487	9.79488185189264	24.31379910535646
C	6.49985314944272	9.11335780199689	22.51126998741676
C	8.87212783077056	9.65968567824533	22.56013165539861
C	7.53079296491519	10.07174754872067	22.53155636507306
H	7.28211847794300	11.13717474013809	22.51315192726608
C	1.62174447698767	10.95502834422722	20.86000482526734
C	2.48971652076748	7.06440862317684	21.90368221697292
H	3.11949586087718	6.16652929054686	21.95845010017488
H	2.10169916489019	7.43872474167752	22.85582252363594
C	1.78496740835351	7.38215786497948	20.70320724052333
H	0.97727153540127	8.12156850294275	20.77042899227785
C	2.41138519841358	7.11674096927446	19.46196391698485
H	3.07427767497471	6.25052244798534	19.34529029972077
H	1.99496739919306	7.54760222909650	18.54665124063643
O	5.54212871120874	11.35026441442549	18.28441970626743
C	5.09190983496550	10.80010478093572	19.44614020774613
C	5.34170806420769	8.98277064400826	18.11380802879500
C	5.55094946248520	10.28163568683669	17.29291863593105
H	4.72823507942765	10.47646617795157	16.58596183901927
H	6.51425059326612	10.33988970510111	16.76495092447141
C	6.58602342291469	8.04771420853515	18.22356667681568
H	4.50257093474745	8.39371398457272	17.70462294823542
C	7.75343235146251	8.78028897122188	18.91100633276983
H	8.63805221913443	8.12251052970305	18.96483228614364
H	7.48732207643024	9.06955372842232	19.93971088371125
H	8.05077087015837	9.69231738520397	18.36194455366584
C	6.20243685788624	6.80030755839226	19.04340442711030

H	7.08335830526399	6.14933324807879	19.18631499642201
H	5.42235441708729	6.21242215498391	18.52641419560772
H	5.80854123231167	7.08240357730012	20.03516946424103
C	6.99181019256222	7.60068228833031	16.80394704345606
H	7.34777126530558	8.44117636989284	16.18167821719440
H	6.14621855202413	7.11991518701861	16.27838653693464
H	7.81362608591512	6.86546530036043	16.86007994168004
C	6.82489588220259	7.74126284578974	22.52990909544451
C	8.16404104290167	7.33383314096875	22.57085463922145
C	9.19031594250498	8.29332318463031	22.57868719140716
H	9.66994906122382	10.40961075445404	22.56383998514031
H	10.23774102973434	7.97489621734218	22.59439643738154
H	6.01816131306749	7.00101714389687	22.49435483188776
H	8.40829727342024	6.26667202338868	22.58215179767757
C	4.43875946962519	9.32163128087595	26.50921970624993
C	3.07055205063301	9.55474248819333	26.71675637566245
C	2.22421611307133	9.79435053561879	25.62080104939681
H	2.07034128981304	9.98330164356966	23.44936754682831
H	2.66360524296072	9.54859046108487	27.73365865411014
H	1.15645039926604	9.97762868125205	25.78049868779449
H	6.03136363322201	9.15414858827430	25.04455731316571
H	5.10188445560350	9.13523723421942	27.36064836966176
C	1.39222345160506	12.47429897296539	20.97610570769002
H	1.74858602801166	13.01459281151518	20.08502690800940
H	1.94034350794095	12.85034013191046	21.85889809153732
H	0.32221962384497	12.68537899893269	21.14198656017852

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Pd	2.19246626376732	5.11959570493252	16.32210054487479
P	1.86140028107275	5.45538378075908	18.47833903169823
O	2.64064643440838	4.90204825641478	14.27294551521374

O	1.84372247332588	7.04520529141939	14.08452675490212
N	3.85198436852935	6.46691490997374	16.52255088134975
C	1.99489035268419	7.25769427181886	18.84657113254874
C	1.15532232947396	7.83470161267115	19.81608373177752
H	0.41842896125153	7.20560267845433	20.32241638062388
C	1.24659162729857	9.19612353682987	20.14256505863435
H	0.57453447848373	9.61908150432584	20.89600999713496
C	2.19822075643258	10.00346034713096	19.50664069730756
H	2.27846627734263	11.06664095905027	19.75263569079167
C	3.05192781961835	9.44556275133365	18.54829167920903
H	3.79907107019760	10.06363481480749	18.04589401058155
C	2.96206873712956	8.08137727351783	18.20040075485434
C	0.29430647117191	4.94307984192241	19.26598101155596
C	0.25505568438029	4.05022362066446	20.35243436363664
C	-0.91134218828660	5.39878806017385	18.68882949037685
C	3.18660903064299	4.71217966974045	19.50846342294202
C	4.94231052924560	4.84418847371358	21.18756716860218
C	3.88794962539338	5.44598885376887	20.48356739371673
H	3.62014788218789	6.48802600836903	20.68213113960998
C	2.44976524856709	6.04297009330135	13.68194486380515
C	0.63887834062336	3.79505087397139	16.02926479746310
H	-0.23590829951736	4.03818065345367	16.65184571162100
H	0.42469359410686	3.94494154707970	14.95934223246181
C	1.21775603654794	2.47190073638533	16.33426588193057
H	1.96166430361024	2.09724708628253	15.61592662919577
C	0.92370830966527	1.71438941369686	17.42033878055164
H	0.18250695829594	2.04188956859131	18.15906604135663
H	1.40237849453650	0.74454555403819	17.59363410460317
O	4.96319465906459	8.39475523879992	16.91108916442255
C	3.90592438921750	7.58138328471418	17.18563289093022
C	5.06586722784418	6.35391374050124	15.67766522923284

C	5.66771491722936	7.77616947317003	15.78649264054103
H	5.46859262474535	8.39060371029376	14.89362332137812
H	6.74047700398094	7.80247543424513	16.02599672648767
C	5.99646702615440	5.19167755730432	16.14473189754138
H	4.74826229601191	6.13361738856191	14.64616064484920
C	6.42887074583476	5.38620083143342	17.60955431537581
H	7.08754050269580	4.55837269384827	17.92427303172914
H	5.55688320170332	5.38968773243198	18.28289496491789
H	6.98682982518635	6.32859208027780	17.76030198213316
C	5.25022201106286	3.85108240640628	15.99494995433587
H	5.91989362796182	3.01383487347438	16.26235669326333
H	4.89010400350485	3.70823884293566	14.96251744987404
H	4.36743621372387	3.80990033802085	16.65743797379367
C	7.22792610532232	5.17359193692871	15.21471772832405
H	7.83736470627088	6.09163397613899	15.29984363280410
H	6.92539690458349	5.05846020031766	14.15831134608718
H	7.88198818566585	4.32262241063470	15.47346998880088
C	3.53653070669836	3.36975091740190	19.25081579958140
C	4.58233303809495	2.77268726733569	19.96596127192933
C	5.29188884666520	3.51034255749823	20.92836480774476
H	5.49384369825741	5.42185046489251	21.93651846212781
H	6.11901580194512	3.04554859153118	21.47488124135637
H	2.98174256231879	2.80463096175333	18.49200710309444
H	4.85259477037425	1.73165204078647	19.76133655547627
C	-0.98084715813666	3.61994747666995	20.86025728865867
C	-2.17691562784746	4.08265211237886	20.29227011151543
C	-2.14073511607199	4.97776033900525	19.20908553398304
H	-0.87618453274100	6.07888769604488	17.83027347830538
H	-3.13911834598752	3.74266650028539	20.68861549253816
H	-3.07228073171042	5.33557928289112	18.75921982182885
H	1.18832230894832	3.68984947107754	20.79450051361682

H	-1.00653578594997	2.92070989870302	21.70233037794268
O	3.09537919315254	6.03138970364906	12.42984495131439
C	3.08400103343349	7.24090540320837	11.71937393091053
C	2.43417771036816	7.31340472672680	10.53872428706726
C	3.92330928104724	8.34068705535503	12.32021839993885
C	2.53021829885677	8.55971251773053	9.67980618764000
C	3.67650364333807	9.68834677735922	11.62431912703001
H	4.99624823650497	8.05863312029346	12.25227689360564
H	3.66962762137945	8.41134743075403	13.39292150519176
C	1.57754057077637	6.19168010185405	10.01406624741645
H	1.54864552567038	5.34340867593045	10.71368113757270
H	1.95390211792802	5.82712659554877	9.03801972329213
H	0.54048628380252	6.54015047262508	9.84073635110456
C	3.66660757683260	9.50667865287452	10.09994712114769
H	1.55895526319181	9.09832531259065	9.71569129048980
H	2.65867103662763	8.26145024189248	8.61961281567639
H	3.56042326739925	10.47969680655758	9.58619964547296
H	4.63692220297731	9.07846611618892	9.78031821907735
H	4.44202397425837	10.42423733323541	11.93200184215138
H	2.69598429764517	10.08398547833758	11.95132599244467

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Pd	3.61317286547095	9.10954824559644	20.42159009870215
P	4.79901449700449	10.01830886289720	22.13760847741410
O	2.78726878754817	11.82560083098348	21.28916256816022
O	0.77914521242979	10.78674100149527	21.64576135224475
N	4.91241719928436	10.11871189477123	19.12744638374044
C	5.33446967440781	11.73362184899345	21.76442706527854
C	5.52177764094338	12.63230209960230	22.82450163647708
H	5.32761101667493	12.29492381712204	23.84631013608527
C	5.91599188836841	13.95780315162627	22.58965999971219

H	6.03530224700409	14.64545652686193	23.43296381586306
C	6.14456926470764	14.39578793394431	21.27895332766221
H	6.44952077958464	15.42786757522936	21.08177547152992
C	5.97793951741938	13.50625266397693	20.21284052782049
H	6.16092935861335	13.83793917227965	19.18943911033149
C	5.56228027131414	12.17455765989522	20.43280351905114
C	4.15983827843886	10.03549784515120	23.85136063271289
C	5.01575918196057	9.76204176235611	24.93897921295548
C	2.79444619667940	10.31729491233867	24.07200782065674
C	6.40930839394766	9.12825979779025	22.27004648555290
C	8.84560346114126	9.05803742923664	22.33819302935449
C	7.64975790825243	9.79354141276396	22.31995306713839
H	7.67974278625704	10.88703034565177	22.33481650785095
C	1.61296534773242	11.45503988287348	20.99994823559517
C	2.26819858919665	7.86493668885899	21.50868214427441
H	2.79593341157736	6.90459317487140	21.59309578895038
H	1.86528064907632	8.27727848521569	22.43749900975739
C	1.64604164969014	8.23921079002313	20.27670162582171
H	0.88139990720052	9.02759082289669	20.31587286330602
C	2.28426124215930	7.91377230017487	19.06166900378971
H	2.88313746648335	6.99944224106204	18.97268352433914
H	1.93171208351417	8.35875827325443	18.12700756946383
O	6.01389417577658	11.80480860897817	18.12075128268868
C	5.43708197135957	11.30962584442183	19.25029582004059
C	5.27469233039493	9.58063303026098	17.79091979789442
C	5.70836709608081	10.86185435277416	17.05032505478822
H	4.89584645498893	11.29723249258402	16.44718974471685
H	6.61758248109259	10.76247430980290	16.44176744396884
C	6.37215334697891	8.46942757610815	17.88004047518404
H	4.36905718920148	9.14551430214089	17.33660300965832
C	7.62548025811847	8.99332498163651	18.60710083528570

H	8.40653797582741	8.21378960215163	18.62228926003118
H	7.39864319195816	9.25264121627032	19.65359996241340
H	8.05267077203037	9.88429684806478	18.11343630623738
C	5.81980126937857	7.24755853738055	18.63790920033395
H	6.60886324909239	6.48319925325192	18.75081835617587
H	4.97584684744118	6.78962103322977	18.09212940695414
H	5.46554271700466	7.52628579064673	19.64633768634311
C	6.72861057963889	8.02816699536575	16.44428491253310
H	7.22382578712766	8.82660479011661	15.86411425632879
H	5.82830107404545	7.70859782071743	15.88789403220003
H	7.42391235363476	7.17139851280943	16.47745710481949
C	6.38487158274566	7.71765336447266	22.24914924311511
C	7.57817044124852	6.98613068013893	22.27575752092203
C	8.81272993928097	7.65620471786247	22.31337459839801
H	9.80512370909385	9.58481552561854	22.36761376087497
H	9.74671530489743	7.08496317832856	22.32099830435548
H	5.42038781956542	7.20047729700643	22.19653435091539
H	7.54653245212725	5.89184673690369	22.25611562829721
C	4.51063771605041	9.77837680359638	26.24721913868473
C	3.15449260646261	10.06153059512298	26.47176220886836
C	2.30461492960110	10.32747707665757	25.38588960162628
H	2.12057700267237	10.52986708746140	23.22842689293073
H	2.76014298699854	10.07051134010661	27.49364973125964
H	1.24505724151663	10.54502749873028	25.55585003723350
H	6.07205738226198	9.53620507759400	24.76295783782246
H	5.17807325221817	9.56654602034690	27.08924415026178
O	1.14354784845973	11.81247020692965	19.67534254050618
C	1.91004333784227	12.66321161686329	18.89612172836647
C	2.29220354257013	13.99797386208736	19.50004422052344
C	2.61967704032788	15.05166124617887	18.42997545122333
H	3.14622379778922	13.84998319245294	20.18283009957070

H	1.45443210903866	14.33699695669128	20.13772824434045
C	3.52476925506685	14.45305096260058	17.34470919664582
H	3.09805978941166	15.93047834974202	18.90068890353171
H	1.68432672122460	15.41094824734985	17.95749572960039
C	2.15165502224330	12.32121857457462	17.60440465656708
C	2.80830897636416	13.29127636077903	16.64301895698616
H	4.45162944485791	14.07162910626455	17.81231019401417
H	3.82461190292138	15.22074576958876	16.60739444619572
H	2.03935222009672	13.69244984949691	15.94598618576869
H	3.52126282963988	12.74844643096693	15.98683058546127
C	1.67911043622021	11.01524116780269	17.02249570372144
H	2.52473404118854	10.40860247928465	16.63616414339180
H	1.00138309502209	11.18067497579144	16.16078197627889
H	1.13944632771527	10.42622229609142	17.77808007153513

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Pd	2.63578926334802	4.74920718007397	16.18078094886954
P	2.10453959869232	5.32391024171582	18.23159806149449
O	0.49946901268832	6.63627440780797	15.44102247200843
O	-0.69759594163262	5.09874022017061	14.23828241708335
O	2.96040789815962	4.38337215796130	13.95770752513682
N	4.18550153437680	6.22982024382299	16.25545901966994
C	2.19791790881435	7.15773638704905	18.40765284350776
C	1.26994846425548	7.80047904193974	19.24534613944377
H	0.49616164082916	7.20457298967802	19.73583530832085
C	1.31513056957757	9.18701924992554	19.45405310452779
H	0.57306420612499	9.66034409972513	20.10471614339784
C	2.30433210128582	9.95613981934880	18.82880869862767
H	2.34743132970588	11.03858888776110	18.98273210762565
C	3.23921798179909	9.33459334754006	17.99406030930804
H	4.01106431908652	9.92285945380239	17.49311602792823

C	3.19633511766939	7.94298677592897	17.76623966326630
C	0.45110947101100	4.90139082476978	18.87119604060004
C	0.26955496703782	4.26754908570281	20.11465851826791
C	-0.65492839533339	5.20138457517151	18.04376937837819
C	3.32244228135173	4.70537226848688	19.45428571555888
C	4.84197123368798	5.00011184336354	21.33137347528519
C	3.85425659092090	5.51377879505379	20.47712018156501
H	3.50547445340246	6.54421440734423	20.59559105361768
C	0.23370506145204	5.90497328569869	14.45019985968781
C	1.36340114542843	6.04318464231242	13.20399021960960
C	0.59434254160967	6.39824108842378	11.89999592847822
C	-0.15461684558941	5.23504411329574	11.23999663573916
C	0.79611368913722	4.05275199386574	11.01707451717968
H	0.27507881399116	3.20683556023218	10.53293254313576
H	1.62017543878290	4.35005666051617	10.33791264525375
C	1.37769203640645	3.59381639678426	12.36474050950661
H	2.11246596228937	2.77623123217024	12.27013491421859
H	0.54261895558146	3.22372940103428	12.99653725576010
C	1.99287743286186	4.69826834340480	13.19410080972383
C	2.35770459332146	7.15958292625981	13.53914577817669
H	2.84025465128605	6.98345833660607	14.50663934068315
H	1.82488281070014	8.12194627610528	13.60117756492282
H	3.13217260585169	7.23348030173169	12.75103031077914
C	1.28359525192989	3.16910289450078	16.14771328333814
H	0.70913588555734	3.05756690576772	17.07887582303810
H	0.60443433795912	3.46888139314886	15.33078980941454
C	2.16148914967177	2.01846115098686	15.87296201713012
H	2.65696433315369	2.00925650533706	14.89240872381360
C	2.42119886699224	1.01316584057783	16.74630830730317
H	1.92915770980630	0.97210189896088	17.72645590630765
H	3.10133901523524	0.19171288480986	16.49877428072088

O	5.27367710960877	8.18017561165947	16.58008175928565
C	4.20395905437806	7.38190550067201	16.85496057168077
C	5.44219987643063	6.06646548501105	15.48823482711270
C	6.02043062720783	7.50331020920585	15.51956114781685
H	5.83896715285179	8.05677828639098	14.58320683913864
H	7.08482188233620	7.56455440123628	15.78662369135209
C	6.36369346065314	4.96218184814765	16.09817060834329
H	5.16627609454920	5.76431849275723	14.46352312897245
C	6.67558177603996	5.26678129716804	17.57600530466586
H	7.33933380140577	4.48907588129881	17.99154665043796
H	5.75501096292942	5.27464146127725	18.18227241618194
H	7.18386013839831	6.23985335210193	17.70389138636572
C	5.66655956638240	3.59235590274899	15.98865038960462
H	6.32963023175155	2.79601052385200	16.37162338911492
H	5.40333905077212	3.35611365120436	14.94316102344040
H	4.73102737621049	3.56836082312828	16.57750593768375
C	7.66488357304667	4.91431718808786	15.26929345815830
H	8.25536317753628	5.84481780050393	15.34745766856629
H	7.44971472120403	4.73294325111850	14.20043981298768
H	8.30687821366772	4.09053461917351	15.62677298924719
C	3.78031781786338	3.37973961123749	19.29571569531096
C	4.75638581879116	2.86967625748948	20.16048574979349
C	5.29326693791550	3.68056546379942	21.17454495016157
H	5.26215824790099	5.63471041947283	22.11854120611262
H	6.06842801045462	3.28541528603135	21.83927990495235
H	3.38630203052464	2.76348181153558	18.47932752559556
H	5.11047265275994	1.84188000886324	20.03073864041142
C	-1.02658789952047	3.93584152983685	20.53844620724730
C	-2.13012814689490	4.23721655878467	19.72541682989405
C	-1.94209875283660	4.87025452631566	18.48420637258358
H	-0.49151590282674	5.68501151381411	17.06711218103170

H	-3.13965495812450	3.97177637461111	20.05695374751320
H	-2.80046000694492	5.09567350792566	17.84348398457186
H	1.13458037339855	4.03493854928077	20.74377751567208
H	-1.17195521914283	3.43964505255134	21.50375492711785
H	-0.10300703779472	7.22545978723273	12.12624564664494
H	1.33313816087715	6.80491015279592	11.17815813594024
H	-0.98002770015697	4.92480413400281	11.90203780537733
H	-0.58863132387885	5.57030753099991	10.27954783650009

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Pd	2.64394833883021	4.64160448145685	16.13764647372260
P	2.06989261984587	5.31365691823581	18.14971988991980
O	0.87210108623381	7.01860722562251	15.53488692724984
O	-0.39432230060625	5.30514453194077	14.71599101535391
O	2.75525889463491	4.22003472923905	13.90240427653612
N	4.21566836134882	6.11368131983919	16.18792903642035
C	2.16824109048905	7.15108833448342	18.24344447726654
C	1.22577153677511	7.83490800791753	19.02901089486685
H	0.43554529612551	7.26686487395738	19.52596106425463
C	1.27359513946675	9.22924679230998	19.17264981805356
H	0.51845824194450	9.73600497164840	19.78189000358105
C	2.28042763546337	9.96417361312074	18.53446849305936
H	2.32521258153975	11.05261431106221	18.63760361696369
C	3.23114954024154	9.29973255581011	17.75299291746364
H	4.01702570513460	9.86085213834628	17.24286799723254
C	3.18556650061932	7.89940999946466	17.58975796863893
C	0.41440103461214	4.91687188739560	18.80418731888168
C	0.23168296720258	4.49691510140681	20.13648845392510
C	-0.68921700539994	5.04751235190465	17.93166885524588
C	3.26920017847230	4.74828801236960	19.41843980085449
C	4.77763298445778	5.12697091806919	21.29037401259860

C	3.80454063851187	5.60510877177414	20.39904627836837
H	3.46954240999354	6.64534841646154	20.45540938238875
C	0.53397360376672	6.16392332807724	14.67333319199220
C	1.40172685282068	6.16148803382042	13.29849254460273
C	0.48123188930908	6.54399050675182	12.11259217366282
C	-0.62082055069040	5.51309957985504	11.79047096962940
C	-0.10870338941171	4.05079788305766	11.88071396630232
H	-0.46551754332996	3.44413456423416	11.02972380362227
H	-0.49430553140082	3.59556137403599	12.80643082673090
C	1.43751029635551	3.97747430596319	11.92729316723585
H	1.85518857019239	4.42876976084973	11.00366882884935
H	1.80641443334172	2.94128934173129	11.99809197282342
C	1.93818812558929	4.76604402848834	13.11347639339017
C	2.56684401186128	7.16034166109001	13.40142160906486
H	3.26725954930154	6.84977043692788	14.18678637673208
H	2.16623731648459	8.14636119471909	13.68296867971442
H	3.10862938930960	7.24263887894911	12.43939015820270
C	1.29585607694932	3.05801518474744	16.14897925368903
H	0.74063736970158	2.95450733524115	17.09264989385645
H	0.61455779987914	3.36674602748093	15.33903787815304
C	2.17789661957774	1.91254819999145	15.86946264841681
H	2.64303271459983	1.88923861947555	14.87409955730137
C	2.47156734831149	0.92279258541049	16.75000397633167
H	2.00841254016836	0.89261116667341	17.74451974470339
H	3.15144364748918	0.10320337898452	16.49566093295462
O	5.30617563393247	8.06856478369140	16.47741495422241
C	4.21580928945211	7.29171196702373	16.73735220505957
C	5.50839758456519	5.90740848657433	15.49374324721949
C	6.10243854051020	7.33867389886762	15.49445315876878
H	5.98452746469233	7.85064047478507	14.52486833300618
H	7.15084713204225	7.39904246377370	15.81951816272483

C	6.38741583652320	4.81852408038509	16.18698285411348
H	5.28917827734537	5.56836670839943	14.46574963126533
C	6.63398715895804	5.17797297289326	17.66439658998675
H	7.26305312537511	4.40779164404383	18.14288754113862
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C	5.67694599236028	3.45452262303109	16.09599960966954
H	6.30243958302396	2.66592201418325	16.55103630352222
H	5.47680260810068	3.17380047687545	15.04666697708642
H	4.70739167733280	3.46717943784634	16.62771490714085
C	7.72533784844332	4.72418420854779	15.42324430887214
H	8.32280865775973	5.65075616460224	15.49428494156560
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H	8.33923639316024	3.90797193238500	15.84215016089970
C	3.71009828955957	3.40988446605512	19.33988059456279
C	4.67160756343016	2.93566512181939	20.24033890205246
C	5.21146032355300	3.79476039074743	21.21251685208232
H	5.19990814633500	5.79932973512278	22.04444160832701
H	5.97509142476907	3.42682799838026	21.90564465776885
H	3.31629752696785	2.75509710694186	18.55425453508267
H	5.01262077438980	1.89755068470551	20.17164987482978
C	-1.06034868659097	4.21668125653000	20.60533662687198
C	-2.16268274666028	4.35519834205923	19.74741910052566
C	-1.97344500879991	4.76832717533601	18.41787690959400
H	-0.54813658873621	5.34165989338278	16.87935354685667
H	-3.17050913532854	4.13298614533566	20.11445760014835
H	-2.82986095884837	4.86503261907083	17.74278125352371
H	1.09484056555262	4.39247044803547	20.80151597057544
H	-1.20369328005631	3.88850541202733	21.64024433314617
H	0.02953977146002	7.52986658347537	12.32455804047827
H	1.12104127400475	6.69033920736958	11.21834957234474

H	-1.44916309748816	5.63805414561397	12.50311250014713
H	-1.01055253361460	5.72515208145212	10.77765317707025

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P	1.99477217221119	5.08923161412777	18.32061699497268
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O	-0.59489846885225	4.38864965736039	15.11878086297818
O	2.49984624803102	3.46866862698060	14.22330668828355
N	3.85973260242518	5.76952731189892	16.03350267294644
C	1.91772926670125	6.92186111130135	18.13599997725352
C	1.00340899712100	7.63308898396563	18.93131870799548
H	0.33571499155016	7.08020815639516	19.59683796550730
C	0.92183755090094	9.03200658113831	18.87351592520383
H	0.19116937467511	9.55730159982479	19.49683306853395
C	1.76877233454955	9.74656796606845	18.01721760729657
H	1.71136991157481	10.83789521318749	17.96084234890881
C	2.69059493867679	9.05642633484285	17.22383532158882
H	3.35248123865838	9.60067997321145	16.54684775351964
C	2.77433380760456	7.64885506271070	17.26410202638827
C	0.42853599989393	4.66226433431102	19.15178372934254
C	0.36601319401874	4.43390155702185	20.54026997141065
C	-0.73238821031783	4.57069267866453	18.35115663905398
C	3.32532249876516	4.82980875658152	19.55764462025830
C	4.91014776585125	5.61430146984486	21.22997671115699
C	3.83425241953686	5.86560256323745	20.36435177902262
H	3.39807346891824	6.86742666465625	20.30406812555984
C	0.26028063446993	5.28354618784488	14.86021503650927
C	0.92536749600315	5.16294627272955	13.40469065056204
C	-0.24371974616182	5.15462459905515	12.38088299292239
C	0.11825348043115	4.65921147778632	10.97632652161935

C	0.68656047992758	3.23780916340220	11.06570699318802
H	-0.07417134667899	2.56653525821273	11.50752897703503
H	0.93443303178075	2.83197013936467	10.06815329450389
C	1.94608117758214	3.22876451025489	11.94744639922206
H	2.74789174897858	3.79465277424583	11.42572456934663
H	2.34267810719446	2.21454424221551	12.12418203457535
C	1.78592857495982	3.91578154383060	13.29608075046171
C	1.88787780747741	6.34958545621379	13.14475085737671
H	2.73462563851534	6.31711989987871	13.84561467563099
H	1.33609149006011	7.28223564142739	13.34014942171817
H	2.27112271499233	6.35853511851673	12.10707492095516
C	1.29308247694719	2.47554805904827	16.75397732172973
H	0.82604521348557	2.46982358077123	17.74965127250313
H	0.52860660474498	2.60187254651359	15.96921653806280
C	2.26012725991080	1.38129077921471	16.56272146161430
H	2.63897910054251	1.23739422108768	15.54070692078793
C	2.72699385360443	0.57099031838658	17.54587808790376
H	2.35863804304366	0.65976274136299	18.57581359868644
H	3.46019481702281	-0.21774509882025	17.34860400298280
O	4.74112891323709	7.84349179629253	15.90313954730250
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H	5.27734400694812	7.37078926185004	13.95153301987813
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C	6.15596832562503	4.71525130630891	16.02704888447562
H	4.85013788084844	5.05249150763750	14.32163418012553
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H	5.56049138785311	5.36170504234186	18.03553529559871
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C	5.60577344452833	3.28766437842217	16.21024644946428
H	6.35096710585094	2.65330585309757	16.72255117947424
H	5.36562795557485	2.82110683886110	15.23816910000819
H	4.68149144820474	3.28532952361253	16.81810877580907
C	7.43757869147443	4.63846098290791	15.17050489885801
H	7.92944444298289	5.62031158655521	15.05017243567231
H	7.22150242935976	4.23710752370847	14.16321980409140
H	8.16891335013630	3.96451973757276	15.64953752203116
C	3.89809068060049	3.54156663671377	19.62641694956379
C	4.96274307160303	3.29436131149299	20.50143814810651
C	5.47436683089839	4.33141069316589	21.29987159612750
H	5.31043619195898	6.42504883499964	21.84769181826591
H	6.31751148354291	4.14055705427405	21.97197089085620
H	3.52249877148154	2.74726933085153	18.97126143623381
H	5.40509839013627	2.29386452934254	20.54755546503058
C	-0.86506020511560	4.12474247827069	21.13791838422505
C	-2.02498897362989	4.04441012248875	20.35155899667964
C	-1.95428892708481	4.26566383235927	18.96568639814045
H	-0.67769935666597	4.70996073490677	17.25843173500780
H	-2.98490265452666	3.80054682616910	20.81955933165826
H	-2.85558417143964	4.18956960268779	18.34877260645905
H	1.27421194531672	4.50010520921226	21.14798389701292
H	-0.91584082859852	3.94528622784556	22.21708841459063
H	-1.02611217007055	4.50417492015487	12.81055858308509
H	-0.66266289023092	6.17710141394334	12.34322552727734
H	-0.77982580402159	4.67386930664072	10.33181991754623
H	0.86101972875525	5.32835758163903	10.49672930637020

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Pd	3.54054390132318	9.28030987692947	20.30642415366756
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N	4.92531902400295	10.39250542312597	19.09132910713515
C	5.33560970846673	11.56909752443035	21.89766222570917
C	5.40929523690876	12.34755822678329	23.06698500642101
H	5.14283654926445	11.89394149099902	24.02498190710654
C	5.81430343790302	13.69034428540557	23.02537630559112
H	5.85386908664854	14.27234468654116	23.95158830301147
C	6.16743196257963	14.27635901833101	21.80319404110026
H	6.48532779706697	15.32245507414012	21.75929261458363
C	6.10534624488920	13.51803903626999	20.62877331021414
H	6.36879877546493	13.96234643806202	19.66640815629005
C	5.68398174053360	12.17198198522315	20.65490236647204
C	4.16324966671846	9.67028530720779	23.72309774904122
C	4.92280670143034	9.14113544185437	24.78342603261826
C	2.84696803931390	10.13082604152687	23.94834723997741
C	6.41098317259805	8.88697714899371	22.01989326934787
C	8.83863706271898	8.77523774069851	22.12932857227433
C	7.65275622948220	9.51977713204111	22.21978153577298
H	7.69181877998098	10.59268155690881	22.43156361489065
C	1.82598986673433	10.20377541749394	18.13107296826187
C	0.68017335832194	10.88760625186467	18.97432911290966
C	0.16450366482883	12.16644633159730	18.24771699937855
C	1.16073882137121	13.33593534681863	18.23420147206997
C	1.62023185325249	13.69826073588322	19.65263088554515
H	2.37265144308435	14.50840980688419	19.63508792571940
H	0.76378508768516	14.06725879575015	20.25039558161102
C	2.22218232407886	12.45164529568290	20.34104992239631
H	2.54555853703273	12.65671450660099	21.37450973332710
H	3.10106375276406	12.12610731571235	19.75863133830770

C	1.20503469575127	11.32023066258793	20.35332876608127
C	-0.46148354614281	9.86735389056414	19.12600789472886
H	-1.25296124408311	10.26576788290976	19.78222584228516
H	-0.08719582784266	8.92867392702482	19.55876798911369
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H	2.46029240071423	8.03734066083022	22.44424273359745
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C	2.53495977576250	6.74482343405262	20.71509455829466
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H	3.37479715123569	4.76901505992773	20.76621875224885
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C	5.59679077592104	11.47074873357707	19.36319265778696
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H	5.09361533966115	11.94383920948345	16.59819403852598
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C	7.39599460559339	8.89578177696719	18.28606039801111
H	7.99799854102341	7.97556234279493	18.18799947230489
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H	7.99248912988053	9.72831890331727	17.87035109151136
C	5.27634425205409	7.53918158384945	18.16698818414151
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H	5.11628622874931	7.67641764081396	19.25124927338932
C	6.27386935342508	8.44682582864837	16.06040798578386
H	6.86824348978152	9.23648493743769	15.56629831075892

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H	6.82376695783135	7.49759787259388	15.93441665770637
C	6.36202981191170	7.50591547326215	21.73587139622039
C	7.54910341385232	6.76716725845317	21.65851638833571
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H	9.80371715679228	9.27187135884191	22.27347785319009
H	9.71591638442343	6.82479957867236	21.77122901118054
H	5.39546769175203	7.02110025301767	21.55348414033386
H	7.50625694382196	5.69703948437660	21.43177841370363
C	4.37090799751720	9.07999893463353	26.07205353761292
C	3.06816931821310	9.54894130824627	26.30172284446635
C	2.31046565069352	10.07428423772899	25.24114918933725
H	2.24207987700024	10.51417281595586	23.11511068307378
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H	1.28965348229397	10.42889976720495	25.41563996213667
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H	4.95994952417262	8.66450743435941	26.89626818367474
H	-0.09270992084780	11.88016041149153	17.21363489233753
H	-0.77082840516572	12.48620358364987	18.74944071748395
H	2.03099068133136	13.04063010730712	17.62259385977163
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O	2.96834583546580	11.53418370530535	17.32120067593230
O	2.55497544792760	12.02853746676073	20.70845338585200
N	5.29030120247389	10.37772843451130	19.03962710662522
C	5.77204990199516	11.49049903033291	21.84077434968430
C	5.97721333843224	12.20596363468170	23.03396254543396

H	5.70226755551346	11.74362275607723	23.98544899668174
C	6.52285418923373	13.49863645918290	23.02505900815524
H	6.66377774981318	14.03329329673146	23.96990221430204
C	6.88490341886006	14.09529377331008	21.81082570891064
H	7.30964486550033	15.10369431916103	21.79183520166650
C	6.70138232421723	13.39459168030248	20.61334099036396
H	6.98066297651624	13.84371479186563	19.65761234963620
C	6.14380422099930	12.09977811232738	20.60901810304505
C	4.36203550925180	9.69511446156210	23.59976316181640
C	4.85706548424117	8.83247048959129	24.59314042802267
C	3.21494293139942	10.48093969661255	23.85034804893507
C	6.56221189579796	8.70882004920733	21.94684739013974
C	8.97146187992807	8.36701254113075	21.98429570382682
C	7.86563139820654	9.22707216080531	22.06640151701796
H	8.01550326828736	10.30143008178162	22.20799803527090
C	2.27051082724762	10.92103738970546	18.15145896795072
C	1.05693043412783	11.66972547267084	18.80091842946103
C	0.63342111926563	12.86335496777860	17.89121578416838
C	-0.40442266123964	13.80066447556228	18.52690842776426
C	0.08860174879739	14.33694025239370	19.87875605748180
H	0.99046502311396	14.95987480942119	19.72121588321862
H	-0.66987044695229	14.98516698650493	20.35436451992759
C	0.45051629737697	13.17151228757808	20.82991313662304
H	-0.46746535565898	12.59793840380909	21.06347744139551
H	0.88096252520195	13.53166175297837	21.77902101735191
C	1.46634703180912	12.24534535615808	20.16965743665944
C	-0.12620544864877	10.69044586988307	19.00599730075033
H	-1.03584740696873	11.20938973537447	19.35294231225381
H	0.12947527453227	9.90542887454729	19.73194462379967
H	-0.35947555977363	10.19694348527023	18.04756007519483
C	2.21206677622854	8.53986735217364	21.20634795461317

H	1.87489724929154	9.13180772573780	22.07283190123639
H	1.45556302533221	8.53632773991251	20.40521191204563
C	2.65571477472441	7.18002473828900	21.57028028622954
H	2.86587014707294	6.50514039293618	20.72609533736570
C	2.83112845730665	6.70991296892908	22.82900229674751
H	2.61981062057957	7.33247912694293	23.70475385642893
H	3.17791076400423	5.68844348658969	23.01969471121988
O	6.69697144768771	11.96339042548592	18.27084384859571
C	5.99986088789190	11.42865464134655	19.30713846399650
C	5.52028714306278	9.98362685320475	17.62945912027873
C	6.25281876205874	11.22663183395355	17.07719996689952
H	5.56196760109861	11.88463477229590	16.52785657321346
H	7.15290582807157	11.01650038676837	16.48193523467900
C	6.27596216955353	8.62584575046859	17.52487919539548
H	4.52646321919080	9.89590240342185	17.16212589455839
C	7.62258247968102	8.67566760923913	18.27014352012944
H	8.15278949267035	7.71228889345861	18.17031378643430
H	7.47376785499780	8.86218946640155	19.34584442036343
H	8.28687198247235	9.46433113461572	17.87166003245557
C	5.38996888738829	7.51382463964398	18.12194647414226
H	5.89308092504581	6.53358394758072	18.03464132840616
H	4.41764202105921	7.46079291938768	17.60238625019853
H	5.18085570507348	7.70219154355539	19.19158197403168
C	6.50240127830747	8.32268877467141	16.02887120312675
H	7.17698688550549	9.05451897133798	15.54895329726953
H	5.54636819781127	8.32393675806500	15.47503634558180
H	6.96269856403102	7.32585348756092	15.90988448784996
C	6.37291313151921	7.32337639473389	21.75655957753444
C	7.48045525441745	6.46945880226283	21.68838439490588
C	8.78121638834182	6.99037551744874	21.79322510050773
H	9.98379671131890	8.77640901317173	22.06462287371468

H	9.64619460142129	6.32275263216713	21.72281688893557
H	5.35479257709608	6.93015776668205	21.66739989783620
H	7.32862771807784	5.39546457295841	21.53913425964059
C	4.20884443252071	8.75506940625979	25.83618939234296
C	3.07161690958293	9.53649203843183	26.08722824376828
C	2.57965887734667	10.40369565083254	25.09508303949387
H	2.83518146947890	11.14430352750733	23.06365063736838
H	2.56452236157374	9.46982870519330	27.05537842266527
H	1.69126414536737	11.01320661986564	25.29030517923412
H	5.74048384633451	8.21986984405121	24.39120463045219
H	4.59178812008029	8.07765126049206	26.60641583414394
H	1.54963911233635	13.42318890409396	17.63619639981052
H	0.25456705374807	12.44834071727223	16.93930486921663
H	-1.36841281020914	13.27460354936135	18.66954346817749
H	-0.61021776806165	14.64157523386904	17.83898466850172

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Pd	3.46215941758350	9.63250280880241	20.76630555729619
P	4.88578935119433	9.90135171583200	22.44331755453835
O	2.92970976189465	12.62812729226448	16.98621838282185
O	3.14195191074822	10.78679158574965	15.63969334769126
O	2.17952653467831	9.55720045556713	19.07028333264187
N	4.93870200466843	10.60969319466113	19.57225015936405
C	5.51706762735447	11.63217223139493	22.41066401875530
C	5.74626389439561	12.31204930563476	23.62054671466623
H	5.52669800828432	11.80779915921581	24.56532399367829
C	6.25131027924691	13.62114656165419	23.63388788868978
H	6.41392055127030	14.12912151352623	24.58971952113527
C	6.54793448207485	14.26715001008000	22.42693717579018
H	6.94129630178918	15.28816708850419	22.42586065245555
C	6.34001699746366	13.60137160135088	21.21318251640411

H	6.56968580482928	14.08990421475321	20.26367914951332
C	5.82189839795187	12.29024804177827	21.18408385448113
C	4.32399223511903	9.64240627072362	24.16211614912146
C	4.93145059676324	8.70062908570478	25.01277949388885
C	3.18730594155397	10.35438482038855	24.60401793086913
C	6.39199355450433	8.87449395701760	22.26341730274980
C	8.80485744574319	8.59797186192883	22.14884523462603
C	7.68647050384443	9.41915072629504	22.35648194756680
H	7.81904796232835	10.48274165106992	22.57556213501777
C	2.63087076140536	11.50237888539181	16.52159705979762
C	1.24100456807164	10.75314894422584	17.24063063108675
C	0.04025427356286	11.70957412893444	17.00779612484807
C	0.04751471591921	12.98077517421739	17.86778110729109
C	0.25557413901184	12.63378017332972	19.34870404656298
H	0.27684859857644	13.54764219050158	19.96992912853219
H	-0.58636030276483	12.01451415190274	19.71774496959335
C	1.57838517050240	11.86192599338972	19.52803418544062
H	1.76613499656928	11.55831910810161	20.57586351570894
H	2.41140256995631	12.50982348143257	19.19028528450614
C	1.65287041657153	10.64247073189762	18.64508617549430
C	1.01759286625131	9.40142323066580	16.56409577841920
H	0.14365799732851	8.88841754302329	17.00836708597271
H	1.89728877783680	8.75231081781284	16.67112868604569
H	0.83800639889669	9.54945184678023	15.48802949451313
C	1.99610474183202	8.64243486906914	21.83935354192797
H	1.93214938985524	8.99286267152812	22.88078092879272
H	1.07908047628466	8.89308953083686	21.28135735763822
C	2.37206074457149	7.21794488227326	21.73123451301225
H	2.25386976517124	6.76161722510632	20.73752261848077
C	2.86581148878486	6.45821712103921	22.73982952598689
H	2.99226191072557	6.86557385151184	23.74991134578870

H	3.14135678042214	5.40916725181549	22.58885761340252
O	6.29114634852270	12.25467560270064	18.83288650991496
C	5.64688000490979	11.66290575497075	19.86054516793552
C	5.13017865568125	10.29135250482516	18.13353581985481
C	5.82275810268384	11.56878878312493	17.60876087834306
H	5.10636683878090	12.23997876491098	17.10608744474824
H	6.71302868785750	11.39073044220170	16.99046241364859
C	5.88989987730377	8.95081254341221	17.91271287284566
H	4.14551606744118	10.17829147740599	17.66395585923672
C	7.27400951581360	8.97150560404554	18.58389086680021
H	7.80277799887111	8.01958459866672	18.40181279832923
H	7.18754799275001	9.10040022007522	19.67478432267356
H	7.90998816218977	9.78475448887563	18.18943743572694
C	5.04302234910201	7.79800237491049	18.48765177235797
H	5.54329393272386	6.82888888459252	18.31059576772659
H	4.04470010976499	7.76880222080551	18.01850252580967
H	4.89761582433428	7.90982913109166	19.57819286966478
C	6.02125496228757	8.75220193513835	16.38670426652256
H	6.71746762280761	9.48039373130672	15.93390352300198
H	5.04360143733519	8.87095706385102	15.88833956112433
H	6.41378403596261	7.74293536753036	16.16942291348480
C	6.22098455251831	7.50453598752746	21.97340609660262
C	7.34313397082401	6.68961226249689	21.77831437130828
C	8.63481824715920	7.23591346876901	21.85778739620711
H	9.81050752796768	9.02631320199229	22.20864663500530
H	9.50964267351642	6.59979594650117	21.68883728946308
H	5.20869712847741	7.08871894287541	21.90521154921517
H	7.20779201029666	5.62772439972022	21.54938024200846
C	4.40764543827948	8.47600735097996	26.29562214140451
C	3.28474376752692	9.19208896362292	26.73528824062082
C	2.67824751410614	10.13687990047713	25.88949327156821

H	2.70701772859914	11.07580365455048	23.93353375400351
H	2.87746799335950	9.01275353781827	27.73539646146538
H	1.79892946966423	10.69414654349097	26.22767735021892
H	5.80784677095287	8.14342885868627	24.67001914500916
H	4.88120059297443	7.73889237301807	26.95199028519358
H	0.00623253390037	11.97163548710972	15.93451784979779
H	-0.88537354330754	11.13340594018364	17.21533279377677
H	0.86907542562325	13.63413619524026	17.53130913771962
H	-0.90504914018897	13.52579653181278	17.73051566705603

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Pd	3.47202550091232	9.83569618958101	20.74914684301807
P	4.90552675287635	9.94749485130646	22.43625374898270
O	3.09019633457383	12.87578030858187	16.89858414524334
O	3.19242984737979	10.87576986775823	15.77300183138600
O	2.18678909303218	9.91419062312245	19.06050456926236
N	5.04297440334645	10.68103628044411	19.58029722239722
C	5.70323172600090	11.60954451826146	22.42724667264156
C	5.99370929082094	12.24738751272464	23.64674737912705
H	5.72103335967751	11.75491991641544	24.58389078656489
C	6.62671644131256	13.49934730296679	23.67980217575843
H	6.83500541193899	13.97548249866349	24.64313286336546
C	6.99156352448970	14.12902454920484	22.48295913533667
H	7.48497887894287	15.10551176205688	22.49733701518527
C	6.72270149103578	13.50416030683608	21.25950479050299
H	7.00334205741936	13.98053574541444	20.31752240189865
C	6.07696282736828	12.25145161612110	21.21074809078945
C	4.31119024509464	9.72618725226591	24.14949566967516
C	4.81744859052808	8.71894805567337	24.99137179452254
C	3.24621331558748	10.54023695302790	24.59379721126692
C	6.30906936330328	8.78363596398226	22.25510774470530

C	8.68553069467811	8.27796609775722	22.16026416769684
C	7.64879758618138	9.19956553551147	22.37009047237812
H	7.88045551305608	10.24200341202186	22.60770279526427
C	2.73023902364927	11.73779006421537	16.53865929923372
C	1.22290704856914	11.18764886499594	17.30416887902843
C	0.17601670686855	12.31807053258742	17.09780852068689
C	-0.21761546612853	13.04697497331759	18.39175683283810
C	1.04291907444681	13.48339430201606	19.14759045438460
H	1.67497534673018	14.08297886757292	18.47298279647050
H	0.79240044339640	14.10033273306887	20.02978464671231
C	1.83475402509582	12.24075831479272	19.59170643246250
H	1.50057273439154	11.88065944570728	20.58544064792099
H	2.91049214354605	12.47304571402814	19.69868375827404
C	1.72795157834351	11.04467417824949	18.66488442601165
C	0.82196591141886	9.86856279199830	16.64800631049678
H	-0.09926698817053	9.47159733067161	17.11576476555134
H	1.61922985666975	9.11984246211401	16.74438745825199
H	0.63368104971646	10.02784040165991	15.57437734107426
C	1.90986250193934	8.98050742497780	21.80173347987581
H	1.86976996188520	9.32952656407966	22.84494893754490
H	1.02376590744387	9.31572304112514	21.23805427689975
C	2.15339618111900	7.52783975272723	21.68710075819468
H	2.00268445122514	7.09097248849128	20.68904223751614
C	2.56481969627121	6.71910875094605	22.69449927171341
H	2.71883073170191	7.10644672249679	23.70857773517092
H	2.74333802301177	5.64999143104326	22.53837519404647
O	6.52614662511774	12.21441966216163	18.85240251034066
C	5.84249091958126	11.66351932040075	19.87916147407401
C	5.20146617731194	10.36399406011627	18.13766986276025
C	5.97900378283968	11.59558095409608	17.62465353997437
H	5.30726648752564	12.33089610277076	17.15055035036974

H	6.83844673306368	11.36628383966419	16.98039743344083
C	5.86485503096732	8.97455672541045	17.90529418203330
H	4.20930376966614	10.32251187075241	17.67239512962346
C	7.24174757438494	8.88490120208796	18.58554660348545
H	7.70301030928759	7.90120529348398	18.38918082823892
H	7.15753830265789	8.99986782756902	19.67819695138603
H	7.93643469349881	9.65799942499195	18.20954260300759
C	4.92780830833540	7.88330861432975	18.46036354227952
H	5.35883767891927	6.88107979217348	18.28551898191203
H	3.93823467449573	7.93027250654637	17.97431529298862
H	4.77283342298788	8.00067757758118	19.54876681946851
C	5.99351147125577	8.78194419873514	16.37838441193992
H	6.74839818596626	9.45808200166050	15.93879759267969
H	5.03138521704954	8.97949408797356	15.87542147554405
H	6.30949956268583	7.74762255345451	16.15406858222257
C	6.01085827171346	7.44101249889654	21.94144404447594
C	7.05173233749536	6.52501085391175	21.74396935720851
C	8.38889012850128	6.94325489031766	21.84498617232584
H	9.72690505880240	8.60665344018496	22.23716331297182
H	9.20047708186843	6.22862819437411	21.67420307334750
H	4.96418646190329	7.12545652489310	21.85739558429959
H	6.81762816283150	5.48470229803393	21.49641273063270
C	4.26472364752134	8.53047908849911	26.26788188440138
C	3.21376556344584	9.34716777823509	26.71001263472090
C	2.70876604958963	10.35732570298075	25.87310772580734
H	2.84370943990958	11.31355777327497	23.92997964442954
H	2.78338268667017	9.19577477196201	27.70505568091903
H	1.88555770837550	10.99353066747055	26.21326033258594
H	5.63763596823554	8.08298066188493	24.64662037310471
H	4.65909495705985	7.74236229848686	26.91731554110763
H	0.57254226979586	13.05990288895607	16.38323823740653

H	-0.72189414153077	11.87056246414823	16.63338359734388
H	-0.85441165898758	13.91882757547511	18.15427250145875
H	-0.82147111349657	12.37278773947230	19.03417541635323

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Pd	3.26950843604510	9.76495175299426	21.00419457583790
P	4.88760379688076	9.91056143608204	22.52617853020251
O	1.76323089045818	9.85273395150916	19.56727544961257
N	4.73672077332216	10.54415332504924	19.63123718078958
C	5.66479716159015	11.58043266656630	22.37210655628401
C	6.05286776841761	12.28298227144990	23.52750210444541
H	5.88044346623243	11.82935278494911	24.50705137912432
C	6.65502707296398	13.54760121695888	23.44624823669792
H	6.94006550973100	14.07152046747479	24.36423644109913
C	6.89414150294726	14.12910917932956	22.19424064883262
H	7.36371961850387	15.11462856551206	22.11935991477293
C	6.52949531405581	13.44156355992346	21.03130283255324
H	6.71323922845150	13.87918586505401	20.04749317569378
C	5.91009859557560	12.17592995841910	21.09953109400620
C	4.49621148079386	9.76586128277550	24.30762889493065
C	5.12573133223182	8.82710859888075	25.14580093157923
C	3.45590693711213	10.57164900582749	24.82053068256393
C	6.29779064189354	8.76383604753914	22.26744745932536
C	8.66169191708101	8.28093487949923	21.95189129910073
C	7.63576535709550	9.19902316151298	22.22341950025806
H	7.87325732712447	10.25431421205814	22.38831736338143
C	1.58241148549900	11.02631471877723	17.51134963414896
C	1.47195730710228	12.31523694111276	16.72287231157369
C	1.29849235553325	13.57134345806962	17.59270767032353
C	2.20906744918311	13.50486731690466	18.82587500043443
H	3.26531289202085	13.40315993290202	18.50141914943214

H	2.14624966749978	14.43727428164700	19.41761424495447
C	1.82359468325013	12.29371346547166	19.68308398030360
H	2.55333448148556	12.13753501363801	20.50301557428847
H	0.84928814927450	12.47477558523721	20.18302482740430
C	1.73167499679114	11.00121732300634	18.87697298656825
C	1.49457185141478	9.75071568180307	16.71544060807573
H	0.49077882104206	9.61383527184904	16.26234797065140
H	1.69102250022378	8.87873312148177	17.35968880892329
H	2.21397743291877	9.74376290392780	15.86788628761892
C	1.82915786962066	8.93256276815405	22.23151323449021
H	1.89049733374997	9.30935738238343	23.26436409134669
H	0.90406472498266	9.25359705043085	21.72957898501449
C	2.09319963673235	7.48510683052055	22.12472463706674
H	1.83540561644794	7.02146901941782	21.16107947340613
C	2.64311364824027	6.70730064271308	23.09189653994621
H	2.90762680928226	7.12067097449099	24.07262177128419
H	2.82860859695204	5.63889024188339	22.93702542209656
O	6.19166281413700	12.01280597861536	18.71732308070533
C	5.56708897833342	11.52327859032996	19.82455615481979
C	4.79194013712495	10.14827787682043	18.20161644670126
C	5.57520241933480	11.32567497108784	17.57675632938724
H	4.91112467256001	12.05035377293644	17.07678738998792
H	6.39053679122207	11.03368849230939	16.89974947561382
C	5.41718257874618	8.73504315551870	18.00408414001768
H	3.75774421412525	10.13907926776809	17.82656552699593
C	6.85149092773487	8.67654479772681	18.55985242808422
H	7.27553757736611	7.66731714949206	18.41879125500943
H	6.86856743909342	8.89352007186076	19.63934909696724
H	7.52399822575393	9.39222980540689	18.05226449971651
C	4.53539314928156	7.69089676370638	18.71641267414561
H	4.94051312171359	6.67568683559995	18.55430069922119

H	3.49877988107736	7.72374371413501	18.34067483091555
H	4.49243137279576	7.87671477084974	19.80394619549529
C	5.41423826388735	8.42950294389303	16.49131592164270
H	6.06277712373666	9.11872092045825	15.92037980261030
H	4.39260016842658	8.49606540548781	16.07646930602692
H	5.78778750915385	7.40587407418682	16.31265593443035
C	5.99347087068581	7.40317047970344	22.05123957983136
C	7.02404105774907	6.49024883574242	21.79375551863943
C	8.35763202052763	6.92832633213497	21.73505992516174
H	9.70011731504658	8.62525648356685	21.90636810454922
H	9.15978327879321	6.21530764070771	21.51810133401737
H	4.94779772396009	7.07289497365211	22.09059722957732
H	6.78358388324544	5.43545451333298	21.62521701567122
C	4.72030731309721	8.69788210776159	26.48339737109613
C	3.69435736062084	9.50787308352162	26.99208976486263
C	3.06644531886547	10.45020259861152	26.15949875396680
H	2.95495457680878	11.28867171860542	24.16056178932473
H	3.37889915788328	9.40295709349443	28.03517512713574
H	2.26100184380325	11.08007924779594	26.55059800289344
H	5.92701899392818	8.19644533883680	24.75026943723703
H	5.21028130174062	7.96150117146977	27.12877123500411
H	0.63043004853618	12.24663180626808	16.00089762427773
H	2.37806799098562	12.43371062029024	16.08235893827716
H	0.24775241185730	13.63629620569583	17.93689838934686
H	1.49649772850582	14.48135627543095	16.99591621019111

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Pd	1.83220876688141	4.74868184896878	16.21049029097799
P	2.04425743257189	5.39270335900609	18.32581430823276
O	1.60763817972589	4.28732034241013	14.20965079356126
N	3.71777637900370	5.75134910107363	15.89380437730664

C	2.49999224160219	7.17921793840952	18.34034720662876
C	1.94412209516743	8.04137022756253	19.30355871588798
H	1.23204333360046	7.63809173007494	20.02836024364431
C	2.29020117046746	9.39932292904174	19.35499492415752
H	1.83830647613312	10.04561449432781	20.11419698314048
C	3.22003444674475	9.91809967724676	18.44238464414568
H	3.50016421532264	10.97543159463878	18.47541671243895
C	3.79228242932317	9.07738119957651	17.48309320397616
H	4.51839247104004	9.46731506632867	16.76625934060974
C	3.43808517536474	7.71219117318954	17.40681015863619
C	0.61312804846195	5.28713248077162	19.46127006853965
C	0.66545133445456	4.58412276734196	20.67867240474627
C	-0.60457128010618	5.86611594914935	19.04169693312269
C	3.42121552214544	4.59719307225404	19.24475233658912
C	5.45584374272915	4.67532417033235	20.57716598645071
C	4.38937770878312	5.33712061596982	19.94945472690445
H	4.31644553167759	6.42784949727488	19.99574041252597
C	1.98703207429946	6.49025792286005	13.25836350151154
C	2.56127294658040	7.31336765091370	12.12013670197481
C	2.85811102548528	6.51308517379041	10.84421988035700
C	3.58162745918289	5.20919801400413	11.19658222043481
H	3.86798839670726	4.64876751013673	10.28696032502847
H	4.52678706607422	5.45235160451793	11.72594841111385
C	2.69063785624245	4.34742167871756	12.10086806196087
H	3.26128418389208	3.49981941812899	12.52719575691113
H	1.87753640997344	3.88551734060060	11.50504995208729
C	2.06321689427701	5.11473911932211	13.26664677219844
C	1.32916763472079	7.30093027927772	14.34100224353401
H	0.87032127906264	6.66452755475169	15.12063899137978
H	0.53794403467910	7.95453932895178	13.91905829670731
H	2.04610070081057	7.97736973399887	14.85557736951392

C	0.08998848273769	3.66025723389702	16.47407832166217
H	-0.59210795641730	4.13294874338285	17.19783544483990
H	-0.32259777866882	3.67848434522275	15.45388522216365
C	0.54755078628003	2.32356753929094	16.90068836192459
H	1.07066185606773	1.73156050931678	16.13504289517024
C	0.39724993357627	1.79238890331479	18.13988836433489
H	-0.12478225316928	2.33867592252968	18.93440916205226
H	0.77865278138724	0.79652446382323	18.39062462127625
O	5.23440267073073	7.42905145203427	15.83808635381084
C	4.09446884915418	6.90106742563957	16.37095410428456
C	4.75956583358115	5.26996498144204	14.95183108559759
C	5.59463302710448	6.55029681764561	14.72467320541622
H	5.31848409148927	7.06872255799808	13.79075776473749
H	6.68369368419143	6.40669903657890	14.76644264770002
C	5.53998057156292	4.03628424289290	15.49562684632786
H	4.25558480780242	4.97180934400846	14.02355925267624
C	6.25500272183604	4.36355435612543	16.81844978200030
H	6.79286235597041	3.47542025393399	17.19277161660832
H	5.53445811136454	4.66437640106274	17.59475548394411
H	6.99576626017088	5.17544738521672	16.70088145779170
C	4.55322474749053	2.87119467106726	15.70426914971484
H	5.09462022470386	1.96827295366951	16.03976813593777
H	4.01160317272163	2.63463328067734	14.77194677953394
H	3.79156251772251	3.12210100270869	16.46284612195377
C	6.56463259701278	3.62402489213207	14.41736041003828
H	7.33191460880736	4.40042908429538	14.24486205554735
H	6.06467785607899	3.41678565734241	13.45358389900843
H	7.09239253887973	2.70558135962561	14.72871229298593
C	3.51866836463353	3.19107303066304	19.18280216090606
C	4.57880416486837	2.53647866870684	19.82273307489523
C	5.55295792216147	3.27700014713972	20.51307093451509

H	6.21392019316465	5.25520991401039	21.11384325628797
H	6.38891465199804	2.76376339180815	20.99963249847209
H	2.75566905908530	2.62297948760298	18.63667187858603
H	4.65115911846936	1.44512315167672	19.77186088737757
C	-0.48813673055725	4.46381585608926	21.46949671018393
C	-1.69310306444447	5.04942817488807	21.05458823360937
C	-1.74820702707690	5.75684645069144	19.84129702126344
H	-0.64664081511405	6.39776032211936	18.08453733265117
H	-2.59166694880757	4.95171426865820	21.67235041852352
H	-2.68806815995689	6.21045098208927	19.51065598297587
H	1.60501193603260	4.12809841582003	21.00322296482512
H	-0.44230266989499	3.91023988118155	22.41303810171766
H	1.86504130928435	8.14451205415362	11.88229541829773
H	3.49712574146622	7.82399391445803	12.45427937151215
H	1.90494644201890	6.26732754768558	10.33676780526605
H	3.45269602941768	7.12155795876093	10.13721185215800

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Pd	3.56114220719750	8.32753066014149	20.53361219270897
P	4.64745766245821	9.55727574778863	22.08505434068056
O	1.68460956108458	10.19472319955745	21.14486264544913
N	4.46640026158286	9.55196167325630	19.10779905071581
C	4.73441605309946	11.31985750031649	21.63748084242321
C	4.97131232496702	12.25667613156624	22.66657519153161
H	4.98933596254523	11.90395718410225	23.70248397325298
C	5.19459702836799	13.60833481035302	22.38831706156662
H	5.38100720309487	14.31419181298489	23.20332942549978
C	5.17259875389153	14.04441810385344	21.04991104784882
H	5.35194963174296	15.09718326943903	20.80917858500687
C	4.92265210405582	13.13951914544325	20.01957568789288
H	4.91019326668093	13.47736047326516	18.98171799644989

C	4.68101494768589	11.76485308012407	20.28114187760122
C	4.04291630774894	9.52853127256068	23.81130988354127
C	4.89159887923932	9.25192883249705	24.89998758434504
C	2.67007026200241	9.78689484963038	24.02115723276503
C	6.41022148183945	9.03691056959800	22.18701341651036
C	8.80198777100704	9.49293315205377	22.12130997383744
C	7.47605277871768	9.95390234849742	22.11893725512988
H	7.26604073629182	11.02551154906628	22.05291973646625
C	1.71426873688598	11.43254776835403	19.12152211934394
C	1.64127304640006	12.75441614342001	18.39100952949036
C	1.67280228317879	13.99954924981247	19.29904018846560
C	0.89864935130706	13.75902674553746	20.60057155136094
H	0.88784660215679	14.67489907297340	21.22128970740455
H	-0.15735761389806	13.51645642039651	20.36852653708896
C	1.53659509260533	12.59296166225959	21.37027360190757
H	0.94328771236241	12.32697397320175	22.26368864605503
H	2.53587525826495	12.88973089577546	21.74013975189698
C	1.66069412591882	11.32694279138359	20.52242628825735
C	1.50911883053095	10.19431785189356	18.29621423374137
H	1.56078922244230	10.41399638015234	17.21382016988779
H	0.52074865959854	9.73245022547538	18.49902317229573
H	2.25357447951332	9.41310201818510	18.53710099924439
C	2.70011776485904	6.84524288907800	21.81287974788899
H	3.42942128798000	6.02509020510739	21.85140709828306
H	2.33129545231978	7.19620185145747	22.78154309725262
C	1.88031957319936	7.01465905231158	20.65330641569755
H	0.96611514871538	7.61493814445434	20.73556599951486
C	2.42824927446393	6.76560935711456	19.37468577273442
H	3.20358510208461	6.00219543108836	19.23996294693244
H	1.86956325466804	7.05657685270217	18.48020890530164
O	4.79085966523688	11.44900652139179	17.91304802005926

C	4.53488115818205	10.87308418774628	19.13277580211659
C	4.81312646411831	9.08055114188059	17.74978238879151
C	4.72766668748159	10.38553828401841	16.92455006639905
H	3.77227000482933	10.47682110177432	16.38274631637767
H	5.56419691137840	10.54528569938574	16.22832650082987
C	6.20342700385386	8.36592716350557	17.72790853885463
H	4.05078609316955	8.35573581985800	17.41407559785115
C	7.29579911741819	9.28694545641835	18.30410401712521
H	8.28105061562140	8.79194901674786	18.24785124523033
H	7.09629107698150	9.51622410823492	19.36351152062771
H	7.36741929820462	10.24118573303532	17.75193778828350
C	6.12481432104070	7.07886501548671	18.57179341955220
H	7.10989690372148	6.57980715892541	18.60198586705631
H	5.39402142409489	6.36831669151494	18.14396837216447
H	5.81624979573852	7.30055403417562	19.60845084330680
C	6.53653823267978	7.97796969755798	16.27227284407933
H	6.69629928340870	8.85880040888367	15.62543289040103
H	5.72914359180612	7.36826159584241	15.82584264395082
H	7.46379618502750	7.37921878891761	16.24286316209031
C	6.68826147162523	7.65551178810252	22.25932684532607
C	8.01198306580404	7.19983200700111	22.27500047435926
C	9.07240449148768	8.11890949552849	22.19951128480812
H	9.62533845217611	10.21202961352199	22.05711625251515
H	10.10759224351371	7.76213801319512	22.19559061057172
H	5.85560918671439	6.94393234878342	22.28534931369606
H	8.21791474566946	6.12586335018825	22.33153394467517
C	4.36804994979683	9.23341239349046	26.20242276576365
C	3.00609665826883	9.49280453266785	26.41712451835445
C	2.16292642432758	9.77084785217939	25.32695581478930
H	2.03677817739104	10.00457582018444	23.14543333609194
H	2.60061576111269	9.47736889324127	27.43451460634580

H	1.09979987989178	9.97413703629277	25.49514963554935
H	5.95455388744649	9.05394796049184	24.73064997337644
H	5.02796096932518	9.01782856059469	27.04949836810177
H	2.46901459374341	12.81418050576891	17.64876243119151
H	0.71074408682463	12.77292776452168	17.77900082776284
H	2.71643086376239	14.24324359077455	19.56212067118495
H	1.27044342626622	14.87185049993984	18.75072899911852

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Pd	3.53879345190053	8.52110422398277	20.53586298890355
P	4.70564837104183	9.60992278461747	22.13404080788706
O	1.60599697888312	10.18813678389642	21.12233881078509
N	4.40861526021264	9.83009953312766	19.17058428832742
C	4.86653306989119	11.39473524930516	21.79488010049571
C	5.22538725115435	12.24154991573335	22.86454405453215
H	5.31934120744823	11.81007312547003	23.86653806347645
C	5.46230640029570	13.60567841179133	22.67246229141150
H	5.74544777813503	14.23896526587711	23.51851074616038
C	5.30522523036496	14.15481572897258	21.38408431409661
H	5.47278148180185	15.22357773161618	21.21614653240636
C	4.95010173187214	13.34136539251774	20.31036308433008
H	4.85160186220268	13.76369746999243	19.30850695955092
C	4.71833445263183	11.94875114874747	20.48382827652113
C	4.04789902135501	9.51202660031440	23.83674340956325
C	4.86188478686086	9.21820994054936	24.94677632522763
C	2.66410443403164	9.74492482470175	24.00232274128046
C	6.43812155791855	9.00019786528756	22.24446457845334
C	8.85129572617790	9.33050959986063	22.21264651994944
C	7.55140500830694	9.86083451385999	22.20681374831428
H	7.39853048557718	10.94319807133149	22.16309143813393
C	1.67555922975345	12.48276147811452	20.51838332735853

C	1.45611929942739	13.57584872073856	19.50344583937193
C	0.71267549744956	13.10455285972744	18.24484354503792
C	1.33521164713759	11.79768545751483	17.74242730973441
H	0.88722306203955	11.48136764327129	16.78083022217437
H	2.40713920294002	11.99157132697876	17.55412678115180
C	1.18876947037997	10.68955171596581	18.79724674492279
H	1.84066720526926	9.82807013674591	18.55740077307695
H	0.15178915188951	10.29485194987423	18.79302240073705
C	1.51648903768180	11.12558498162554	20.22749519490045
C	1.93954319977957	12.93032217493790	21.92233157187516
H	2.62478063227286	13.79840982129190	21.93851514383670
H	2.36971055228664	12.12067292819500	22.52950625367806
H	1.00353018844526	13.25566390107670	22.42545968110885
C	2.76981620201701	6.89955779740360	21.71249497092414
H	3.51173527739785	6.09449501258178	21.62716598323952
H	2.45167358644041	7.14559258214597	22.73033589833336
C	1.88414912620657	7.16884650274548	20.62359453009153
H	0.97963929198732	7.75828323055404	20.81439832481182
C	2.35947699713146	7.05695111193587	19.29757397248930
H	3.12805846898381	6.31922228580450	19.03987666377797
H	1.74694757738326	7.43298363047899	18.47235208179623
O	4.81700994655889	11.77853773856565	18.09958981337684
C	4.56719577650322	11.13284631481084	19.28351018281252
C	4.75057028173643	9.42249176438387	17.79073999713157
C	4.74936946016968	10.77750224593260	17.04482416290421
H	3.82251990095567	10.94424560124555	16.47216435649202
H	5.61943277095313	10.94309384713899	16.39308179510157
C	6.10971904934972	8.64745095022703	17.73497655564180
H	3.95649842825141	8.75814534320431	17.40792490203661
C	7.23394478234519	9.48190269300545	18.37863716612298
H	8.19883237522602	8.95338069758060	18.28783567317662

H	7.04141682536154	9.64042539631577	19.45221160919891
H	7.34759348438846	10.47030019218789	17.89826955661051
C	5.97975706531118	7.30828421383453	18.48567388676959
H	6.94878123944070	6.77800899158235	18.48708591918449
H	5.23290876385320	6.65313973326972	18.00148790549727
H	5.66572703296898	7.46498926951055	19.53353543646435
C	6.43957412307351	8.34556708736500	16.25763620253752
H	6.64497957227588	9.25879338793774	15.67168871081548
H	5.61136181049068	7.80262815191004	15.76571230749026
H	7.34009450829657	7.70988104042170	16.19556208711588
C	6.64249654080304	7.60445088252764	22.28547208352844
C	7.93995074009695	7.07964816301424	22.30488452033158
C	9.04843687646221	7.94296054451062	22.26279481828645
H	9.71179271283557	10.00668879498603	22.17392125995015
H	10.06337999922147	7.53211364395887	22.26248982687630
H	5.77386843440624	6.93717327311600	22.28594527717002
H	8.08848010271491	5.99529205279878	22.33950696767659
C	4.29289098982390	9.15968843746250	26.22896677574755
C	2.92059758829481	9.39585463578591	26.40082023349657
C	2.11184112261662	9.68924194730545	25.28867513412594
H	2.05359166936433	9.97377650037030	23.11382356867011
H	2.47983577587294	9.34946183258347	27.40242662366195
H	1.04064277037251	9.87330333469690	25.42328906085755
H	5.93219774930449	9.03482994738259	24.80838645670804
H	4.92488786013411	8.93028814360864	27.09353548747825
H	0.90167964079874	14.41309468363940	19.97688493710951
H	2.43892284563079	14.02148701643909	19.21202888197760
H	-0.35380699186056	12.93316027786885	18.49034579376963
H	0.74395692323258	13.88531979625302	17.46176677186102

(exo)-15

Pd	3.61139312815659	9.28260965597612	20.44382933381304
P	5.01965918497125	9.76122806407128	22.16997126603481
N	4.94165819856223	10.30979395786565	19.19440223581410
C	5.51594946679407	11.52449624491146	22.00416086716801
C	5.70257714253353	12.29560722682150	23.16382170938030
H	5.52222022532367	11.84199414169043	24.14218474991073
C	6.11500395388525	13.63558203345925	23.08339624618207
H	6.24690274030932	14.21725338091072	24.00058098752513
C	6.35657781674812	14.21878464834154	21.83338612957371
H	6.67837852493706	15.26143988896989	21.76066300282654
C	6.18479218023965	13.46227430460720	20.66755342288983
H	6.37539971679747	13.90822614449799	19.68903290111751
C	5.75773110094448	12.11907209778597	20.73286762041345
C	4.39214123122425	9.60802764457074	23.87441963573064
C	5.14054670540821	8.97649067870321	24.88575239369319
C	3.12138334127900	10.14928598965616	24.16712158620931
C	6.58522165464587	8.82539405509399	22.10243801210103
C	9.01336453056049	8.69911275503305	22.09561307132736
C	7.83915717348512	9.45894185046512	22.20424612813991
H	7.89772605684551	10.54015638961813	22.35945769964019
C	2.15047498801979	8.08876070230529	21.42435925750499
H	2.50941081047527	7.06604381008536	21.24498452692857
H	1.90290269832625	8.31787818507693	22.46525704134765
C	1.49810981945751	8.80297995427771	20.37007819982864
H	0.84779503996716	9.65170779690673	20.61679604574425
C	1.96295149318194	8.64923463166266	19.04758691933322
H	1.61304666389753	9.32662023873717	18.26296103139804
O	6.28095089431638	11.93803423613203	18.40925594623399
C	5.61968112198219	11.39625552763852	19.45559060112461
C	5.24539902501984	9.88789505032517	17.79764767075895
C	5.89420917087586	11.16843399004588	17.22341218071946

H	5.19253827710908	11.79044334459958	16.64408958995543
H	6.80875392962903	10.99900414402833	16.64021546862616
C	6.14755272053722	8.61325877997771	17.73866888690504
H	4.29077372089256	9.66379488083936	17.29227838408604
C	7.47965065498413	8.84559313505937	18.47669403824510
H	8.10858014746132	7.94220056287562	18.40981175458328
H	7.31808214470036	9.05451942976393	19.54602103834832
H	8.05819654672321	9.68011244070051	18.04308282269684
C	5.40630853037213	7.42219335599466	18.37485671796614
H	6.04467425621099	6.52238153313878	18.35448713648223
H	4.47661897074332	7.18895487296929	17.82612499015641
H	5.14614787527281	7.62102949894207	19.43227393601249
C	6.40717452259829	8.28510748607617	16.25230284685168
H	6.99911559048868	9.06523551367962	15.74280832705316
H	5.46137660680711	8.15403345494933	15.69609544742168
H	6.97644160265968	7.34363853076728	16.17135060631308
C	6.51441294897815	7.43020694934629	21.90212635911776
C	7.69051368398389	6.67695810851076	21.80431635769967
C	8.94052691993529	7.31230955668810	21.89341669998887
H	9.98686968392192	9.19334778411003	22.16839502772519
H	9.85911229821304	6.72430916808188	21.80553853119310
H	5.53788054988424	6.94091829971233	21.82031335333583
H	7.63274002537246	5.59515840289154	21.65062494536028
C	4.61486674992994	8.88527374742094	26.18391140583054
C	3.35429378751174	9.42755559334676	26.47515912265097
C	2.60920170205617	10.06426203529081	25.46713031654854
H	2.54485766670302	10.64363296131216	23.37677605312457
H	2.94873314196225	9.35395100698682	27.48871377423226
H	1.62679069583548	10.48906572499430	25.69475827580760
H	6.12613731995864	8.55938028759879	24.65911473740619
H	5.19471360536352	8.39020740912539	26.96875560446969

H 2.37875732402947 7.69112672397853 18.71453902339266

(endo)-15

Pd 3.53324460405904 9.64811527414043 21.56996690437598
P 4.90531042680132 10.16606727266896 23.30998968781679
N 4.86604259959788 10.69104112260087 20.33340586773039
C 5.38908753038174 11.93085455036971 23.14656856945274
C 5.54804040454744 12.71195219882479 24.30358229391213
H 5.35342579306882 12.26386541263340 25.28172115222114
C 5.95327359956623 14.05373528819089 24.21987025067009
H 6.06485043862586 14.64368040019436 25.13445023493599
C 6.21512799300356 14.62793916984491 22.96963086943093
H 6.53237281685103 15.67181632577597 22.89437982922320
C 6.06905478858161 13.86169486060423 21.80677468646038
H 6.27385021120434 14.30196730277795 20.82864978006119
C 5.64876145558716 12.51617261217976 21.87452672317450
C 4.29945974568280 9.99139494774242 25.01928327171889
C 5.08303870767488 9.38644929859009 26.02113846397497
C 3.01717854537018 10.49243448893505 25.32970570893523
C 6.47680237824239 9.24140239414600 23.21728166069873
C 8.90558854352839 9.13378671304366 23.18561910093179
C 7.72662244134329 9.88458777379788 23.30658539428929
H 7.77865615443571 10.96599385394559 23.46270640701237
C 1.92207594800202 8.69670504064215 22.57487984577226
H 2.14766548742964 8.00862440638123 23.39550268309526
H 1.26584883105550 9.53522758782703 22.84324462073421
C 1.93094154774604 8.21399585083616 21.22670866860080
H 2.28380027485124 7.19511283841476 21.02236214783703
C 1.84385314603595 9.13465792719167 20.16571980591963
O 6.18971070147140 12.33706209261712 19.55698634876988
C 5.52964830048737 11.78595861587860 20.59924666838192

C	5.16506585524615	10.28502583058601	18.93004706724705
C	5.81731429218350	11.56947583436497	18.36653208063372
H	5.12069181534744	12.19100311834159	17.78072323151074
H	6.73839026959609	11.40339028519694	17.79259622088443
C	6.05685658318928	9.00550850597531	18.84603842370592
H	4.20709813841258	10.07461545099666	18.42574622032282
C	7.39470191921159	9.21801151430851	19.57927506487019
H	8.01424921235003	8.30888641057510	19.50276076813353
H	7.23873908622977	9.42107985768780	20.65061656559825
H	7.98010650479569	10.04980971263322	19.14943188837810
C	5.31305601659348	7.80813604691210	19.46811914020886
H	5.92782699578105	6.89558541265857	19.38314489267559
H	4.35386786070028	7.61839289282797	18.95356541769058
H	5.10429125559046	7.97383218151028	20.54088845790237
C	6.30324113237528	8.70103712042778	17.35224780247793
H	6.88805659473460	9.49012992285025	16.84833611011793
H	5.35235354522135	8.57593879426590	16.80326178911771
H	6.87377836567494	7.76227742016695	17.25162787778859
C	6.41463569158955	7.84583267466675	23.01740902056299
C	7.59542616380120	7.10175967937963	22.90697506690372
C	8.84140980567383	7.74658650558907	22.98359194241045
H	9.87590223953156	9.63554260357263	23.24892891044221
H	9.76354297562460	7.16569072298691	22.88618644638040
H	5.44078171906400	7.34964626434287	22.94538344790574
H	7.54432161698333	6.01967566190656	22.75299615679477
C	4.58021059806325	9.28225303604290	27.32693336677058
C	3.30736569387685	9.78538036752259	27.63560331846266
C	2.52750905339776	10.39475444498921	26.63740236974955
H	2.41264111728592	10.96451296704328	24.54769455978336
H	2.91940977240835	9.70171025510304	28.65527391722975
H	1.53514810884562	10.78783700696588	26.87831207919212

H	6.07765570459378	8.99980141622810	25.78057742831355
H	5.18697348753770	8.80780120426593	28.10412172063684
H	1.27814697437982	10.06818346095512	20.27670262510359
H	2.04025041887613	8.80667979535738	19.14084095795430

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O	0.92277253701128	10.06692913454111	19.48073703630849
O	0.80450071899885	12.01440915020097	20.67229128755976
O	2.31510224057838	12.11454088427419	16.59562952858845
C	0.81308238074195	11.31687972913181	19.62849421515386
C	0.54393470783046	12.21026801563927	18.24810299149262
C	-0.99463367559756	12.13937533493290	18.02420529078112
C	-1.48945285468406	10.74806492891984	17.60324698546940
C	-0.76769933398700	10.29074062174764	16.32603292695690
H	-1.11486432662960	9.28431232870841	16.01634095938614
H	-1.01942660406631	10.98116283407227	15.49258707565656
C	0.75775344521765	10.27890806543205	16.55143813475409
H	1.31846968036916	10.01098409032019	15.63808530219560
H	0.98177109942494	9.56495480006950	17.36926745595967
C	1.28905796895286	11.60927793758264	17.08000855225727
C	0.97339780661664	13.65931660999558	18.48332014444784
H	0.64947451270560	14.31433052386621	17.64915217936300
H	2.07084992625456	13.72607327257270	18.55237291091930
H	0.54093661287327	14.00966323954719	19.43301929872502
H	-1.48704245279411	12.46109724947330	18.96213483221528
H	-1.28106684905149	12.87908477697012	17.24289529796062
H	-1.26369667777769	10.03516881628832	18.41573171684013
H	-2.58719086298782	10.76191765571378	17.44646587700886

(boat/ax)-16

O	-1.85914992201708	12.00474465792720	19.92417878949567
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O	-0.57709674678301	10.11493199770745	19.70865283782864
O	1.56024924893029	10.56595533440811	17.15473084242266
C	-0.92183506434353	11.30132361879849	19.45783326541440
C	0.05762795021279	12.05250953891369	18.36787193836593
C	-0.69263336963592	13.23314431412456	17.70147714906251
C	-1.48258818565065	12.83935856789266	16.43160156443361
C	-1.98701600067164	11.39102741478008	16.53938989440341
H	-2.56264675560333	11.28854289600058	17.47584170968445
H	-2.66674990856917	11.13740968628573	15.70161470274292
C	-0.77318737231310	10.43900169259462	16.55362550733803
H	-0.40950837514405	10.23280817570661	15.52844410945610
H	-1.03389989914118	9.47002032765089	17.01549437999814
C	0.41774432849962	10.99422728818054	17.35742297800007
C	1.28835464749743	12.53166419425911	19.14397708226684
H	2.05510263463448	12.95789814918844	18.46880755173978
H	1.73932339002607	11.68176727917407	19.68152049323102
H	0.99195743522994	13.30171763640820	19.87971047717034
H	-1.39342517996092	13.58315635424959	18.48413625251724
H	0.01171261498779	14.05518461367370	17.45879845630576
H	-2.32414223887009	13.54212457350000	16.27338214038605
H	-0.83408323131474	12.91884168857563	15.53335787773655

(twistboat)-16

O	1.51316471150643	11.03074762191200	18.51438280242009
O	2.05945299645582	13.22642373360330	18.89453378822396
O	0.65970793874531	13.26321857041879	15.35097380092974
C	1.36823352992546	12.28295089665905	18.44925159879295
C	-0.01736930023581	12.77642415587756	17.63990496441530
C	-1.19669293138300	11.92388038074792	18.18734446723733
C	-2.21893451954386	11.59798598007238	17.08563801580294
C	-1.57724229099236	10.68351478465465	16.01473151577163

H	-1.69985847164372	9.62258333568511	16.30771061803700
H	-2.10452130531419	10.80759596781384	15.04925477937360
C	-0.06248714333202	10.99582691324103	15.84470322363614
H	0.29618694840687	10.76444193684395	14.82750439012162
H	0.51632616234993	10.41786318214117	16.59339118931006
C	0.23100713106018	12.45249609308499	16.18770148154540
C	-0.22945442228501	14.27653602215347	17.83917505277602
H	-1.19345243997197	14.60673444056403	17.39864155993548
H	0.58190337865607	14.83463140062781	17.35070692780831
H	-0.21932885218265	14.52153840747404	18.91413725132353
H	-0.77887754676853	10.98684643273120	18.59908514865092
H	-1.68046010256555	12.46688245899840	19.02261474705961
H	-2.54811928728857	12.54602526341652	16.61343574592811
H	-3.12951418359882	11.12005202127880	17.50031693090022

(chair/ax)-16H

O	0.13551799086052	11.30549813281947	20.58613874550995
O	2.28061105689156	11.36661927334350	19.90709469058021
O	2.56614232121388	11.40198103516972	17.21119112435698
C	0.95406004750620	11.53834446087482	19.71460795628852
C	0.56153142673609	12.12993385168947	18.31018993447209
C	-0.97242330395561	12.11069086739717	18.14220107734247
C	-1.52091563080307	10.76737755634920	17.64891506345113
C	-0.90523322471459	10.42607626984645	16.28518980514958
H	-1.33531907880342	9.49820433552227	15.86825633617836
H	-1.14017420927429	11.23477089626080	15.56648673883424
C	0.61751025323689	10.26898330748022	16.41278246587872
H	1.13864328781497	10.21586054430535	15.44093485961633
H	0.84041117013145	9.30624436054549	16.92043863707915
C	1.33017160963302	11.30607443594680	17.26512937201314
C	1.08043423960260	13.59547924451886	18.29279016200428

H	0.82218233678450	14.07175702122125	17.33190796655692
H	2.17163503170180	13.64689307414362	18.42073982036097
H	0.59925936248307	14.16645285527903	19.10415407256372
H	-1.41847871502479	12.38390762364693	19.11227815284069
H	-1.25057669661307	12.89671755558854	17.41388370053589
H	-1.28823267115890	9.97574278433244	18.38685229711707
H	-2.62144771370522	10.81948389375123	17.57432567738517
H	2.73865110945642	11.53057661996735	19.03260134388447

(boat/ax)-16H

O	-0.51865901890402	11.85214772727448	20.69831408747750
O	1.32542168259136	10.57163497749761	20.54541159336393
O	1.92770059988817	9.72459349991765	18.14260941305642
C	0.36290570745110	11.35193808908504	20.01884994678387
C	0.50004927704182	11.65718986990266	18.48811886251930
C	-0.85390442870003	12.14295803092106	17.92846691944613
C	-1.77421518662030	10.94432528641413	17.65301572051372
C	-1.20368588342627	10.02629915623526	16.54054621722769
H	-1.44373620664032	8.97182288907476	16.75813151920210
H	-1.66758801484234	10.26163450137126	15.56710730903167
C	0.33883278950094	10.17359983180718	16.38427901375415
H	0.54856913148405	11.05284486418274	15.74299891325980
H	0.80049555399805	9.29361326428523	15.91048277254979
C	1.00640730152034	10.43627676878913	17.71112255875576
C	1.58667273223149	12.76665575525709	18.36494023905232
H	1.73964362657636	13.04169618122454	17.30676327685555
H	2.54780518241584	12.43063537545889	18.78516699974305
H	1.25215725469652	13.66274559962841	18.91344971352020
H	-1.30386107863432	12.81904928227161	18.67213070398535
H	-0.68707470106509	12.72527247417912	17.00226001630109
H	-1.88220744485088	10.37884416353863	18.59708602255716

H	-2.78713563967870	11.28698357394635	17.38176459680565
H	1.85049676396624	10.18171883773714	19.77637358423779

(chair/eq)-16H

O	0.01577947511607	12.61615893593189	20.68131496806410
O	1.20579183673560	10.70911778348944	20.64324921329788
O	1.39250789922511	9.45630034586956	18.38756168616521
C	0.52736561114255	11.70506852281426	20.04789740843423
C	0.46142161442474	11.71064322468224	18.48774058339160
C	-0.96390013345872	12.18968315256161	18.07715349127295
C	-1.22681067925704	12.13192092639500	16.56702823804252
C	-1.00709610671090	10.70963077749635	16.03342084610980
H	-1.72992133831294	10.02065344259915	16.51089574782397
H	-1.18615601319747	10.65512773661733	14.94518538367026
C	0.42758207229706	10.23027197352692	16.34104409479011
H	1.14263593406284	10.84946365514570	15.76164730777266
H	0.59853596804056	9.18012118001709	16.05370834882678
C	0.79689351658577	10.37758596187600	17.80615501689226
C	1.54167729998599	12.73764463801711	18.02817087400864
H	1.51030592101246	12.90528132078208	16.93939798315272
H	2.55396176730366	12.39436816105217	18.30032722671800
H	1.34648149607124	13.69423078160891	18.53950190677487
H	-1.70437152784975	11.55079698553398	18.59512407533039
H	-1.10134055231752	13.20546135675624	18.48040729766499
H	-0.56692192528400	12.83911105339599	16.02850176682074
H	-2.26232496731644	12.45973896880548	16.36553852328891
H	1.46608283170116	10.05164911502545	19.92030801168640

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C	-1.43917743136595	1.75646533580337	-0.05839285108041
C	-1.32814623266214	0.28780508699595	0.37637194020319

C	-0.10375387094047	2.55455035549151	-0.02024770720186
H	-2.15972396429083	2.30670741326236	0.57914566287037
H	-1.85478683161932	1.80825721673452	-1.08939354162200
C	1.09102960345078	1.82044746184936	0.03821030466625
C	1.16873001748542	0.31701481050316	0.07332239413486
C	-0.14287604246033	-0.37363798510431	-0.33884689938738
H	1.45901267553332	-0.08401426660584	1.08741698173402
H	1.98800714250240	-0.05363269416127	-0.59446612992968
H	-0.10089247698005	-1.46269099512289	-0.12120540615387
H	-0.28704054909914	-0.26483052005241	-1.43376808019528
H	-2.27203492406346	-0.26876685373959	0.18333355164958
H	-1.15087482213436	0.23645679990217	1.47128549814065
O	-0.22666410582642	3.83083637804899	-0.06568593527017
C	2.39092866309959	2.56910996997132	0.11929395635811
H	2.16068665918948	3.64904841123338	0.06360168106043
H	3.10617210293467	2.31662272122040	-0.70413390211041
H	2.96313438724684	2.38488135376983	1.06489848213358

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Pd	3.52889617543610	9.21978068591655	21.45080246593847
P	4.91184173033927	9.72703079982704	23.20410370468534
N	4.79436614366268	10.55017752092798	20.32156240459920
C	5.21962232020145	11.55278959422706	23.22824611392529
C	5.31152334756855	12.23845597844068	24.45273981613803
H	5.19264277214624	11.67633146254385	25.38312505954725
C	5.55320837010077	13.61975159434864	24.50349504947576
H	5.61310773267734	14.12497920321566	25.47296815884494
C	5.72182235133026	14.34210644020734	23.31536780105977
H	5.91378891600694	15.41916759490108	23.34124349057160
C	5.64091847449948	13.67946369180956	22.08557824961189
H	5.77105262388206	14.23120379349050	21.15201487481896

C	5.38093300839835	12.29320673195982	22.02010759174000
C	4.43105849158181	9.36808482013772	24.93595231214878
C	5.32559587610988	8.86252775853566	25.89873685886838
C	3.08285699087263	9.59445667057167	25.28679986995633
C	6.61577384059686	9.04826489658286	23.05979545057731
C	9.04329539118596	9.25435519140625	23.01949751093763
C	7.77831390400993	9.82474401448114	23.23011822736833
H	7.69284293984330	10.87770030819016	23.51561912379361
C	2.10333638324569	7.93271429820993	22.19068401283624
H	2.50863300360130	6.91182834619335	22.07257997193580
H	1.79843170701882	8.11372987144685	23.23396804982047
C	1.10877083719595	8.27482449127107	21.09667304285305
H	0.47006607564844	9.12579789970638	21.40631681868287
C	2.07633164896308	8.72197882571533	20.02278369806920
O	5.85527716013716	12.44232885136887	19.67231491207257
C	5.31149163914534	11.68949527079739	20.67658618192054
C	5.08731961449664	10.33628946531335	18.88295035154037
C	5.52376992672540	11.75014299206923	18.42998061941580
H	4.71030346174503	12.31287219005208	17.94023798543715
H	6.42185569396713	11.77540868990978	17.79695829589162
C	6.15756658010833	9.21744509855654	18.66109298213976
H	4.15180107071610	10.02340432555594	18.38959488441238
C	7.46189938101594	9.55169511504442	19.40980906404887
H	8.21542508006499	8.76681976966212	19.22523759275356
H	7.29479744823321	9.59890557677202	20.49735231888974
H	7.89702119726489	10.51363262267618	19.08350421195601
C	5.60828271391334	7.86778967118890	19.16047360486933
H	6.37315365887513	7.08018869115538	19.03654477366706
H	4.70800001912873	7.56878890484421	18.59589474116963
H	5.32324602427309	7.91805042824723	20.22638329085704
C	6.42533764438686	9.10304157750396	17.14502102957811

H	6.89709652337878	10.00963786263340	16.72531319025645
H	5.49036368333409	8.91249437467543	16.58706554856486
H	7.11023415952465	8.25965812181638	16.94900628423546
C	6.73611514832592	7.69237183897063	22.68683476452546
C	8.00037743537371	7.12318205978417	22.49029561674597
C	9.15628039643944	7.90580433055912	22.64884130631260
H	9.94240754142877	9.86726079055006	23.14278167675642
H	10.14413447178397	7.46516982577304	22.47900487981577
H	5.82879853690128	7.09759505216035	22.53515700211824
H	8.08362290762133	6.07147478316846	22.19762917796097
C	4.87564386652704	8.59034373255640	27.19969270846164
C	3.53672824902218	8.82741756468294	27.54748951425942
C	2.64148540943429	9.33338070496522	26.59015392376490
H	2.38945966404483	9.97126862271851	24.52728221613761
H	3.18842074552380	8.61227345508812	28.56302447238851
H	1.59459736015132	9.51212110988056	26.85634221792328
H	6.37057270940344	8.68268480657985	25.62735272116690
H	5.57410089577375	8.19299444098732	27.94373683572759
H	1.74822095660814	9.55292849678019	19.37560785126832
H	2.45617597157592	7.87054601677975	19.43262473126690
C	-1.28878278856735	7.28260967893264	22.57256936849981
C	-1.77398211431150	6.45216312463457	23.77137727875235
C	-0.41532514421496	6.47649151676432	21.63298743421201
H	-0.72913212581338	8.16496077518581	22.93435913527090
H	-2.15378710431874	7.68782676979974	22.00686118242236
C	-0.31259720633063	5.12421236095492	21.67739394744603
C	-1.14341905681100	4.29512386347855	22.63673051141090
C	-2.28395035629413	5.08517816845022	23.29790999871897
H	-0.48086170990193	3.86754786903085	23.42129262395383
H	-1.55663748533797	3.41644249950787	22.09938187440464
H	-0.93053479420397	6.30089154135015	24.47341878013535

H	-2.55838299344553	7.00209703880132	24.32359593202050
H	-2.71389170481630	4.50841949810884	24.13767717869959
H	-3.09813059153937	5.23973864499425	22.56290594515751
O	0.24423274934969	7.17625981244464	20.63925211063701
C	0.61381974213524	4.36539017311280	20.76362485373143
H	1.26866735279272	3.68428212272107	21.34352901255883
H	1.24328883180343	5.05501947517642	20.18168950058523
H	0.05127049732825	3.72636535045863	20.05313012229967

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Pd	3.46255242964848	9.40011121502846	21.69689869406675
P	4.90672302254475	10.01651451645224	23.36477687437765
N	4.81796066763939	10.47757062468319	20.40833683632375
C	5.30610095584816	11.81340321833686	23.16876303931861
C	5.42050783335070	12.64588248308893	24.29582342174158
H	5.26728851070061	12.21508487051854	25.28912830386314
C	5.72937088896377	14.00933025545626	24.17140361309696
H	5.80477143555586	14.63259981843127	25.06838815064710
C	5.94535569989454	14.56260332317536	22.90315071110948
H	6.19173368948837	15.62314680514457	22.79308838856009
C	5.84022342174337	13.75154436856533	21.76735404134066
H	6.00407695108802	14.17141135323409	20.77247036459773
C	5.51005674539209	12.38346173581989	21.87709751692498
C	4.48231319998918	9.86586849452045	25.14242526604274
C	5.43815178698615	9.60470541955346	26.14441571392750
C	3.12425980854582	10.01064884224818	25.49327726546242
C	6.57216903911833	9.24079715497250	23.25263807764129
C	9.00477950153138	9.31706853424276	23.12909157494380
C	7.77444699293322	9.97306918594715	23.29198557048526
H	7.74729743380606	11.05720628652978	23.43872770165838
C	1.92555938863246	8.35534757667691	22.59496867806183

H	2.22950113709450	7.68855102229719	23.41895889748056
H	1.20677963766358	9.11538042754417	22.94527299338090
C	1.51259810947571	7.70868761835357	21.28584784927386
H	2.08821373895189	6.78085384241592	21.13053536921403
C	1.98957465451424	8.78687474859422	20.33578937731117
O	5.99211444869937	12.20497251758390	19.53276866728584
C	5.40675154064866	11.61788889149084	20.62036818081246
C	5.07429681152165	10.07602090261828	19.00340041674950
C	5.61320363858531	11.38807631529239	18.38342675367202
H	4.84407092170096	11.94244084128375	17.81856007483046
H	6.51153666712847	11.26860532514176	17.76134551973664
C	6.04594569879064	8.85539522550760	18.90531614665209
H	4.10941873178313	9.78607065681492	18.55514982186954
C	7.39104894551911	9.17279016673291	19.58547333016923
H	8.07293299713732	8.30962695366886	19.49709499892053
H	7.25488204388233	9.37758693480943	20.65860956358588
H	7.89598838086382	10.04276777861601	19.12784496014469
C	5.40425426426014	7.62598581188864	19.57694992111198
H	6.10245436420770	6.77039374054221	19.54291750553859
H	4.47132871461401	7.33173285707547	19.06523950762088
H	5.14775102727564	7.83169668871012	20.63156902815817
C	6.26475480956162	8.53648129504689	17.41087988911516
H	6.78818319840941	9.34823783964940	16.87429726498622
H	5.30409925714051	8.34904651939675	16.89723803960135
H	6.88266204663445	7.62733133482663	17.30853716054779
C	6.61793859221842	7.84388723931723	23.05790724853092
C	7.84751783154573	7.19107760650729	22.90752014858483
C	9.04338304594771	7.92800932066359	22.93589469339586
H	9.93484154007246	9.89482631962582	23.15028398166607
H	10.00394358595499	7.41965703026974	22.80276247108322
H	5.67986776186200	7.28054030229627	23.00719503899775

H	7.87252060928346	6.10750593987756	22.75275863418400
C	5.03808874336031	9.49966106329280	27.48454240136031
C	3.68650715463110	9.65751810328302	27.83114927599517
C	2.73070743198749	9.91432074116694	26.83475998015179
H	2.38639805797732	10.18532170887111	24.70357675546059
H	3.37682874234953	9.57199182164318	28.87797622096461
H	1.67470368831254	10.02636443760765	27.10132810362769
H	6.49117131592298	9.48195366181426	25.87135439363576
H	5.78327400717542	9.29270679974308	28.25994332257716
H	1.27505405372333	9.62317474675596	20.24850582188583
H	2.33905611885800	8.45238946990373	19.34436307677879
C	-1.53230737512482	8.46118283242234	22.45367794180675
C	-2.91015251075789	9.12491970712342	22.30769641827899
C	-0.89203866605972	8.14927714149640	21.11496359188167
H	-1.60089409786462	7.51482383675453	23.02235847302787
H	-0.86210108400990	9.11495251082780	23.04891940427801
C	-1.33736866484229	8.65633124248698	19.93695159814253
C	-2.47212124219092	9.66154611808892	19.88786737366319
C	-2.83728064286469	10.24561308884864	21.26156965161516
H	-3.36706505955151	9.17981717045269	19.43578060312413
H	-2.20253493281290	10.47989911020302	19.18890473983154
H	-3.65020204699850	8.36953473069168	21.97788843136216
H	-3.25774635980396	9.51099525818054	23.28377135648366
H	-3.79304678241330	10.79817863180178	21.20030569489300
H	-2.06207941265012	10.97528435370511	21.56867217386063
O	0.11862490517016	7.20667543435677	21.16008071383125
C	-0.78126731163117	8.22043968614960	18.60636969986644
H	-1.60071289485668	7.91144852647964	17.92620038349255
H	-0.08443087169381	7.37813281997568	18.72958134560563
H	-0.24236241969113	9.04336914878630	18.09691779411192

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Pd	3.40892821984617	9.57548180994135	20.63708137423307
P	4.84593533321281	9.79648201908891	22.39467584511297
O	3.72121715500973	12.10929642182155	17.76164834581262
N	5.19863442987848	10.22736089300746	19.45410200953097
C	5.60750763629421	11.48086667325468	22.25115597994107
C	5.69592805542466	12.32728514020735	23.37125677904141
H	5.32772089945508	11.96915954521793	24.33629927115776
C	6.24850212031137	13.61395298205514	23.277424444546726
H	6.29458925032951	14.24978402392602	24.16778885514220
C	6.74570177325324	14.07368666891647	22.05149476088817
H	7.18524188860840	15.07248156009153	21.96753037224923
C	6.67389926572365	13.24677006445060	20.92410559721537
H	7.05018617831925	13.59074590141271	19.95801111939930
C	6.09639667958848	11.96160478637347	20.99991108123387
C	4.29513244063977	9.74735606637389	24.14941702044027
C	5.14207640491821	9.40414709839555	25.22237129427582
C	2.94700565201092	10.07018704440548	24.40379135034721
C	6.33013870592848	8.70490264048157	22.41219925611539
C	8.73168119807324	8.28782974203697	22.45055158685528
C	7.65130966727384	9.18225825123993	22.51114826416465
H	7.83483884037841	10.25512305831720	22.62467765182594
C	1.39933668244652	11.51472730954684	18.13004322753791
C	0.48499025360100	12.77550794929948	17.94808873920420
C	0.42350108471802	13.67901939931408	19.19370299302099
C	1.82642350144789	14.11638424814738	19.64954862904691
H	2.26451189638659	14.78916718009596	18.88646478918058
H	1.77194646060617	14.69352923408393	20.59046380508886
C	2.77756911872315	12.90332008504502	19.82980940627712
H	3.80816342495517	13.23311445389370	20.03229499853076
H	2.45038247666115	12.26767578640207	20.67419431516601

C	2.76140977289175	12.10160311216322	18.53758653275498
C	1.52240375586956	10.76175437906711	16.79980764244113
H	0.53039228107476	10.40472449743852	16.46973016897448
H	2.18686008071839	9.88782162542038	16.90595243188864
H	1.94802984330979	11.40849203966424	16.01581701515308
C	1.46660664872501	8.85307474989263	20.92932340384906
H	1.53083638359487	7.77645428264424	21.14017539338617
H	0.88606648516123	9.41788749921577	21.67370453060018
C	1.52997925447675	9.33027251887933	19.58362570519831
H	1.64878434054261	8.59259858774980	18.77748582148616
C	0.77917867217335	10.59848756547767	19.21686884553761
H	0.62030860044023	11.17536312387277	20.14451125661726
H	-0.23873947905966	10.33398893689353	18.85210778438655
O	6.87215517631868	11.58773394657944	18.75910791431981
C	6.01419130441858	11.19327446281953	19.74224560238274
C	5.48851682565873	9.77007793739730	18.07594119280332
C	6.48555146618170	10.84111168931777	17.56209155743612
H	6.00935805072447	11.55154279054394	16.87143550329406
H	7.41052027828996	10.43653577587442	17.12460728172655
C	6.00706941297575	8.30099776483311	18.03487590543506
H	4.54514993142261	9.82813557169816	17.50833320716369
C	7.30630727234765	8.15561854093982	18.84813395892141
H	7.65472811202569	7.10838876048460	18.83012573012424
H	7.14663609546928	8.43649850823804	19.90018662676940
H	8.12132855259047	8.78247423870561	18.44337346725440
C	4.92737419174689	7.36453617069685	18.61013298179947
H	5.27460562116382	6.31566206669788	18.58154134734334
H	3.99083647535687	7.43388370644379	18.02764214036510
H	4.68399855429023	7.62727690917917	19.65654513345953
C	6.25428639366204	7.92296878203579	16.55943986291501
H	7.04960296746653	8.53506308192094	16.09691355095989

H	5.33553865712328	8.04621797448163	15.95716203214114
H	6.56807200182852	6.86669279909721	16.48534828251532
C	6.10679548203821	7.31973759245566	22.26031096784333
C	7.18532401305821	6.42811630404683	22.21664707292259
C	8.50166334527760	6.91162392553700	22.30464252496925
H	9.75620499363189	8.66935285771535	22.51650253636760
H	9.34623123455324	6.21668185440797	22.25279215210035
H	5.07928406586081	6.95345092337835	22.15759579277393
H	7.00055967907282	5.35557066507219	22.09580205013044
C	4.64536242375417	9.39396093181183	26.53394442652993
C	3.30515824219112	9.73205368959254	26.78323383551776
C	2.45669242550519	10.07192375755660	25.71683866553102
H	2.29478305017913	10.30414991516969	23.55440270148741
H	2.91998514745839	9.72198750638516	27.80835325948386
H	1.40850384670283	10.32532367512722	25.90795941032653
H	6.18737959396861	9.14408159613316	25.02589897379470
H	5.30593825060969	9.12155781691829	27.36411005272814
H	-0.52951949829738	12.43323246967131	17.66630218325726
H	0.87227257305116	13.36229073369384	17.09177376839953
H	-0.08649513997127	13.15005829272420	20.02007640010707
H	-0.19370328510800	14.56928102095648	18.97153032362477

(S)-19

Pd	3.19786378040030	8.62175825193197	19.84689559937232
P	4.22345921950733	9.38171681359213	21.71176550595840
O	2.28474864919786	3.08899966348348	22.38370514346721
N	4.70160707636192	9.89328680100826	18.76913960500753
C	4.59423582415026	11.18591367817029	21.62504888384051
C	4.46983013599596	12.00071469263805	22.76561850948697
H	4.16624589002449	11.54022157308841	23.71023182867225
C	4.72864655447691	13.37806396070281	22.71562694829733

H	4.61922249325276	13.98536310120809	23.62019589469507
C	5.13668149329723	13.96582060435437	21.51096449792619
H	5.34688181580675	15.03852209149992	21.45819023717318
C	5.27617333414029	13.17322317507357	20.36606284043772
H	5.59624186843058	13.62179937434885	19.42319939954374
C	5.00033728154264	11.78820336812787	20.39513709599581
C	3.41312827010591	9.15774433965395	23.34533583384498
C	4.00085488769135	8.44089603743628	24.40630222715213
C	2.08148823153753	9.61214877413002	23.47513515564908
C	5.89321055792576	8.64505243734926	21.94770016842996
C	8.29905346999896	8.78376432996710	22.31104316878335
C	7.04311129542021	9.40577604911958	22.23422680942957
H	6.95676459345721	10.48616008563362	22.38533297832155
C	1.13972569613690	5.03022475690615	21.47106143221709
C	-0.20943356833268	5.59749686462991	21.99219827443914
C	-0.08142256866038	6.35806400149984	23.31874851484190
C	0.50052103425702	5.44917679823939	24.41110504838562
H	0.63147155740319	6.00784257116798	25.35566247136365
H	-0.21180274085975	4.62657251055948	24.61884160908178
C	1.85399167871466	4.84722920504056	23.97645522277784
H	2.21900449063028	4.08643838082266	24.68625609649537
H	2.60648716310855	5.66106214805023	23.95169762701918
C	1.79752130054745	4.19981487649759	22.58854306997720
C	0.90727746514776	4.17242851483234	20.22220899928185
H	0.51244844636292	4.79824547556984	19.40408366037042
H	0.18774583765096	3.36101112838060	20.42815183190722
H	1.84757799326834	3.70388195285671	19.88933748117184
C	2.15835505021691	6.18415707920226	21.14488694053653
H	3.05030862994793	5.71433284023564	20.68865192580870
H	2.49491699824342	6.64785763691155	22.08833428851184
C	1.64312572323594	7.29050028362112	20.23843898683394

H	0.80125917221279	7.86288262893083	20.65781762812333
C	1.80067342779749	7.30148820930138	18.81945203823472
H	2.33049761556552	6.47862922607218	18.32243603229875
H	1.07974536806862	7.83877956791176	18.19155300380887
O	5.93737690524339	11.70510411937513	18.19090792429868
C	5.17375792371608	11.05132706614811	19.12427651371423
C	5.26148513723249	9.55406828092266	17.43962592848342
C	5.86362161028217	10.90456536801524	16.97491304781057
H	5.21574183188352	11.43867323481866	16.25850757105575
H	6.88314512021492	10.83972883079549	16.56801999650768
C	6.28292047513569	8.37232904607128	17.52049465053447
H	4.42710964789240	9.24040639318006	16.78878206804020
C	7.43311034516361	8.71148824169784	18.48749323828438
H	8.15537961447031	7.87788858050949	18.52439345679734
H	7.05714297077309	8.86877918494886	19.51047811737213
H	7.98641672098140	9.61667953061096	18.17797936949396
C	5.56273221346980	7.09996193352637	18.00531386703197
H	6.27813665776539	6.26051994550389	18.07016854105995
H	4.75172932486174	6.81135950863921	17.31329883471624
H	5.10671453296658	7.25242643840422	19.00092380775500
C	6.83354070727372	8.11358280916411	16.10197670370253
H	7.42203884220461	8.96363344202425	15.71224521450389
H	6.01618573253199	7.90606825483656	15.38708401538967
H	7.50039159891517	7.23375462642378	16.11324341106122
C	6.01683292480773	7.25167989847582	21.75349605163165
C	7.26849589890278	6.63140834178485	21.84921751363232
C	8.41436387860787	7.39862443110863	22.11916039793485
H	9.19004549711726	9.38487826515681	22.52139332763097
H	9.39592664549700	6.91681769411774	22.17636206073153
H	5.12388627253681	6.66503372162927	21.51202775878579
H	7.35211245526173	5.55037022226619	21.69712479171866

C	3.26871925934328	8.18508971688042	25.57721302373950
C	1.95588146019806	8.66181642981244	25.70944229196115
C	1.36633091642034	9.38386470291381	24.65661701660343
H	1.60990063610371	10.13283772271537	22.63382821590527
H	1.38972037448996	8.46715240746685	26.62599079359031
H	0.33763470247460	9.74735317067818	24.74881807454964
H	5.02907498565083	8.07890773895304	24.31230137831166
H	3.73127513859734	7.61772487482130	26.39170264469387
H	-0.64808013080580	6.24159539579872	21.20829931727606
H	-0.91164128550673	4.75003870571812	22.12596720328561
H	0.56849574598928	7.24275168648305	23.19019342684170
H	-1.07161710757676	6.73929023703577	23.63113007324480

TS1

Pd	1.92426851745018	4.84194645324793	16.39545559556877
P	1.98317715338195	5.55106562395326	18.48358698773690
O	-0.44844803242199	5.17988990330528	13.67955110148908
O	1.40334275087022	4.06968251995508	14.43499880564901
O	4.11399485814947	5.17719049076853	12.77406510284533
N	4.12204031579250	6.22152805538840	16.72399779644422
C	2.19461927108409	7.36206288784380	18.71954681845631
C	1.33545778757838	8.06052379811840	19.59287989574361
H	0.57174970094588	7.50340992601162	20.14232235569793
C	1.44818533866854	9.44386621184369	19.77927529577810
H	0.76956106084465	9.95419139653831	20.47065872102532
C	2.43576638903239	10.16645742689204	19.09070172450003
H	2.53372343864258	11.24723943786228	19.23332131818328
C	3.29962090386746	9.49763583393236	18.21963156866747
H	4.07289183766229	10.04431311820166	17.67462843783286
C	3.19625490559250	8.10352987971920	18.01663894598469
C	0.49569602050596	5.12636031099269	19.47807340306236

C	0.55438245129390	4.48303357924216	20.72898906735853
C	-0.76141570265847	5.33827595572958	18.86888361921165
C	3.36331187099145	4.82819163000460	19.46444911225979
C	5.21893435551989	4.98419490724971	21.03393330934817
C	4.15921760486962	5.58899876640659	20.33988742592319
H	3.95653225952896	6.65663595109841	20.46862732814234
C	0.76231507407360	4.97702244937474	13.67532986161469
C	1.75100275242499	5.75993534522349	12.76902555244492
C	1.03241038772455	6.13011054339351	11.44175864866644
C	0.69948867622380	4.90272052626510	10.58059349015119
C	1.95776330894417	4.07843174006302	10.26985896696450
H	1.70619333187662	3.17887919580804	9.67944111743075
H	2.65307059603098	4.68058556985510	9.65310218359368
C	2.67762466741094	3.65821065090405	11.57394893752814
H	3.62882652712465	3.13864384978808	11.37433082680964
H	2.02246439337875	2.97592169565746	12.14769002972717
C	2.96778265159059	4.87707520518792	12.43768025104102
C	2.16770442321623	7.02640682898634	13.54272919835872
H	2.56131278450269	6.76745167358851	14.54116553876341
H	1.29290316026096	7.68324703154702	13.67939180211848
H	2.94933056913043	7.56973321582616	12.98620928031750
C	0.17281817317250	3.22290821513836	15.61656703527791
H	-0.53016955022056	3.92526720965013	16.08048449956976
H	-0.24919650518765	2.76205987954973	14.71602105326425
C	0.91182606590948	2.32734929583038	16.51317268737985
H	1.71625211676019	1.73780344692980	16.05391290907022
C	0.51993145915816	2.04937489071120	17.78561020705608
H	-0.29338841358366	2.59682357639457	18.27149856628440
H	1.03266427942665	1.28592611310982	18.37780693357141
O	5.04454322748951	8.29286410097549	16.46840769296021
C	4.11505635724030	7.47127309430571	17.06689220688898

C	5.16379158068014	6.03968145452372	15.69418978544212
C	5.89567021788482	7.40949876811292	15.67360114327857
H	5.98188386858421	7.84395234256062	14.66662418682549
H	6.89203658393810	7.38924811384805	16.15085898766137
C	6.03345442549715	4.78507098173310	15.97325165242444
H	4.65821319810599	5.87403853835362	14.72544815803631
C	6.65624191094857	4.84728758070286	17.37911286701446
H	7.23674650995638	3.93023845537207	17.58301494516700
H	5.87286874355105	4.93608976482898	18.14854385210179
H	7.34586782392472	5.70447860255232	17.48971469718344
C	5.11633960367756	3.54880154767920	15.86388255951321
H	5.67969523547741	2.62482243341732	16.08952968844054
H	4.69931959408602	3.46426319065386	14.84512901127630
H	4.26994271317384	3.62583699278150	16.57130219130701
C	7.12547113900373	4.70124273185043	14.88805856905629
H	7.82497344948569	5.55628963954993	14.94089595747723
H	6.67284079157533	4.68403858987630	13.88080715249208
H	7.72276389224873	3.78025649695186	15.01352255834486
C	3.63207791459984	3.45398593446419	19.30078243462487
C	4.68097486930290	2.84980405306765	20.00520281635891
C	5.48117301489889	3.61563012892177	20.86918124598508
H	5.84240574067621	5.58600168903147	21.70366769033341
H	6.31107217740184	3.14727108586158	21.40849922140612
H	3.01444917351489	2.87152557860292	18.60921958733338
H	4.88549116660825	1.78274430617901	19.86774988712601
C	-0.62573130443588	4.05623919514652	21.35867658692180
C	-1.87139724969404	4.27871661078457	20.75276428887938
C	-1.93828952132553	4.93020511798477	19.50809987274115
H	-0.79769972553182	5.81233236542441	17.88026822642994
H	-2.78942079880998	3.94063374480789	21.24462368646310
H	-2.90771284897646	5.10338970700951	19.02899542922033

H	1.52469434213631	4.30877045430565	21.20344134525824
H	-0.57023893744058	3.54706799552423	22.32682833092993
H	0.11224587163139	6.67891016267322	11.70550815118309
H	1.68851824283077	6.82103997092363	10.87724421940172
H	-0.03701398751531	4.27660154840590	11.11884545711092
H	0.21385500705781	5.22684471716287	9.64224034548699

TS2

Pd	2.33698681628077	3.83414969802973	15.93610527668928
P	1.92675210158141	5.19349743012855	17.64409033912776
O	3.12076796337220	2.94455971571330	13.93427964481558
O	1.42251417336613	2.01477761279220	12.74373755346308
O	0.71358821666797	3.87136262128104	10.07162308321960
N	4.13483462107380	5.27792752583210	15.67233052862831
C	1.99863480427069	6.94895788706757	17.08102173221912
C	0.99606395655107	7.85263986123878	17.48544158229496
H	0.19533395823845	7.49709009931468	18.13886563686764
C	1.00946987023234	9.19441114895213	17.08168655520511
H	0.21431479735504	9.86811704547618	17.41713992860237
C	2.04569451277318	9.66999816550269	16.26476915894028
H	2.07059826096245	10.71762398028769	15.94967654979775
C	3.05123583751099	8.79272265796896	15.84796995175733
H	3.85933783315463	9.14388939107374	15.20234181745546
C	3.04058676755045	7.43293946520618	16.22983929960096
C	0.34881531570513	5.10427717609423	18.57131142655527
C	0.26678216436173	5.20472713381767	19.97407244492415
C	-0.82646650089276	4.88403640808294	17.81948984960143
C	3.21393716665200	5.13118704463523	18.95444138918491
C	4.83841530963931	6.16374043506706	20.44850880525965
C	3.82494193536151	6.28377846490745	19.48513244061302
H	3.51370186106719	7.27327953921946	19.13711976136751

C	2.30264354348457	2.95056314320849	12.97760851771585
C	2.28414635133570	4.08145279015311	11.91665048047750
C	2.56729426135581	5.46996673970728	12.55459495945694
C	1.44134255027781	5.98211950260353	13.46208666994595
C	0.08957927372548	5.99815099091582	12.73938355020638
H	-0.71439600371269	6.32312797572636	13.42514464415954
H	0.11510063059542	6.73016429579255	11.90789973169127
C	-0.23817378959018	4.59715254571229	12.17374694103075
H	-1.17971176064253	4.58996862636284	11.60080573220315
H	-0.32895593652603	3.88350630595217	13.01484129298500
C	0.88656573900690	4.12444276849254	11.25989314302405
C	3.36676208162013	3.73974307359174	10.87519849887886
H	3.16072830597276	2.76724255626793	10.40175312987942
H	4.35705086164266	3.70131021321282	11.36113291898447
H	3.38382329498647	4.50419595355670	10.08070821768999
C	0.95051464500225	2.26846247311487	16.31714386625814
H	1.75539512453483	1.58023195091270	16.64588458854240
H	0.30779219080619	2.59759162573382	17.14495363953112
C	0.28105068164849	1.89641979767958	15.12033593494523
H	-0.71579507859594	2.31115330687104	14.92169711911270
C	0.87963627074711	1.08730674252408	14.10782678517658
H	1.80368040871112	0.56714333731491	14.39119306406204
H	0.20863176796066	0.48036749416393	13.48968349230135
O	5.14316094895905	7.22075691525037	15.07342926818326
C	4.09901143075441	6.57293750001560	15.67951961015436
C	5.38527857419282	4.84233474399938	15.02033250015210
C	5.99147143044320	6.17609808868216	14.50205216779439
H	5.94495566965675	6.27395106097342	13.40502228207672
H	7.02027814911708	6.37073354348545	14.84234957596193
C	6.28222958024822	4.02410946931988	15.99722610639697
H	5.09978214199020	4.17619007181564	14.18748853322394

C	6.62527059781040	4.85134234738817	17.24943313561203
H	7.24662540788654	4.25726845557735	17.94187209411135
H	5.71155705996566	5.14741272397517	17.78832479744649
H	7.19234730096757	5.76729420714790	17.00089165847967
C	5.51773263807683	2.74978065286893	16.40788806679010
H	6.12873049377138	2.14019436454881	17.09792363784092
H	5.26342994516333	2.13729103669169	15.52576040475397
H	4.57025154747935	3.00673287935693	16.91604151557445
C	7.56787316824371	3.61731984361471	15.24910437165482
H	8.17790946833906	4.49158352791330	14.95700561426505
H	7.33166376516119	3.04316014002020	14.33471093132700
H	8.19778407106030	2.97994248851751	15.89436248726402
C	3.62225949664217	3.85974820608320	19.40965802157834
C	4.62284800717278	3.74383063633728	20.38234230009758
C	5.23867000850308	4.89627809557881	20.89826933045590
H	5.31680998781482	7.06443204356531	20.84731948307771
H	6.03305185868634	4.80549897882953	21.64618526898672
H	3.15961630849083	2.96466386521505	18.97998803200647
H	4.93515383039799	2.75228728532259	20.72579853238108
C	-0.97674541774509	5.09622872972360	20.61395066251114
C	-2.14422134581728	4.89345702958612	19.86077495694935
C	-2.06787278246833	4.79136082214677	18.46166069549397
H	-0.75138989059934	4.78429119512380	16.73044002164071
H	-3.11284323444299	4.80815505991081	20.36402348548785
H	-2.97510128381595	4.62460811423279	17.87177711113144
H	1.17602957718826	5.37151921400506	20.55982533477160
H	-1.03438682652029	5.17399149186121	21.70479567440014
H	3.51100078628617	5.40041438019367	13.12030401562104
H	2.73215741117924	6.18843893416505	11.72729391891424
H	1.37419775262188	5.32805328672355	14.36231167790345
H	1.69399520995593	6.99013385297246	13.83590104307845

TS3

Pd	2.25233045590384	3.42891728132080	16.36090735763613
P	1.92381333262682	5.04313974076011	17.84220032958514
O	0.85721067857255	3.89574774650870	14.04488716595375
O	2.61468471121527	2.67015629435274	13.28639064275806
O	0.68542925191000	4.01793973732260	10.06405062850257
N	3.91723856132408	4.69233630400333	15.62451579745447
C	2.02247008178841	6.70067262072081	17.03618594648863
C	1.11861299180574	7.71697036508401	17.39534306915178
H	0.35086539224678	7.50323881352963	18.14374077391430
C	1.19128596057837	8.99537706025256	16.82275285820504
H	0.47114627951491	9.76434099214562	17.12043679036423
C	2.19055945194429	9.28408960618258	15.88454177301805
H	2.26325353937645	10.28008034553002	15.43730839240800
C	3.09413525575315	8.28480888903075	15.50662648432576
H	3.86390686690227	8.49034216509434	14.76010031723408
C	3.01647670639427	6.98619822156514	16.05425022708734
C	0.38435361332781	5.12912514905370	18.82896256241992
C	0.35377268410011	5.55398842704507	20.17146908318590
C	-0.81012667950328	4.74227446513061	18.18630377196389
C	3.28206660679924	5.12822813423141	19.07949551798446
C	5.00713814755063	6.31675108835342	20.32323863902580
C	3.92909144283283	6.33063334493795	19.42424782666792
H	3.59801347536446	7.27453011202022	18.98079349585156
C	1.78927386718940	3.66737540516273	13.23295772370935
C	2.00054713200949	4.63203814817793	12.00882366540669
C	2.20233431271674	6.09683104303157	12.51236687529224
C	0.96869774507948	6.74361018040749	13.15466024099734
C	-0.22578763846899	6.69850029997951	12.19166286687056
H	-1.12571618077072	7.13515220323282	12.66267232292473

H	-0.00589232639533	7.31326717179572	11.29580525208350
C	-0.52396682359183	5.24691613230045	11.75217018813568
H	-1.33637567816178	5.19331361453934	11.00876513536632
H	-0.80577802406583	4.66716251346965	12.65031137654155
C	0.70449054353599	4.57292080592593	11.16117283693186
C	3.19617352976679	4.19987059675668	11.15262419821486
H	3.06537335975667	3.17460144036199	10.78088365016392
H	4.12558698793947	4.23365321527189	11.74589718590389
H	3.30319494056442	4.87128673266491	10.28315916713800
C	0.98289799266139	1.84603505988207	16.73532212366899
H	0.94946401987515	1.53599029120641	17.78817097463586
H	-0.00435715296342	2.07907072280367	16.31134709438591
C	1.94875129956334	1.20043849988541	15.86810893507155
H	2.80440644104133	0.68573230189035	16.32139747995289
C	1.82648449059337	1.18058167219103	14.46244517901924
H	2.47705715732389	0.52652070447303	13.87823134531903
H	0.85562501953932	1.41936570512512	14.02292460596071
O	5.01902135176312	6.50181242403102	14.82721625869134
C	3.96927866766861	5.98739463849502	15.53676011007799
C	5.11580642236473	4.12583763712703	14.95772402964284
C	5.69497562982894	5.35856451800742	14.21920748738849
H	5.45047175340599	5.36347077486059	13.14375828833460
H	6.77472120975610	5.51396114256841	14.35424927419372
C	6.09333039792581	3.45955000627809	15.97704621852669
H	4.75784901492301	3.36332942741704	14.24469364597377
C	6.51964819949176	4.46598605523444	17.06308644771586
H	7.22324476540173	3.98990862808857	17.76789772722046
H	5.65012185431901	4.81359604339307	17.64386309854677
H	7.02630670326080	5.35027293260340	16.63594338740750
C	5.40218970772165	2.25310298722488	16.63842213383881
H	6.08791392434822	1.76618932346589	17.35519256709182

H	5.10286836476431	1.50567100678252	15.88250603725298
H	4.49051964742428	2.56471970864078	17.18067384040529
C	7.32505887667316	2.94937505905961	15.19929263244701
H	7.91602107381082	3.76927931320521	14.75352438798140
H	7.02614180100315	2.26238064914870	14.38681993836397
H	7.99664402285471	2.39624991108397	15.87914307458939
C	3.71957391798122	3.91590675031320	19.65342900107913
C	4.78550528686980	3.90781119428643	20.56105224957017
C	5.43673622838095	5.10822190050598	20.89149744030843
H	5.51394962396951	7.25380158847231	20.57650555743443
H	6.28238704300476	5.09973924711632	21.58685787861963
H	3.22975872125032	2.98169122063679	19.35813425656577
H	5.12105814752277	2.96156290380581	20.99771702444264
C	-0.86607626164060	5.59575185919021	20.86303308531489
C	-2.05570283345456	5.22328234515709	20.21706139389555
C	-2.02720172106913	4.79999218213890	18.87755536996857
H	-0.76714694186631	4.39464763282909	17.14796054477470
H	-3.00588821946750	5.25619350319071	20.76019549916210
H	-2.95334589338222	4.50275674340564	18.37494471332723
H	1.28296494825997	5.84871110685039	20.66964730998562
H	-0.88751015035863	5.92047494775084	21.90864731829515
H	3.05921570966945	6.11796369627851	13.20763729448110
H	2.50747984638134	6.69880884069221	11.63220603798275
H	0.72005959763522	6.20464539276820	14.08347292766652
H	1.20345573853636	7.78903339318390	13.42605463655351

(exo/t-N)-TS4

Pd	3.86418515968508	9.47783888986366	18.90929290673223
P	4.26611687551358	9.92791668538739	21.11692872438993
N	5.89903731873825	10.04504655842229	18.56623850695710
C	5.15111518259716	11.54766897683556	21.18059482664973

C	4.84000228396181	12.46536248849619	22.19891764107815
H	4.06513811006233	12.20527272331061	22.92529299221212
C	5.50216164552425	13.69861462972116	22.29777715845725
H	5.23225848855092	14.39548091503669	23.09750072168286
C	6.50487532861605	14.02948111126713	21.37709680377264
H	7.03025424190079	14.98664989568879	21.44681267178829
C	6.83160282166357	13.13003605084690	20.35618287755019
H	7.60826116225597	13.37909338730469	19.62967715556487
C	6.16006034030379	11.89413741004097	20.23341308163444
C	2.90837368932430	10.09350517990486	22.32599507823319
C	3.06300071851310	9.73861053813151	23.68308344639661
C	1.67031058986401	10.58000390237422	21.85997383187820
C	5.46159109442054	8.77497375619908	21.89835570453399
C	7.52173942408255	8.26904322102121	23.09443957626281
C	6.61787248909862	9.20878822593479	22.57463375282412
H	6.81493787330811	10.27918770383309	22.68691098719575
O	-0.60385338286595	8.22966226207642	18.84933116026818
C	1.82188155499410	8.56196389726203	19.04459326036717
C	1.96059077878353	9.41123034809282	17.91522858876197
C	2.94366371598073	9.12660473322292	16.93535717894533
O	7.76993758607581	11.31109212554395	18.55340494934083
C	6.55883842335531	11.02763656229841	19.11035583772559
C	6.75356679092664	9.41857039136902	17.52864526301382
C	7.88995279144496	10.45966088686508	17.37217985523569
H	7.76619437357113	11.10277544222478	16.48477700503211
H	8.90427436145858	10.03640745444375	17.38115233576293
C	7.22196147835998	7.98564771420853	17.93756755284676
H	6.15799241475622	9.33491059249511	16.60332184738852
C	8.01411968423927	8.02490165710310	19.25778331999098
H	8.33943744766438	7.00763482578186	19.53430787865036
H	7.39515083483530	8.40916193016670	20.08326476745869

H	8.92044149977901	8.65227038166429	19.18265404242778
C	5.99241984072438	7.07161007288007	18.10073164064947
H	6.30958824089782	6.05551987912008	18.39444576402174
H	5.42311812748487	6.99340133993435	17.15760077018972
H	5.30589606844999	7.45295795158043	18.87996353536467
C	8.10172708324204	7.42693149588991	16.79932626556305
H	9.03277191316337	8.00543705581190	16.66179646807920
H	7.55727546377985	7.41990944660855	15.83743737623267
H	8.39501525970365	6.38742520992492	17.02654155425738
C	5.21474512203779	7.39267732747087	21.75812096546212
C	6.11329766038959	6.45880747932993	22.28783367564076
C	7.27261071721560	6.89596215456222	22.95052319511277
H	8.42323689192988	8.61260791015705	23.61214639772233
H	7.98158239145119	6.16545245731899	23.35314826595765
H	4.31862664260476	7.05724162719940	21.22469332241298
H	5.91460337631862	5.38830295011792	22.17456127783860
C	1.98105359231063	9.87651049223657	24.56384082759034
C	0.74702401500653	10.36150173546180	24.09672228144014
C	0.59294813688486	10.71143983685352	22.74675577456654
H	1.50589930503210	10.81900335895391	20.80499970658625
H	-0.09972299841744	10.45047970377624	24.78519965138928
H	-0.36491533485469	11.05753639607801	22.35044537393320
H	4.02134118327172	9.34979017197328	24.04223645988562
H	2.09904545852939	9.59470106091984	25.61547299190200
C	-1.07833068217770	9.31391394639258	19.32980371311473
O	-0.44477381606045	10.34701640198888	19.69741368209126
C	-2.65409847561028	9.37651274148555	19.44146990178623
C	-3.02958317756891	9.95383175093026	20.83001500293487
C	-3.22683715799790	7.96082855262741	19.30115487412110
C	-2.93115789389532	7.01044088738750	20.46216311566515
C	-2.63913315227548	9.01819526954736	21.98383764509099

H	-4.12240187536046	10.14216471439694	20.86083136954464
H	-2.51816698742332	10.92848683547013	20.92385268058302
C	-3.30074113603599	7.64098521247620	21.82257072111564
H	-2.92390366049569	9.46989318719952	22.95365118185515
H	-1.53825268459176	8.90072489441364	21.99705980874340
H	-4.40134876166187	7.75623368379637	21.88579573050916
H	-3.00597560524007	6.96256080652434	22.64550257413735
H	-1.84541222027835	6.80487529769044	20.43472650700799
H	-3.47257021857115	6.06657117479421	20.28270686555125
O	-3.91290162134706	7.61439530697425	18.34042352671205
C	-3.16087789913051	10.29066243520207	18.31557926981407
H	-4.25834728771320	10.40235849380757	18.36481713038901
H	-2.91351729037683	9.86336637681611	17.33064714519300
H	-2.68918462425820	11.28310082128428	18.40868176423363
H	1.42680836890328	10.36814543864577	17.94269109587225
H	2.07059633655789	7.49612626228374	18.98035720063861
H	3.12763403707968	9.84033367214904	16.12545871550402
H	3.21988512132996	8.08493452509038	16.72631333349326
H	1.26939901569940	8.91173074202603	19.91061861348873

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Pd	3.46206580183238	8.87356270038980	19.30234169477824
P	3.96362614710319	9.63996366234333	21.40239702690101
N	5.30242434559011	9.75776090511379	18.67401345582731
C	4.54666753974269	11.38519462559010	21.22173852800710
C	4.18177052507445	12.34086723621025	22.18565916008543
H	3.54272062710821	12.03427415429324	23.01791081235159
C	4.61748000062525	13.67179684660909	22.09632086704552
H	4.30814029679546	14.39481168138946	22.85760100899356
C	5.44509026949412	14.06650957894697	21.03782549596000
H	5.79286813998351	15.10087101174189	20.95911071191649

C	5.82455549984392	13.13012344400699	20.06970389998176
H	6.46701244482181	13.42719667612740	19.23798932690497
C	5.37734175680718	11.79255397913593	20.13675862898582
C	2.74302866213769	9.72301888680535	22.76057056959668
C	3.08327414721203	9.40471792711429	24.09203762888622
C	1.42871895133384	10.12812571469536	22.44550312901363
C	5.42658623791721	8.79790977696292	22.12601668751812
C	7.64627377976508	8.78841508706818	23.12834422964152
C	6.53430506813029	9.49536300107712	22.64505229052885
H	6.53026093333022	10.58932482009606	22.66345525260867
O	-1.02812726015953	8.16389011747421	19.57993405663485
C	1.26249298738607	8.38296015569587	19.62680427741699
H	1.07080380924803	7.96319781203320	20.61308037077582
H	0.91550288854418	9.40735590173465	19.46385436941581
C	1.86012010403050	7.58436804154527	18.61343376671989
H	2.02239059684856	6.51570539965311	18.80339166750452
C	2.45902824823942	8.18869109671160	17.47877513936998
H	2.99329924977192	7.56395709900685	16.75484675085874
H	2.06203184325973	9.13543271127826	17.09045900915742
O	6.90034617205396	11.32068765703688	18.34749074571669
C	5.81815278870093	10.89097123775814	19.05620685606309
C	6.15726510351270	9.18698872860691	17.60308672286770
C	7.05758583447263	10.39161050232091	17.23198541676106
H	6.72615246266924	10.91080714576739	16.31695461753625
H	8.12876896435063	10.15830676672236	17.15509914567518
C	6.92649763602567	7.91045092974123	18.07156475879597
H	5.50212546878917	8.90472531800749	16.76140178360056
C	7.81301442540105	8.22464338640247	19.29116694603852
H	8.35409678060803	7.31746274548358	19.60968382037562
H	7.20854171043329	8.56582985172488	20.14575606972758
H	8.56889178567599	8.99934935932083	19.06948525040663

C	5.91876725101437	6.80345729167890	18.43644583780882
H	6.45551632224343	5.89616301032471	18.76579243519687
H	5.28882752276148	6.53366996619499	17.57006302146783
H	5.24581751305928	7.12328046317039	19.25316055487535
C	7.79106648368239	7.41490312561147	16.89264291408297
H	8.58020292335849	8.13541221871087	16.61272318998396
H	7.17391789053344	7.21747393414694	15.99709752919778
H	8.29442427053129	6.47185149435493	17.16748933828728
C	5.43993832825410	7.38705836128663	22.10805955596012
C	6.54569135191317	6.68521242261017	22.60334080630612
C	7.65451376500741	7.38556389557765	23.10711835813338
H	8.50826940874157	9.33693189183574	23.52186505609421
H	8.52509662801159	6.83717265653003	23.48099900667534
H	4.58198302382967	6.84752323041420	21.69228562162906
H	6.54796222437741	5.59068106035832	22.58482443489038
C	2.11082104526049	9.49179851054619	25.09892782570458
C	0.80447633735381	9.90268891523723	24.78564310799893
C	0.46796468989643	10.22295231736119	23.46107367676973
H	1.11059086198250	10.35411448695314	21.42189084575897
H	0.04723390614755	9.96443510850454	25.57420483998517
H	-0.54450354210521	10.53242184241482	23.18872436515731
H	4.10218347109711	9.08911420921102	24.33710853813758
H	2.37560924845871	9.23681919966876	26.13053095070050
C	-1.47079247120021	9.27173194681087	20.04449125692839
O	-0.80774093141742	10.30735832161712	20.33762073851413
C	-3.03437074907229	9.35844047295338	20.25293904197043
C	-3.29353211286092	9.79984555199692	21.71783633893121
C	-3.67151747098806	7.98447214740933	20.00366479813528
C	-3.38660035673435	6.90923575074899	21.05273180433149
C	-2.88318478272222	8.73056199625485	22.74113789264122
H	-4.37158270815425	10.03031400155467	21.84064283637349

H	-2.73259251155771	10.73858680352172	21.87601880917567
C	-3.63822666458895	7.41693962054234	22.48845115551872
H	-3.07500661391958	9.09360736763896	23.76914466748653
H	-1.79345924106729	8.54840124995619	22.66472341244103
H	-4.72367381643529	7.58838462145926	22.63356123381266
H	-3.33978339699150	6.64252691220228	23.22011860462296
H	-2.31983058062936	6.64248637332903	20.94021160778677
H	-3.99846874728115	6.02371605509903	20.81230003689381
O	-4.39296150026014	7.76002825435876	19.03247581906658
C	-3.58123685739409	10.40443695690909	19.26940684815736
H	-4.66530188569270	10.55284082140420	19.41855488111424
H	-3.43118752568855	10.07415644737595	18.22916636281596
H	-3.05517277526635	11.36018503440679	19.42537809552027

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Pd	2.65669853533299	10.68279904742784	21.39406790364591
P	4.53488254727955	10.15698406124721	22.55317486667898
N	3.96604325030168	11.10018876179447	19.73697088069333
C	5.71503719755229	11.55505001755058	22.26519116621105
C	6.50843978576229	12.02765604640801	23.32534223897124
H	6.40529718862101	11.56701519241521	24.31151426320532
C	7.42887449461597	13.07148556050257	23.14236740876004
H	8.02707966588183	13.42122796479176	23.98983304264647
C	7.57979516665545	13.65425943925808	21.87842268320413
H	8.29683393809011	14.46575247884843	21.72156122254057
C	6.80303066940283	13.19574211366746	20.80785649737026
H	6.91063803326819	13.64139016961608	19.81650521669221
C	5.86036036628599	12.16025743142460	20.98112575783659
C	4.53726192046488	9.95530526546714	24.37501691227564
C	5.41586363945043	9.08100895981522	25.04493668170990
C	3.61278643673869	10.72018249366181	25.11529241978584

C	5.47948482065108	8.70519165400269	21.94269943659513
C	7.50959543901000	7.62443699664121	21.14131543800751
C	6.85841988824008	8.75431697491090	21.65930085079597
H	7.41852477150516	9.67821829044147	21.83214846564933
O	-1.07666849164723	10.64355123283292	18.90478485667209
C	0.84245420599250	10.42011406202761	22.44970661190885
H	0.62724362052351	9.34868989321298	22.33075742676999
H	0.76292691151860	10.78328045843173	23.48032989442322
C	0.55205287000119	11.32081083548041	21.37253401672130
C	0.67696239917864	10.91899127830985	20.01851260002053
H	0.85320033671962	9.87391790413221	19.76992963087079
H	0.92093192021395	11.64752426945895	19.25026273409367
O	5.61245197673681	12.14214320401639	18.59343472966672
C	5.08713568225955	11.75793158600445	19.78856849828547
C	3.65395958464222	10.81901226469403	18.30311673929825
C	4.59746556457910	11.80900726141136	17.58668238716384
H	4.09593628630123	12.74948370938792	17.30180954108580
H	5.12875912102672	11.39469546890130	16.71931251398367
C	3.87905075383639	9.31846776402696	17.92613888414227
H	2.59375089028004	11.04614655854031	18.10081557604244
C	5.33252789197249	8.88530862954964	18.18844294708619
H	5.46873435390197	7.82852489374668	17.90068961331717
H	5.59243097753264	8.97193583649389	19.25558787016181
H	6.05802759095017	9.48177500377994	17.60629144963778
C	2.91411207152366	8.43701824644354	18.74196882294876
H	3.10920114030046	7.36935371384207	18.53693331291069
H	1.87253975520779	8.66268465409249	18.45923063056537
H	3.03259359838806	8.60338232786016	19.82864203692876
C	3.51517894194747	9.15999771260608	16.43272794400988
H	4.21095286818004	9.70478935899503	15.76886132684585
H	2.48896465505928	9.52093448875812	16.24442107552492

H	3.56796049938922	8.09374550297798	16.14930770107814
C	4.76425621488202	7.51176689539549	21.71138140147793
C	5.41975171529204	6.38380038487911	21.20297472853531
C	6.79243784651713	6.44080258970945	20.91060445535681
H	8.57918847948009	7.67237624528903	20.91243808509038
H	7.30112821539656	5.56396909680150	20.49740989247462
H	3.68898400588642	7.48091081771844	21.91720454883086
H	4.85562344246534	5.46384395766545	21.01970757331276
C	5.37008887086731	8.97904935603637	26.44324863925278
C	4.45683246878530	9.75195187896751	27.17758898170296
C	3.58003013076609	10.62513601603125	26.51244930363882
H	2.92090860604512	11.38092209835609	24.58141463749064
H	4.42299406887835	9.66881498869155	28.26872385470579
H	2.86186577838549	11.22304142613444	27.08285502445515
H	6.12996681327885	8.48242825738867	24.47071820907470
H	6.04987665006542	8.29378005132819	26.96019760766533
C	-0.67075186628737	10.42132289672529	17.70179237339401
O	0.51082712292033	10.51558884550025	17.26513971299569
C	-1.78972073572866	10.02993669575064	16.67994048339513
C	-2.87614858023301	9.15666499932159	17.35934865829497
C	-1.12005584591616	9.21576211040625	15.55782442725942
C	-0.59783631340074	7.84202520008636	15.97501242792687
C	-2.32830183844356	7.80268425870861	17.83536159329930
H	-3.70132051168655	8.99091860324677	16.63728607508409
H	-3.28473443504393	9.72709020652928	18.21085395216541
C	-1.70268622762458	7.01627418897318	16.67291160235187
H	-3.13646575892781	7.21158603040794	18.30508976013733
H	-1.56864104399224	7.98475533429829	18.61963149783698
H	-2.48970843904494	6.76819853697290	15.93347920950527
H	-1.28534891275206	6.05437374741126	17.02533527371887
H	0.23905515774709	8.00222603489570	16.67993801287759

H	-0.20370318840198	7.33347827688813	15.07954899111316
O	-1.05997634173320	9.61069930639102	14.39627116397645
C	-2.38915518206240	11.33238588583010	16.12496779785844
H	-3.15889579582147	11.11181915268011	15.36572749097960
H	-1.60745502400045	11.94081446922660	15.64310187481446
H	-2.84567974881004	11.91299024873533	16.94435377698666
H	0.40635447062548	12.38612387071407	21.58937217552452

(endo/t-P)-TS4

Pd	3.36658590529359	9.19935705031870	19.67575889173735
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C	4.91431448128100	11.53856562113320	21.45140701339623
C	4.80122109597942	12.45889855320213	22.50876201227572
H	4.28009219988299	12.15487995500868	23.42055656516055
C	5.33436761273616	13.75296395699363	22.41165349815185
H	5.22067401228268	14.44990386273177	23.24792873150460
C	6.00638427235790	14.14530989638475	21.24732754529657
H	6.42500854815327	15.15228091674519	21.15906395955719
C	6.13593767177977	13.24317383908823	20.18560953548344
H	6.65471802144442	13.53921174093246	19.27122701500669
C	5.58884733350227	11.94411369877806	20.26365605156357
C	3.06459400392283	10.02553435715687	23.06858733422739
C	3.38325063677410	9.56609002865378	24.36133749333481
C	1.82270621094854	10.65322236971704	22.81933864000282
C	5.63643206034137	8.86344202741653	22.27049124494421
C	7.92010850697848	8.63962889599261	23.08497944081604
C	6.83617782593842	9.45097542126314	22.71623477957237
H	6.92478520418438	10.54050237218193	22.76424530522018
O	-0.76799468512947	10.32376793481538	18.35417299347455
C	1.53881660127973	8.35668116202811	20.21146243429692

H	1.57577499064656	7.38237442232572	20.71538989663028
H	0.99268411198398	9.13817461758539	20.75214153034986
C	1.49221402998540	8.38524953642550	18.76940185615407
H	1.53356126214620	7.45343494962696	18.19146632204382
C	1.46961400454675	9.62128286706869	18.10314727884352
H	1.53553863190228	9.66371138145863	17.01144025242573
H	1.43699188019569	10.55648930385387	18.66995566087002
O	6.79298637987810	11.43268329205954	18.25518302254266
C	5.77010562932373	11.07777385542779	19.08381817707799
C	5.72597004188692	9.43430324096039	17.52943913734258
C	6.69711509206929	10.55782529366683	17.08973551296657
H	6.30619061666863	11.15953181063398	16.25203606948351
H	7.71636085572467	10.21954301492123	16.85631943709405
C	6.40461787402568	8.06411669393638	17.85563330662483
H	4.94639180643632	9.26021007232699	16.76776700440928
C	7.44107991452927	8.22281747060870	18.98463396013196
H	7.92686709209064	7.25385876021573	19.19137366680865
H	6.96532068789003	8.55906362102717	19.91973148011247
H	8.23694751803885	8.94257740974384	18.72172176954335
C	5.33110151222069	7.04322539073647	18.28009335216570
H	5.79911818921001	6.06670313218763	18.49765104956673
H	4.58026597216790	6.89455817603723	17.48345105379175
H	4.79422791499486	7.37783577413561	19.19138403438692
C	7.08504482971703	7.54781767817973	16.56966889015607
H	7.91661514327880	8.19526498272577	16.23909719748769
H	6.36180935576311	7.46714691880341	15.73766791056875
H	7.50613448576012	6.54294958135268	16.74629523434476
C	5.53159252984512	7.45717404460628	22.20623073281221
C	6.60972373749608	6.65149978044896	22.59136065199823
C	7.80917544815366	7.24227198329957	23.02360549417038
H	8.85414181292586	9.10214036599893	23.42040182948483

H	8.65835164418354	6.61254139941279	23.30797928241345
H	4.60493369469741	7.00626848432645	21.83458764024882
H	6.52059401886863	5.56159943913735	22.53944611587649
C	2.46139750205479	9.73272254678063	25.40608871584035
C	1.23142565242528	10.36473909892259	25.16519346764685
C	0.91806885585724	10.82606218247108	23.87561938206107
H	1.54053040622104	10.99749572745736	21.81466772619291
H	0.51436722150262	10.49399437855146	25.98262200837292
H	-0.04104053892822	11.31475357263053	23.67769789172759
H	4.34682931248568	9.08112468967592	24.54764564726504
H	2.70740875015295	9.36988143071769	26.40960731409576
C	-0.75460741127260	10.89242816968277	19.49877992283858
O	0.25957682458726	11.31673958723948	20.12899023460150
C	-2.13903957901528	11.03485676262159	20.25323823470948
C	-2.14579714987023	9.93418823559462	21.35530805660180
C	-3.31165238597545	10.81460483844609	19.28357413126038
C	-3.56810297320668	9.38526829679763	18.81231469168300
C	-2.24178751841443	8.51116122978552	20.78849779991882
H	-3.00718177135619	10.11720057985943	22.03054532260299
H	-1.22904468663738	10.05721101672296	21.96066872458707
C	-3.52496063487388	8.35393519437652	19.95908761849353
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H	-1.36320133873635	8.30784854081953	20.14880674538317
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H	-2.75483007531399	9.16267179391146	18.09770139845487
H	-4.53071775074522	9.37057864672825	18.27393278517844
O	-4.01515484912822	11.74934439545867	18.89990432345748
C	-2.22306016257844	12.42609240572924	20.89487379972055
H	-3.13137153551045	12.51355021998872	21.51724178230760
H	-2.27192088467428	13.20960415474391	20.12265713018133

H -1.32891190781462 12.59364837920758 21.51556768010818

(exo/t-N)-TS4_ent

Pd 3.82866478060741 9.50648378552803 18.93673352080769

P 4.26413886030277 9.92990591649820 21.14491797912897

N 5.86217092286559 10.06951360192928 18.57423437408379

C 5.15123594047026 11.54817833587874 21.21172942466927

C 4.85313884090156 12.45741644851620 22.24137305534624

H 4.08664106989169 12.19152971768357 22.97458462715056

C 5.51799355562841 13.68903900804238 22.34283047033596

H 5.25847185353224 14.37944537406588 23.15155465532630

C 6.51044483510251 14.02642084026651 21.41342265392206

H 7.03806875575146 14.98220003801587 21.48535374215454

C 6.82396731906866 13.13542414470495 20.38094265867215

H 7.59243814516211 13.38972055974543 19.64755050407905

C 6.14912223717769 11.90165547934307 20.25548650161424

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C 3.10127418414176 9.71728381860300 23.72813574949950

C 1.67098819384754 10.54278185414024 21.92753604060292

C 5.47105679341697 8.76877279696979 21.89614603390008

C 7.55051221526393 8.24836239386609 23.05195995140713

C 6.64033481245158 9.19440692039618 22.55500256275160

H 6.84248251512674 10.26337719686124 22.67178693558761

O -0.63296963081015 8.26896669520432 18.93580978497047

C 1.77792574151466 8.58564225596038 19.08909635785774

C 1.90866875088275 9.46246714262326 17.98020540228775

C 2.87271269110202 9.19372150912116 16.97612451719936

O 7.73696554189090 11.32980026412311 18.55040460465788

C 6.53194529619799 11.04451858219836 19.11965278090955

C 6.70030110588744 9.45188171684059 17.51835534227054

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H	7.71050651589641	11.14129997269796	16.48008078501971
H	8.85237966574370	10.06066348452380	17.35412140579317
C	7.16609532485565	8.01147681903210	17.90283283700112
H	6.09241361301132	9.38292384180132	16.59978614493958
C	7.97732363068618	8.02986607617894	19.21183218267189
H	8.29964594902304	7.00727880839389	19.47173298377701
H	7.37289740130970	8.40844655984137	20.05055833233579
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C	5.93360745902368	7.10255678774424	18.07249536864789
H	6.24903843886668	6.08044617878165	18.34653347173369
H	5.34880604894111	7.04140339502915	17.13759826288479
H	5.26189828683189	7.47663714586546	18.86801342984757
C	8.02618672711968	7.46222448662656	16.74513716207218
H	8.95768298045682	8.03830855876048	16.60048253280454
H	7.46740001266781	7.46895507520933	15.79148484907751
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C	5.21771692255200	7.38820762627709	21.75030263025810
C	6.12274705185974	6.44804483497582	22.25730055032362
C	7.29487133336516	6.87708784982607	22.90256808946282
H	8.46190725206094	8.58565581733469	23.55631325338943
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H	4.31097663674415	7.05901874447750	21.23111920088213
H	5.91869664417398	5.37897085604322	22.14014451427291
C	2.02667919660043	9.82753904989545	24.62152456964311
C	0.77589425950958	10.28477293288764	24.17052095733604
C	0.59869633372697	10.63901872506726	22.82467531870195
H	1.49001764541611	10.79134997732301	20.87747074882815
H	-0.06469950055584	10.34786803136765	24.86945218842434
H	-0.37128252306647	10.95955449987212	22.43507946896329
H	4.07081622247114	9.34416086326855	24.07371672086076
H	2.16253166804821	9.54266710149800	25.67017772956986

C	-1.10383510885874	9.35535528239792	19.41699583243391
O	-0.46787426524133	10.38803380119918	19.78178298534992
C	-2.66899039911726	9.36152669107808	19.62061034677370
C	-3.22212942248950	10.78076890713667	19.34031996883976
C	-3.29579359449939	8.36658308667468	18.63617450631374
C	-3.18580757514874	8.75802642047966	17.16316545065838
C	-3.05766442930021	11.19482698252228	17.87032893777289
H	-2.67568525083112	11.48064668056150	19.99645131665802
H	-4.29485847341633	10.81250827593430	19.62099385003667
C	-3.73109998183147	10.18508291253016	16.92771990067641
H	-3.47781341709112	12.20597022739015	17.71143233946963
H	-1.97623846931429	11.25743289482989	17.64373927871053
H	-3.58482840014564	10.47435961381275	15.86980120788565
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H	-3.72318664414285	8.00587809330310	16.56186507741972
H	-2.11406268562195	8.72311860385698	16.89340858289477
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C	-2.94250257863288	8.93602486617707	21.07144052335146
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H	3.04542200513785	9.92383466273546	16.17837753216165
H	3.13783911227288	8.15525195276263	16.73854847341228
H	1.25319138421087	8.91614864152313	19.97885511578000

(chair/ax)-TS5

Pd	2.53673510949036	4.74691891757087	16.29844335320693
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O	-0.99966411859784	4.45158149264641	13.40279852652892
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C	2.37113918694406	7.16160541243818	18.65935507833142
C	1.57434917053062	7.82159679923589	19.61833053859421
H	0.83580478319847	7.24399927951507	20.18141602370970
C	1.69532976097661	9.19779435744027	19.86520185766143
H	1.05388828997196	9.67237193768454	20.61505461014373
C	2.62925859453152	9.95282645469753	19.14611963799408
H	2.73319138818138	11.02806613660344	19.32270987861530
C	3.42855523410683	9.32521322546993	18.18495321192091
H	4.15221961037117	9.90680758126630	17.61009406410682
C	3.31428745890545	7.94063495135379	17.92233573206367
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C	0.22467803633264	4.54619713717900	20.42490160386684
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C	4.62856419392486	4.67992616019359	21.73417820590195
C	3.76691871113235	5.30216083439734	20.81728158194871
H	3.46443921562941	6.34210563505331	20.97743897870951
C	-0.44594050715656	5.35216487930186	14.01038867022720
C	1.32644116656234	5.90310881105128	13.03605446871732
C	0.82096686812365	6.28131169344637	11.63138835933631
C	0.50277819198832	5.09986859967313	10.70087798369607
C	1.63550373485798	4.06506035529918	10.73616252294479
H	1.41617931458889	3.21514762652486	10.06289462777999
H	2.57715547441046	4.52341560539564	10.37116494280591
C	1.83282430771605	3.55750807878151	12.17503726320506
H	2.69273998191730	2.87006494531129	12.26056838286856
H	0.93019751060761	2.99396487372966	12.48759902809753
C	2.02440891118091	4.67298795852066	13.19675618610686

C	1.78652952242498	7.10767522188923	13.83602884261563
H	1.93604759631880	6.85995793347700	14.89848978564033
H	1.03590938485131	7.91447587407566	13.78792361156327
H	2.74054049825537	7.50648953958554	13.42981864926127
C	1.14185501173612	3.19452181644898	16.24512253062369
H	0.48620055899864	3.17555191028233	17.12810813848131
H	0.56566475359457	3.44528458591741	15.34075521195629
C	1.96935809880774	1.98174830734092	16.09638111496567
H	2.54296555160529	1.91094311852342	15.16216504052726
C	2.06282129373571	0.97708586296326	17.00281703247608
H	1.48463394272787	0.99121275390357	17.93549136832258
H	2.68894569675314	0.09616762252626	16.82451199606303
O	5.15873501941218	8.25379279474705	16.41597331128350
C	4.19568581091138	7.39915262743530	16.86724160923699
C	5.26694359817931	6.13993968774035	15.31898799641767
C	5.75523496850569	7.60910841809602	15.24762644950154
H	5.38728404940284	8.14178657220220	14.35387203694890
H	6.84466295054523	7.73707514994078	15.32871425569036
C	6.35954194861713	5.09233614391943	15.72295735131111
H	4.82387394316030	5.81221591329798	14.36304094045206
C	7.00121905052725	5.44061683845980	17.08238986286906
H	7.77199890896613	4.69238873546015	17.33942950946030
H	6.24915265791937	5.43416829145884	17.89031230042798
H	7.49504880933392	6.42972070407692	17.07705209207377
C	5.72095697554053	3.68905387178395	15.79804373776306
H	6.49859622024793	2.92760109701777	15.99191366825585
H	5.20228080896664	3.43276613724900	14.85832056074638
H	4.97575151109640	3.63122872416424	16.61137654218521
C	7.43655133555576	5.08238199685019	14.61281129536476
H	7.96482971390714	6.04922237830423	14.52221302098012
H	6.99486010226643	4.84062728176615	13.62888152716160

H	8.19920423834730	4.31517650671337	14.83510860424910
C	3.70857706101936	3.25673864145029	19.49343393091151
C	4.56216684833739	2.63766855476846	20.41841475706589
C	5.02508715736795	3.34757587822104	21.53799646045965
H	4.99225594725468	5.23979425417175	22.60259045228839
H	5.69861587550528	2.86518374393535	22.25453138289301
H	3.35965235769783	2.70302717696113	18.61288041810046
H	4.87277319229641	1.59986053716686	20.25724443701785
C	-1.08812719488529	4.34781817924835	20.88181931478128
C	-2.17677352494673	4.63339039033312	20.04321319309317
C	-1.95297207399752	5.11159041857954	18.74126871977576
H	-0.48346327821553	5.64754205367447	17.24142457735763
H	-3.19981002568246	4.47404128229048	20.40084420524299
H	-2.79708105483155	5.32256302047959	18.07672332566775
H	1.07028549996071	4.32191325206542	21.08319909105900
H	-1.25783042658959	3.96596960373533	21.89439073465992
H	-0.06610194017542	6.93785380593652	11.72415193825126
H	1.60361744826681	6.91324151284633	11.15384124810465
H	-0.43503640452449	4.62065055540911	11.03054572357162
H	0.34276833691480	5.47164363417097	9.67100184663992

(boat/ax)-TS5

Pd	2.47955707716982	4.80796453958170	16.23743775737005
P	2.09433733678448	5.36387892622228	18.32704090715973
O	0.34243190059452	6.55328256525699	15.37981983133258
O	-1.02237950135466	5.40788705978005	13.90617960959094
O	2.84700265729380	4.45999082633258	14.06363701242555
N	4.09005211263448	6.24003388960849	16.27879502693258
C	2.24934898665367	7.19341649421987	18.53608379242114
C	1.39302557828872	7.84603703068493	19.44075591275413
H	0.63504291932701	7.26279667964143	19.96975266071978

C	1.49161196988120	9.22622171479932	19.67282223386912
H	0.80552021130403	9.70647439164765	20.37762370392689
C	2.46359667857715	9.97989417370423	19.00323349587734
H	2.54838788226548	11.05710245507342	19.17547738231133
C	3.32777291417710	9.34933795732800	18.10146508173761
H	4.08624870232308	9.92496776443982	17.56648420482696
C	3.23090349793724	7.96446762321759	17.85075820729288
C	0.46792386781786	4.98767920867401	19.06146023307030
C	0.33133998994773	4.37257375905687	20.31932589522014
C	-0.67322688017036	5.31924109244905	18.29640134606905
C	3.35945377887662	4.69303626097284	19.47245670430770
C	5.00580603674022	4.92388191835808	21.24882431620085
C	3.98789454562093	5.47833992453822	20.45785684707349
H	3.69100790236444	6.52238942871816	20.59626559606376
C	-0.03377334952982	5.97900846318585	14.35213819744273
C	1.39832205344871	6.07322303264486	13.01595212508176
C	0.67438524550101	6.36405570053583	11.68274398240205
C	0.68148353051468	5.18971961227578	10.69086431816362
C	0.27416804004139	3.89760360476227	11.40889324139977
H	0.16237973710394	3.05762240834942	10.69914780547980
H	-0.69752085323882	4.05500238871533	11.90609491975125
C	1.33212260518698	3.55393975862500	12.46694450064999
H	2.20214881658597	3.04505647981430	12.00543227098645
H	0.94098541537083	2.84213584338101	13.21848323693664
C	1.90960784564047	4.74373140217840	13.22165423385773
C	2.28677989788469	7.21182311071602	13.49587246143885
H	2.60706396350237	7.05680824207946	14.53363917969467
H	1.74385139624217	8.17068735572781	13.44902510991476
H	3.18571589015651	7.29418732300764	12.85173925562188
C	1.04916792512506	3.29767501580132	16.18279690143613
H	0.39168487208178	3.28659659371215	17.06416066345755

H	0.46452359536720	3.56416405952204	15.28645627870931
C	1.85947505553024	2.07241879847127	16.04838041411803
H	2.42051882750036	1.96722713075254	15.10919361118658
C	1.98424825972525	1.11380017746457	16.99942718258606
H	1.42615930651974	1.17496608215154	17.94236676615805
H	2.61938998361199	0.23372528989436	16.85512291992782
O	5.22867758366517	8.17212028112547	16.52584805501535
C	4.16719860148774	7.39163216840704	16.87225527666745
C	5.28888657133765	6.05289561174486	15.42979629154161
C	5.88998933566934	7.47986614271868	15.41681829481632
H	5.65116317274895	8.03471693530804	14.49423641483099
H	6.97104040040444	7.52600570251115	15.60958221799820
C	6.22874298913460	4.93550967545864	15.98558064216434
H	4.93338868021321	5.74797741732758	14.43110091544178
C	6.64489035409278	5.24015317010846	17.43751497535450
H	7.32317093413728	4.45340627873516	17.81064401597795
H	5.76742865854161	5.26394501857444	18.10456043331915
H	7.17550901480442	6.20564113949166	17.52744088654701
C	5.50167447752745	3.57750233249721	15.93159537933196
H	6.17894187726004	2.77138458962620	16.26670776436032
H	5.15406212667568	3.34752918982532	14.91019029358911
H	4.61286966950870	3.57180467306134	16.58828810420629
C	7.47025430418551	4.86064150362207	15.07158392187461
H	8.07973499357516	5.78165572537129	15.10397372761721
H	7.18004179836761	4.67741123299559	14.02107553166423
H	8.12129930525813	4.02811582765888	15.39053559377147
C	3.75017620418888	3.34957176743218	19.28772156747217
C	4.75817931173441	2.79997848235752	20.08947401086478
C	5.39179515592923	3.58718699150206	21.06559819433667
H	5.50075240122191	5.54016425879599	22.00652117764612
H	6.19082860215857	3.15983936236557	21.68027031280869

H	3.27567362764263	2.74805229413174	18.50288513325778
H	5.06042969868326	1.75843794974936	19.93970417946146
C	-0.95038385046501	4.09364684888618	20.81893155711477
C	-2.08661270436517	4.43124245564742	20.06788118199449
C	-1.94628750973382	5.04519130905332	18.81077874539833
H	-0.54955152405338	5.77722084164564	17.30466752705422
H	-3.08492887139192	4.20899548112324	20.45913156583274
H	-2.83170992601382	5.29878985772020	18.21927477344066
H	1.22165275172158	4.11486861218733	20.90159289106215
H	-1.05937361269468	3.61123820325426	21.79587250293249
H	-0.37376036395341	6.64565303146356	11.88591408637838
H	1.15637282846828	7.24476289730778	11.21690295765464
H	-0.00003280623680	5.40664300520756	9.84784850265349
H	1.69662751363631	5.06667817592552	10.26029306159032

(boat/ax)-TS5_THF

Pd	2.41486830929922	4.81187971749647	16.20869437624065
P	2.09693406409441	5.34743889894144	18.32954736424208
O	0.04542491942412	6.61673350799223	15.21735368422494
O	-1.11716187242634	5.28004636188271	13.68751325143556
O	2.81740947287222	4.47189520667964	14.09925490125095
N	4.07234288041150	6.21383247498234	16.29418899500573
C	2.21182439979660	7.17749356717891	18.53230497829189
C	1.35049023712796	7.82700442118352	19.43440895225599
H	0.60772185693046	7.24147691760521	19.98185280633477
C	1.42937461138581	9.21245082112664	19.64847587473396
H	0.74181179911210	9.69038952780146	20.35285107477882
C	2.38832031623605	9.97183383940650	18.96529387667489
H	2.45945899031498	11.05159582943812	19.12502635923197
C	3.26246748456779	9.34209925190446	18.07060798674710
H	4.01279018661044	9.92580547151717	17.53277880944204

C	3.18568890712395	7.95263458670466	17.83737466568533
C	0.52542137643987	4.89528622213223	19.14041899828967
C	0.48487178732119	4.11682699091689	20.31184797522059
C	-0.67738967827726	5.28663866563278	18.51006782620964
C	3.43015791778566	4.70974715019464	19.41409306231461
C	5.17301397965669	5.00648913478003	21.08556170358225
C	4.11282691837953	5.53258821684042	20.33048030976691
H	3.82698740581634	6.58199651897110	20.44763189938192
C	-0.29672211714072	5.93432742014915	14.28293927888707
C	1.56734607380902	6.10524864671999	12.85444167581739
C	0.88040681954225	6.42157994782398	11.52458570857122
C	0.92827676483686	5.25852114156862	10.52043567368868
C	0.48318411202188	3.95732895884774	11.19966988030244
H	0.43597388179006	3.12378663077973	10.47483178111177
H	-0.53268963416134	4.09584074865085	11.60841031757249
C	1.45120819115000	3.60697381524667	12.34098698862560
H	2.35398068393107	3.10503184801264	11.93669307553511
H	0.99983517533454	2.87731908749704	13.04061388554305
C	1.95745333743843	4.79300503268837	13.15551993007536
C	2.27601212884369	7.25936348555838	13.52564226404689
H	2.45652344024974	7.05673211201992	14.59106202535336
H	1.68636001614337	8.18969592476029	13.44526291978409
H	3.25902599373224	7.44850596629272	13.04544170769661
C	0.88072250014158	3.41226615801165	16.10943125569568
H	0.06001458324249	3.66927615816557	16.79568304466425
H	0.54810217364066	3.49760438465664	15.06243078340501
C	1.50013368713841	2.10659453389299	16.41568197254704
H	2.17981764648699	1.70426491196263	15.64971884466079
C	1.31979188842579	1.40218818934923	17.56071738548716
H	0.65666586185738	1.77080489586863	18.35347654681093
H	1.83082965861950	0.45031105492214	17.74134605479960

O	5.19179827498950	8.15777612997312	16.52540079273929
C	4.13671371180505	7.37477253870150	16.87361471015349
C	5.27139498478135	6.03176808158244	15.44241493574944
C	5.86885527296122	7.45909299144434	15.42285283844058
H	5.63563307512911	8.00927060961484	14.49729374122109
H	6.94701123233987	7.51143379151528	15.62619437896158
C	6.21688977607945	4.91856369502395	15.99229656600765
H	4.91320388141859	5.72499826480958	14.44561032506009
C	6.66463592935529	5.23698885809493	17.43133875102169
H	7.33641550798304	4.44368306873830	17.80250341161156
H	5.80038682668163	5.28652780927767	18.11353567245005
H	7.21373374277659	6.19404981155238	17.49311629155673
C	5.48122413060484	3.56439490330960	15.96679787812391
H	6.15730334173587	2.75920517739556	16.30645685699255
H	5.12472994972856	3.32567408304688	14.95015197303269
H	4.59916795149493	3.57535350480857	16.63215141578993
C	7.43961855092301	4.83101549680957	15.05445804840183
H	8.04147514570753	5.75709514563051	15.06063543915964
H	7.12699314968852	4.63134053066972	14.01328575580854
H	8.09975677282226	4.00624015676256	15.37578544074520
C	3.80528099665700	3.35752184889069	19.26519631714632
C	4.85718218961817	2.83655959625570	20.02986167939155
C	5.54730796678232	3.66172331584714	20.93471024723665
H	5.70822792013414	5.65124058820002	21.78997725691490
H	6.37824609687158	3.25643710874739	21.52100850453918
H	3.26860207864421	2.72324625481197	18.54971794738970
H	5.14672308873298	1.78762700895886	19.91014195360773
C	-0.75349662228878	3.73618455490572	20.85454759951378
C	-1.94796579707018	4.13651936285770	20.23570035266385
C	-1.90847025801141	4.91637422524006	19.06551637305314
H	-0.63977031684057	5.87114780280012	17.58329912419116

H	-2.91144956181496	3.83822094403566	20.66117742519844
H	-2.83860653734469	5.22484627394946	18.57784155335468
H	1.41546114298713	3.80888519485375	20.79736498627327
H	-0.78189523089111	3.12811785862864	21.76433781797511
H	-0.17660890567232	6.71451868372781	11.68240331006441
H	1.37428833048915	7.31098725065736	11.08520230744084
H	0.29168176818015	5.48501009799934	9.64504137947512
H	1.96477130475356	5.13898302511592	10.14548590951818

TS7

Pd	2.64922365232681	3.89543997834878	16.55455251690574
P	2.08200957016136	5.03479706115477	18.36335161828237
O	2.23827625292656	4.52687766606837	14.25754615221235
O	0.81284830479411	5.99416232691548	15.26719446128172
O	3.81835265522882	6.33997229074451	12.03097073238518
N	4.15145251227561	5.34067151759775	16.21748591299825
C	2.17836290198619	6.84947022265700	18.06160150008678
C	1.30657897374478	7.69828232953797	18.76614903689594
H	0.58554587335851	7.25936529403673	19.46167148499874
C	1.33084703664040	9.08779098474269	18.57705510879222
H	0.63556403719600	9.72418310899049	19.13380281131133
C	2.23729096543018	9.64891574545492	17.66896138474137
H	2.26135232896802	10.73036958014685	17.50386951963971
C	3.11023784215826	8.81964528184532	16.95745371152925
H	3.80971608000770	9.24541696037311	16.23602578807526
C	3.09417117226033	7.41969318897286	17.13719446435193
C	0.37134374161563	4.80844017488217	18.96283220137951
C	0.06922006597925	4.42458576487376	20.28141137328832
C	-0.66195458888421	5.00041219440480	18.01712106490098
C	3.16499444434018	4.78184768600377	19.82742979849501
C	4.33674660225209	5.55683653592655	21.81629930682447

C	3.49062796056503	5.81527965144563	20.72764670470794
H	3.09001441311858	6.82135868880625	20.57045289528676
C	1.53338373674499	5.59954079603812	14.31757290181833
C	1.62689709773479	6.54473853307432	13.05571209017036
C	0.21715921989314	6.62966708679681	12.41502332588957
C	-0.21788327382465	5.31874500920775	11.74768920831508
C	0.78059595271973	4.92595323756966	10.64900688435974
H	0.47171274482036	3.99079948631089	10.14600610977426
H	0.79036177570117	5.71490737871300	9.87062692987800
C	2.19712184996860	4.75848273402556	11.23221405913823
H	2.95867292064524	4.59341453496718	10.45129701628953
H	2.20717999267603	3.88600901008977	11.91179929627711
C	2.65313781332363	5.93244807607819	12.09559555958016
C	2.07109551832667	7.93633071942290	13.53323252015464
H	3.08484671436480	7.90670115814724	13.96022494415919
H	1.37135111980469	8.28988049267000	14.30647641220467
H	2.08402899005826	8.65215321667085	12.69203074273021
C	1.24434913162145	2.37730524948006	16.76307733038735
H	1.42616007498591	1.83997613488383	17.70552571195358
H	0.21157760024555	2.72629285939347	16.65212625954084
C	1.94093628167620	1.92437481167381	15.57222411231444
H	1.50629433264542	2.17849028976819	14.59965997425369
C	3.23731550302343	1.46288511167906	15.61324561719478
H	3.70684743602675	1.16745711761621	16.55769753203819
H	3.81047644767490	1.30509933367906	14.69513946716175
O	4.94069671282105	7.36380512883335	15.61717821357282
C	4.04703613850545	6.63447392645507	16.33531902449731
C	5.33837206993780	5.04148935709472	15.37608767450739
C	5.61260463740520	6.41148202834446	14.72171685435464
H	5.13624788801471	6.50842424917034	13.73126478745115
H	6.67047590455509	6.70643300524558	14.68374348155787

C	6.50616536700838	4.46270546886866	16.23640086836663
H	5.03434486226380	4.30135547196315	14.61816972900690
C	6.90360964931331	5.44550995351853	17.35601189114576
H	7.75416845977361	5.03923388584848	17.93094892283320
H	6.06742997111306	5.59914861405617	18.05976702136500
H	7.20831810122753	6.43005628550456	16.95989850065165
C	6.06890051233939	3.13047508352160	16.87297931455192
H	6.88787169111889	2.71524287704100	17.48783613761200
H	5.80968007504012	2.38830481859602	16.09847534674316
H	5.18353713291646	3.26878768678156	17.51728106315836
C	7.70597106061556	4.19672083612904	15.30390293981867
H	8.11331457682624	5.12494070640233	14.86603872029187
H	7.42264256297689	3.52488136459488	14.47331705685196
H	8.52331182263531	3.71241142617651	15.86672570764863
C	3.69775135903747	3.49190108289350	20.02866527358506
C	4.53142589463416	3.23391890443898	21.12448658311131
C	4.85534715111821	4.26815802928601	22.01782596235687
H	4.59406906903708	6.36637806762554	22.50733388020621
H	5.51879541975049	4.07158060971988	22.86637517530496
H	3.46223198773003	2.70472339586444	19.30338178382620
H	4.94043178592084	2.22930119762501	21.27357341997640
C	-1.26967738558170	4.23182655584381	20.65931827961625
C	-2.29916896556995	4.42848602422443	19.72732019101690
C	-1.99274179142487	4.81490728697041	18.40993729120795
H	-0.39867626614251	5.29332848685730	16.99129913548540
H	-3.34225102022273	4.27928334372022	20.02566673155603
H	-2.79665770502498	4.96803970323853	17.68227754371115
H	0.87494127415610	4.27982240771302	21.00800167488366
H	-1.50580856835274	3.93004630773106	21.68521160025091
H	-0.48528440622484	6.92187066411431	13.21574461455069
H	0.21411488973316	7.44146453630213	11.65912260452939

H	-0.27017541721727	4.51493581658869	12.50795192562106
H	-1.23389828107109	5.42756879321032	11.32501951826156

TS8

Pd	3.54514869797019	8.83318284815213	20.28827566994798
P	4.75283616562166	9.38204096115904	22.04215392344303
O	0.96431992923921	10.64250681296993	20.99605345333229
O	3.00061066444315	11.67665265090498	21.00795071009120
O	2.23684272559025	9.55685796209857	18.25372137540292
N	5.05439206874571	9.72815157294364	19.07407368635899
C	5.53079192957704	11.03450764050560	21.83486890260468
C	5.75725317214187	11.81907502520522	22.97687383871858
H	5.42859718673685	11.44634527223653	23.95063795917716
C	6.37403949768427	13.07517777508477	22.88381491730293
H	6.52754912811695	13.67155356451902	23.78893550038951
C	6.78309484628636	13.56160115462798	21.63532419743842
H	7.26085043775671	14.54244853131845	21.55011977472790
C	6.57357378094843	12.78878724110971	20.48898175874173
H	6.88221300920682	13.15990523507680	19.50951769564405
C	5.94591869211334	11.52728530710507	20.56778231567813
C	3.98344645780406	9.42467902782182	23.69628703392102
C	4.57193667693089	8.77980764739302	24.80174435174746
C	2.75591539627437	10.11018538146299	23.83509161038006
C	6.20951201767383	8.26685914704472	22.20185289513620
C	8.60039747803354	7.85803321359190	22.43627480720267
C	7.51607482917058	8.74922966473583	22.41169064112212
H	7.68491603087493	9.82192906210450	22.54390614827621
C	1.89838457088058	11.32041291214562	20.48146577721899
C	1.64443535933205	11.81306567086080	18.99734794554182
C	0.26844190450806	12.53766584566098	18.97332958313726
C	-0.30087772765517	12.80206073410658	17.57354806187711

C	-0.40896949322734	11.48871494507734	16.78776930482154
H	-1.10591115014386	10.80478845556113	17.30953319852891
H	-0.81952732235282	11.65382545146376	15.77489073381553
C	0.97353024794410	10.81503678826313	16.68133868199262
H	1.63906476256524	11.46631270575208	16.07714646687629
H	0.93169582626332	9.83357111794329	16.17968888486138
C	1.64934377121642	10.62821204701556	18.03562409641190
C	2.77985482477124	12.75288343948601	18.51847849496571
H	2.56258711937882	13.20442034426616	17.53301023559514
H	3.73653019868264	12.21224264376571	18.45890635193371
H	2.90575649109760	13.55292176138031	19.26421916605602
C	2.12555874740144	7.82365777985659	21.40985205841533
H	2.60286369732218	6.97950290906523	21.93509377734803
H	1.62237006641015	8.53071052199893	22.07739316399896
C	1.40517999362680	7.49847965600917	20.18319432007983
H	0.64363405952684	8.22575323839967	19.87787868433659
C	1.73266227321243	6.47122007507761	19.34756899798834
H	2.50017899979862	5.73770433375099	19.62246099852332
H	1.23692050261807	6.33534830121999	18.38173118057623
O	6.49643107294060	11.25619472563380	18.24990553262970
C	5.77858651215359	10.78218281448012	19.31302361040641
C	5.33324909231327	9.25688560218678	17.69802770979122
C	6.08141393343194	10.46886258910360	17.09400055004550
H	5.42642932065488	11.10547315955420	16.47470224462432
H	6.99107035427481	10.21677107460725	16.53042642400965
C	6.12593456053122	7.91058278336303	17.69930020328070
H	4.36558531012364	9.09282638667869	17.19486522664799
C	7.42928845724756	8.04209340651999	18.51034602342233
H	7.99428656440557	7.09445738826313	18.47771307953217
H	7.21649205421042	8.26519386991348	19.56855299820445
H	8.08789969753393	8.83624739715520	18.11433652804327

C	5.24504704529042	6.80836664897018	18.31704835148448
H	5.78473889595461	5.84427057416250	18.32223212160211
H	4.30634902847217	6.67916490773506	17.74988532926676
H	4.97119774803332	7.05742428115085	19.36030439815201
C	6.43499668454474	7.52919236235675	16.23648665595115
H	7.12465399666984	8.24104514750537	15.74860127823551
H	5.50993804652582	7.47935453970350	15.63328532120732
H	6.91373643876666	6.53505153291156	16.19983757100702
C	6.00347548551712	6.88187278901147	22.02726535565469
C	7.08505348578407	5.99421261513984	22.06721231702524
C	8.38809732071252	6.48233573244498	22.26380651370110
H	9.61442357988199	8.24287004290169	22.58719861771824
H	9.23659315578828	5.79043545294011	22.27695012813933
H	4.98956820173773	6.51409641245906	21.83710964360530
H	6.91408176519405	4.92162910961168	21.92874662006603
C	3.93701765197799	8.82553310466274	26.05216666628414
C	2.72099257792964	9.51076870512084	26.19752874106348
C	2.13590958963304	10.14911047081327	25.09064439140648
H	2.30399850737996	10.59471309336726	22.95810936796216
H	2.22605489904901	9.54291129975067	27.17418974023191
H	1.18250598592222	10.67631713907594	25.19991055043525
H	5.52149021860851	8.24819569743966	24.68535699943325
H	4.39437699047497	8.32435487974169	26.91185213366220
H	-0.42619179241413	11.89988832078769	19.54854276692434
H	0.37420606101293	13.48303231912796	19.53756037688826
H	-1.29521403147554	13.27802124943203	17.65989986839494
H	0.33956699108825	13.51421599691734	17.01571471217354

TS9

Pd	2.06223460439791	5.28950075592175	16.19255062049913
P	2.07843453675560	5.35796167720140	18.40348979327585

O	0.93362413731428	6.49487526669890	14.65467922125972
O	-0.44272101084454	6.53764995740515	12.85370209951287
O	3.12451525173499	4.37067038449985	13.94966756240056
N	3.82829126747199	6.53463292447024	16.32621206159371
C	2.22292213378068	7.15389963187425	18.84933315158235
C	1.48319392902258	7.65367626611744	19.93642859110736
H	0.83273838149667	6.97490293590624	20.49388329915084
C	1.56200692161158	9.00253372663417	20.31658462616161
H	0.96666470659415	9.36124452097476	21.16227759473927
C	2.40061610319293	9.87944228200439	19.61750062470318
H	2.46703573674688	10.93320741740523	19.90441526596034
C	3.15932011115770	9.40003348467452	18.54356438551138
H	3.82458393558485	10.06808603302197	17.99159651239898
C	3.07856118643401	8.05044324052908	18.14451288481607
C	0.55980157405077	4.82782677913835	19.27511486807786
C	0.57098616574792	3.85318940706913	20.28945572809289
C	-0.67007618824803	5.37026113567055	18.83902825715538
C	3.43955761226687	4.57873167946595	19.35617341603971
C	5.23916749216661	4.63458040998006	20.99348747963774
C	4.18110746883355	5.27422650139784	20.33025070135258
H	3.93820387224494	6.31559439742357	20.56177167706123
C	0.63731755249527	6.30809885298728	13.41817455982328
C	1.87653267299342	5.81192408606043	12.47667425720657
C	1.42495044239015	5.74549720839530	10.99854955960692
C	0.53222404025771	4.54579705919562	10.66199453289883
C	1.22860061937398	3.23394509691571	11.04099573606457
H	0.60048072142666	2.35816584382651	10.79536933262661
H	2.16670086164082	3.12544971651082	10.46115952367675
C	1.55506923815412	3.23090353150299	12.54444559777042
H	2.14609857758154	2.35238866563034	12.85455290614468
H	0.60224720642835	3.19136041299372	13.11266281801642

C	2.28622595616100	4.47682885561073	13.02872211767992
C	2.97469702783568	6.87781840864399	12.65078321605631
H	3.12051439392459	7.10380327501052	13.71531531799752
H	2.66483252664659	7.80789164622263	12.14325682281347
H	3.93049398244026	6.54254895220529	12.20804389656470
C	0.51612512578795	3.92602281317986	16.04436328000400
H	-0.28436137464058	4.12167481545073	16.77252731749696
H	0.15501400588627	4.13932289814190	15.02605537535808
C	1.14985001491412	2.60482999031581	16.21090335884896
H	1.87043550219216	2.31419740526789	15.43333931561478
C	0.93131305364431	1.76172539434443	17.24989759377927
H	0.21898712297087	2.01020534192040	18.04507329262420
H	1.44632397590719	0.79792838028535	17.32713698915564
O	4.99163430663915	8.42807890191784	16.72726947801656
C	3.93855209407553	7.61923827411440	17.03122595801222
C	5.05361720130004	6.39562154888414	15.49545680895710
C	5.58719407242210	7.84293848863440	15.51780406773258
H	5.23543683665680	8.43815676583735	14.65754556208031
H	6.67681845498561	7.93694825087815	15.62042237963321
C	6.03691137060395	5.32176913497324	16.06356134852631
H	4.74468181150674	6.07445866511895	14.49046284588637
C	6.49786879547049	5.67670750233853	17.48944012014265
H	7.18942746180646	4.90263008564789	17.86479144923461
H	5.64653173687968	5.71482350432303	18.18693890365708
H	7.02659455190292	6.64584070953610	17.53279758722913
C	5.34574587275494	3.94527291546248	16.06860706836333
H	6.01279186622183	3.19053369666562	16.52227695547444
H	5.07822381297420	3.62717154194983	15.04947499505611
H	4.41019934149695	3.97420451814676	16.65028249888202
C	7.25389645492152	5.25603512704602	15.11588315873883
H	7.83829898325933	6.19405846021863	15.10744076846308

H	6.93882684959650	5.03695342083024	14.07976464319358
H	7.93587734001787	4.44985554023858	15.43841643746319
C	3.75622227378695	3.23649176169747	19.05898798697605
C	4.80601389111984	2.60042116633182	19.73343974491054
C	5.55392357688815	3.30014615886201	20.69522121940945
H	5.82019409278375	5.18253938060957	21.74249202679834
H	6.38279924944528	2.80479226700869	21.21136326093817
H	3.17212182980825	2.70259299865488	18.30033286150371
H	5.04865012494536	1.55887183082482	19.49893337763290
C	-0.63687854705185	3.42619422068806	20.86433319227261
C	-1.85495456585643	3.97411592425026	20.43713716152267
C	-1.86900440422020	4.95238279590686	19.42734011093570
H	-0.67764868481690	6.11312978251416	18.03312762429305
H	-2.79507028538747	3.63755214027504	20.88596415443411
H	-2.81763758804203	5.37830309889542	19.08558795868644
H	1.52039789660421	3.42834457298193	20.62701026284805
H	-0.62209200291629	2.66326631068240	21.64953358633378
H	0.89136624282529	6.68410458667945	10.77492617957562
H	2.33284880912491	5.71401790173244	10.36124580445631
H	-0.41545312006911	4.65060525700931	11.21909802324812
H	0.28459881960839	4.55443132552999	9.58444528856218

TS10

Pd	3.46169361422814	10.06892910940671	21.01017281457425
P	5.06319485240585	9.87815741291280	22.51768571319317
O	2.47153734825913	10.27666102806771	16.58017770619821
O	1.92416758297279	8.59975316484299	18.04146811711836
O	1.77029563583214	11.26295135755418	20.16946874167872
N	4.94604700674346	11.05022968108762	19.77706261280730
C	5.85964904802398	11.54119115445612	22.66870526407396
C	6.24690134132625	12.00534918972087	23.93910676159936

H	6.05096189518193	11.38319638029111	24.81615211000874
C	6.88293877532934	13.24600545450371	24.09927156498240
H	7.16798707956140	13.58223701294671	25.10120849985259
C	7.15506159601450	14.04192296988038	22.97950709194846
H	7.65238965276069	15.00990201319012	23.09316149475053
C	6.78711299087556	13.59335375863938	21.70560957495290
H	6.99667745939440	14.19961982544441	20.82137417725200
C	6.13361138426758	12.35608181794413	21.53185535985093
C	4.61488545120092	9.45680500319728	24.24140269033269
C	5.29753308386187	8.47058321634280	24.97726635972738
C	3.52839651417550	10.14238005689844	24.82717033370406
C	6.45804492176254	8.76203568865857	22.11873999443483
C	8.82763664256354	8.27810676132383	21.86745661734179
C	7.80222753654190	9.16997717567455	22.21462951882375
H	8.04473602460124	10.18324435990384	22.54843665908838
C	1.81680591748701	9.72255167816330	17.49951824456889
C	0.59363469587531	10.67081952368709	18.16565513013467
C	-0.19829090266952	11.36308781788716	17.02499686687232
C	0.49127227102557	12.57164536511485	16.37794148508186
C	0.96281139603295	13.56110556320580	17.45112370529273
H	1.44322064580649	14.44617882662326	16.99478711230062
H	0.09691340110176	13.93414424324271	18.03352648053831
C	1.95570450744983	12.86201261606720	18.39634951790350
H	2.83978869230148	12.55924017902941	17.80094590031271
H	2.30729848635265	13.50607979619362	19.22030207053809
C	1.41533104916831	11.57866861567739	18.99728580528667
C	-0.32876052820788	9.77413686193673	18.99804455425446
H	-1.12236905416523	10.38028743711856	19.47399298457466
H	0.22960093077770	9.24522578711306	19.77863819449237
H	-0.80378398037637	9.01984401821085	18.34992856821879
C	2.06274788831896	8.92366377848300	22.00661162611290

H	2.25329107287251	8.79161711652202	23.08182804428045
H	1.15373050323898	9.51829346119016	21.82106851638367
C	2.16674210801066	7.68048309127596	21.22041237083755
H	1.85900981438580	7.73561586554777	20.16533479741993
C	2.66017173580798	6.51415538141894	21.71019320008440
H	2.96733734313561	6.42157059752221	22.76039082908226
H	2.74101001691602	5.61777902182452	21.08687724765865
O	6.46518318735069	12.60445061623779	19.16316485162872
C	5.79669125764224	11.95579926297847	20.15451374503906
C	5.09078350151135	10.85810154161040	18.30718747998061
C	5.84883647969471	12.14238942006033	17.91036489137368
H	5.17852649426768	12.94655647805366	17.56123691511646
H	6.66095015189401	11.99260120670324	17.18618554694601
C	5.82494638143999	9.52558374356860	17.95156125173372
H	4.09501207111248	10.81482756109404	17.83478480657203
C	7.26445104346333	9.51045787898950	18.49898202347070
H	7.75144524864272	8.55434699103375	18.24010973181765
H	7.27859760145392	9.59375996092280	19.59829936949555
H	7.88802888331999	10.32196052199704	18.08130581459086
C	5.03696556742969	8.33691528410844	18.53033957299149
H	5.55775301553152	7.39148599715324	18.29176311579078
H	4.00960092723717	8.28970765622712	18.12811171957725
H	4.96567631562859	8.40664124831749	19.62886293949106
C	5.81546355769249	9.41202459761216	16.41161544314094
H	6.40822007473532	10.21007771123020	15.92609572147494
H	4.77761804269275	9.46237197539750	16.03788544944670
H	6.25637385018795	8.44654513977584	16.10648680915968
C	6.14479325584127	7.45738174907057	21.68480624234553
C	7.17489452639804	6.57016754526794	21.34845638352331
C	8.51542569718694	6.98066904434076	21.43296608883260
H	9.87186480671013	8.60062917026193	21.93135646604478

H	9.31788130360417	6.28936601708016	21.15584708045137
H	5.09550003595826	7.15018837592945	21.59701739247342
H	6.92811249337614	5.56099396398725	21.00388184973025
C	4.89853863753291	8.17696719241986	26.29073540892310
C	3.82755447007651	8.86898226154589	26.87482763348372
C	3.14511530540289	9.85586629042219	26.14229878077154
H	2.98694892256177	10.89293209318134	24.24015020982869
H	3.51833305187181	8.63641432814344	27.89890357063343
H	2.30344349018943	10.39199817425606	26.59214725998491
H	6.13765595899802	7.93657855988889	24.52408756468744
H	5.42943378506282	7.40553152631811	26.85788170237172
H	-0.43699816485588	10.60614763704999	16.25622745643239
H	-1.16887287906989	11.69108047149539	17.45091372891611
H	1.35950719765675	12.21317471082719	15.80061592000979
H	-0.20802099596182	13.06533585949815	15.67755903119292

TS11

Pd	3.89257170862054	9.81491996442508	20.52991319460407
P	5.33218616577181	9.89309219511237	22.19362377581948
O	2.44427772702690	9.93111446043880	18.98826825156175
O	3.07119022831655	11.91897355352619	18.04849959481768
O	1.44824440193597	12.16672423383523	20.93289477042633
N	5.46317756802960	10.58714456894312	19.31585181730631
C	6.26971809100615	11.48344368318423	22.13672348445991
C	6.64187411146795	12.10934972722621	23.34026673548892
H	6.34799397051674	11.65415685893976	24.28970611008878
C	7.37982859811300	13.30269252332288	23.34325536311703
H	7.64983932510855	13.77025032208411	24.29553084032053
C	7.76669691721469	13.88670337011593	22.13042578050863
H	8.34125466861957	14.81800464225444	22.12054837583290
C	7.41184705731458	13.27574499362490	20.92232461409449

H	7.70429547695887	13.72007805930589	19.96848446117222
C	6.66076894793012	12.08206629203105	20.90516967751901
C	4.74450545649170	9.81724288818313	23.92337347933064
C	5.34216927082269	8.99171826690576	24.89296446095731
C	3.63622859137249	10.62228192755975	24.26624547579187
C	6.63914195783704	8.61281254115309	22.06209352720155
C	8.96253288784859	7.89330138355597	22.01641825145575
C	8.00892100773184	8.90580143530832	22.20241916936340
H	8.32794715029417	9.92486703577606	22.44157112802095
C	2.22967351844174	11.13818694648465	18.53250292527684
C	0.74736805123864	11.60810628056740	18.65474230052888
C	0.42422143752747	12.63961533175038	17.53870224336579
C	-0.88791677465260	13.40743960445300	17.75378914529746
C	-0.88513335803411	14.11993994214418	19.11377840149654
H	-0.07244710611114	14.87189625987388	19.13186773457860
H	-1.83099180629482	14.66706905828177	19.28136484158475
C	-0.65811899152580	13.10842045025941	20.25846441500102
H	-1.52087038774757	12.41347364476176	20.29840766557150
H	-0.57812610478773	13.59897202178347	21.24264180069467
C	0.60836432197500	12.28213794782912	20.04129378795701
C	-0.22842192611038	10.40713275661799	18.60950132349156
H	-1.28007515301343	10.72793471931570	18.70615949236477
H	0.00421843681924	9.68689215997424	19.40739975196063
H	-0.12030834533947	9.88422906122083	17.64348006238925
C	2.35781276001596	8.94468851346247	21.60765451895604
H	2.51422163168581	8.94853523696774	22.69675389575452
H	1.51323989951962	9.58928742186900	21.32334397065582
C	2.32212689041781	7.59001148911821	21.02887337031618
H	2.00193473067824	7.52956508949454	19.97939173994259
C	2.68582001924249	6.45375393288765	21.67494215254501
H	2.99161601019688	6.47450386162729	22.72894763244300

H	2.66598042233666	5.47529430678643	21.18377944797159
O	7.04229845273300	11.99780445576439	18.53506626674141
C	6.33668579733316	11.50576161404343	19.58924686336604
C	5.56229969436842	10.24593532310487	17.87611013254328
C	6.42212532051762	11.41178035353361	17.34019550339701
H	5.80057813186078	12.19513772952707	16.87846260843833
H	7.24097792706291	11.12028906471139	16.66725999317138
C	6.13154288518309	8.81195277072554	17.65550550158279
H	4.54218408534834	10.30845955074068	17.46889300494357
C	7.51061888442927	8.64865955372244	18.32214369158596
H	7.90569282989681	7.63374529223021	18.14072803154070
H	7.44272601622625	8.78709341222236	19.41340754088879
H	8.24993538216520	9.36948818681562	17.92749215967965
C	5.14506891650998	7.78181647361040	18.23994135294452
H	5.50778935676421	6.75492009468317	18.05183559756697
H	4.14261925289885	7.89280895457823	17.79252480098465
H	5.03003627045846	7.91053422149465	19.33059404233617
C	6.24080866421474	8.57428211776285	16.13439927163181
H	6.97849214733137	9.24182007057431	15.65372957608022
H	5.26551554240316	8.72751046102592	15.63797476702366
H	6.56168191347919	7.53626289794882	15.93684769959144
C	6.22786562046891	7.30145782227748	21.74308574413290
C	7.18514291270835	6.29392752535766	21.57031884383477
C	8.55253788343215	6.58910995664571	21.69973412047517
H	10.02792991550275	8.12651255477459	22.11370674452425
H	9.29951784549954	5.80298368368410	21.54808234902543
H	5.16057258406104	7.08161749089716	21.61392927722080
H	6.86201949627222	5.27886448166105	21.31759070533748
C	4.83908324002099	8.97773404253017	26.20336745752188
C	3.74693943083956	9.78849439154763	26.54724281569806
C	3.14804398353263	10.61224436072749	25.57831888458615

H	3.15901942292858	11.23990148008733	23.49644066657770
H	3.35577670087543	9.77409230377798	27.56981787659170
H	2.28909740122382	11.23751403341297	25.84207069122930
H	6.19732718782720	8.36497907213472	24.62173115335994
H	5.30294280378143	8.33178154035159	26.95606294353405
H	1.27338619942628	13.34333794677663	17.49061072813303
H	0.40796140002062	12.10502944426965	16.57014510507065
H	-1.75498799850961	12.71990856009281	17.69965710967022
H	-1.02336296392539	14.14330574582983	16.93954341803459

TS12

Pd	3.54289000833998	8.64378804162948	19.91243346686683
P	4.37835889999179	9.45787496519942	21.79757969918216
O	2.02334672186320	9.74813873807012	18.46843839171904
O	1.55730571063665	10.74539467034906	20.46557371059446
O	-0.80585889221009	13.11668173491605	19.86859882761481
N	4.97866046284476	9.83284892595859	18.90576879696290
C	4.51105074593418	11.28802911020703	21.58410698041115
C	4.20217487865795	12.14085608503111	22.65624551495349
H	3.85403321379257	11.70604751142490	23.59657847335686
C	4.31952220464822	13.53439856081027	22.53691929834902
H	4.05474941091719	14.17412951031841	23.38462183868756
C	4.77439417626483	14.09819285891629	21.33858434681835
H	4.87011295667932	15.18298067022944	21.23454302158129
C	5.09171207701912	13.26545424277082	20.26005729571148
H	5.43239314780904	13.69100761935526	19.31415565143863
C	4.95080356105883	11.86496406752540	20.35896696256755
C	3.45368376383683	9.24938630962507	23.35724376535950
C	4.04574468291421	8.71119920115029	24.51565318006731
C	2.08607904470458	9.60933421262382	23.35621221440605
C	6.11178991606892	8.97763749457606	22.17905157812437

C	8.43551716099390	9.49170583869388	22.69958552286629
C	7.11168424980673	9.91478523243327	22.50460652014022
H	6.85579803834342	10.97462702432617	22.59531915108088
C	1.45702648698423	10.62821491698496	19.21312258251909
C	0.52612374878000	11.64032953691199	18.46769964885966
C	1.21490420820087	12.13105837978194	17.16806626301372
C	2.50163519660488	12.91818783004607	17.45596892613632
C	2.21938879914775	14.13203666144554	18.35437636437273
H	3.15420854068088	14.67686940326149	18.58501986622917
H	1.56597899554627	14.84193449510848	17.80955386099341
C	1.52864625416617	13.70551088368365	19.66777619963353
H	1.22036208796743	14.57464553766539	20.27222410976358
H	2.22536015634181	13.09312099486584	20.26681209862841
C	0.29734622998819	12.84192077819723	19.40200473418341
C	-0.79864110854071	10.92775498896692	18.15349114612694
H	-1.49496877238850	11.60974318789908	17.63580829149404
H	-1.28842286814324	10.59483833083614	19.08261692561853
H	-0.60539720952962	10.05169982057624	17.51199702948317
C	2.13153206870844	7.38768787113421	20.75022519232506
H	2.61735392613063	6.70195631971576	21.46018502595403
H	1.29995989505657	7.95196797073269	21.18599832114728
C	1.98340232497074	6.93798614281064	19.37150599128759
H	1.19492835443871	7.40565309218382	18.77143379785678
C	2.91758670644882	6.15771597313336	18.73968258826723
H	3.71995063030825	5.66499061610900	19.29995737635012
H	2.86518153336355	5.96508735932990	17.66390124560413
O	5.93832041484791	11.74073175885577	18.17497342114986
C	5.26875782589140	11.07562686128563	19.16003356200613
C	5.59080007173988	9.46197554372513	17.60706629302438
C	5.93554806163927	10.84911756650722	17.01746671180073
H	5.16258272673597	11.21562110777185	16.32129468991271

H	6.92771168217768	10.92216346663349	16.55090287881258
C	6.80533370789940	8.49772352246271	17.79577193086688
H	4.82161461361228	8.95298837013341	17.00221744333424
C	7.86839568186893	9.12633098115185	18.71790398090390
H	8.73022648955855	8.44443545788616	18.81953837765461
H	7.46491345937262	9.30211156231572	19.72832884604173
H	8.24796787394839	10.08598670209300	18.32370739111592
C	6.31020508384445	7.17728829250769	18.41310807493843
H	7.15894183350677	6.48793294611548	18.57079283252195
H	5.57749781518203	6.68011073497703	17.75325790162085
H	5.81676358574006	7.35519596703590	19.38417488315742
C	7.40752629942188	8.19926473813862	16.40678878802119
H	7.85039246267057	9.09446362115546	15.93499883336846
H	6.64430496671677	7.79164764408014	15.71883546842483
H	8.21147422356388	7.44832104028450	16.49930088468130
C	6.45232427535354	7.61353187898837	22.06350319274101
C	7.77024885737474	7.19192661299187	22.27760977014571
C	8.76678412496225	8.13298450119050	22.58681644969674
H	9.21013079318281	10.22768172287112	22.93906715945606
H	9.80151705907289	7.80703377079441	22.73433516937041
H	5.67529894503222	6.89321310803324	21.78404226543486
H	8.02449809585856	6.13098112453524	22.18573060945603
C	3.27239443945907	8.52991713340167	25.67260765494993
C	1.91685170014598	8.89190937831157	25.67789053406860
C	1.32930339229962	9.43386885979225	24.52144594952424
H	1.64491939193124	10.02815397719302	22.44297831025670
H	1.31713616240679	8.75228342590204	26.58348167377030
H	0.27218283374276	9.71918645076810	24.52403052678362
H	5.10532375489702	8.43762589715589	24.51307467507222
H	3.73366168650550	8.10930186543904	26.57239255912334
H	1.43320828006206	11.24333611198393	16.54964668181796

H	0.50618293138686	12.77075004582089	16.60382894242143
H	3.22143432854359	12.24422530828709	17.95698406423808
H	2.97167774169549	13.24440722390233	16.50860882360600

TS13

Pd	3.21707639151023	9.12254094405386	20.85054762571597
P	4.75563104758807	9.84248164624426	22.27730939309779
O	3.55861784923150	12.53179948276347	17.99631426302736
O	2.26677090110640	14.24402564560715	17.21758170058936
O	1.68616395519821	10.21849535866247	19.26569386220761
N	4.55976814754528	9.72535495060609	19.33102422961881
C	5.22581972285232	11.53971446403445	21.75692377138593
C	5.37566509391884	12.56672694078218	22.70574460923662
H	5.28024364115826	12.33521064045796	23.76987137310442
C	5.62590876604560	13.88624165703498	22.29765465529052
H	5.72806810863482	14.67392006469701	23.05120191896120
C	5.72209086959894	14.19341609936011	20.93337443027813
H	5.87763065854632	15.22663291902319	20.60882245183941
C	5.60075491363025	13.17951467762821	19.97473857839036
H	5.59182404089036	13.39863821615645	18.90528509066451
C	5.36166323017317	11.84948287675229	20.37628572482249
C	4.34217474817167	9.99370276543065	24.05205426538545
C	5.14464127195576	9.42688770869750	25.05984902932193
C	3.16390578223156	10.68736882474081	24.40468804195589
C	6.31645932097922	8.88572399090358	22.22450537994151
C	8.73394089325386	8.74022320669221	21.99454200454010
C	7.56790756636766	9.51525249369408	22.08564930405317
H	7.62487654284686	10.60673975897995	22.03538929490309
C	2.46275749728410	13.13846181509579	17.75743001133395
C	1.13655395792951	12.30782336328306	18.18939524291972
C	0.02296904402769	13.29836382531535	18.59822139664739

C	0.36676034384187	14.08726887322609	19.86922785062590
C	0.68965714480739	13.14380294820300	21.03737092800966
H	0.96521370926207	13.71190580256830	21.94581114639800
H	-0.20917725567801	12.54705868769927	21.29277485900145
C	1.84156296964595	12.19165819160449	20.65530486395623
H	2.04236784694716	11.43304105432319	21.43441636829079
H	2.76802440562147	12.77463122177890	20.50612064137988
C	1.56258935807365	11.46161116137382	19.35212860443690
C	0.72096581283968	11.46459492346626	16.97673328937116
H	-0.17580588787160	10.85583121823917	17.19393213050012
H	1.53400288580730	10.78014872776032	16.68485806602954
H	0.49962986861071	12.13294458486513	16.12776904304870
C	1.86951163120960	8.36476738550308	22.24342357369743
H	2.38872889230207	7.60491715433249	22.84664196166247
H	1.36856805469121	9.12164914291581	22.85907503678976
C	1.17988946342776	7.91873887002064	21.04272017641696
H	0.36514539894950	8.54442912631652	20.66108792086045
C	1.66173367454847	6.91690745681596	20.23807425309082
H	2.45999038333864	6.24899209119392	20.57871570003909
H	1.22612414863330	6.72047349888182	19.25458591832428
O	5.86847937068650	11.13001844314703	18.15495969808248
C	5.22205377709308	10.85147848941813	19.30272476251226
C	4.68994498289105	9.08484925932717	17.99399941472950
C	5.25496261836404	10.25456061276581	17.15542517958057
H	4.45949858440144	10.85902682675433	16.69220757565022
H	6.03929858551874	9.98223653745986	16.43645024217205
C	5.57253876337699	7.79954537433882	18.02791815137437
H	3.67432545839298	8.81749525507194	17.65546273311168
C	6.99042619647117	8.11682861619781	18.54057581244600
H	7.60130900565367	7.19742601934760	18.56220974608052
H	6.95907057622298	8.52037009799125	19.56510037679594

H	7.50905726968200	8.84934515134616	17.89808302200367
C	4.91845859827467	6.75612787073477	18.95046888892350
H	5.53624416855070	5.84111005902422	18.99649915640534
H	3.91500416992147	6.47764716366001	18.58347827185660
H	4.80596402876056	7.15027111861700	19.97517928747153
C	5.63807518597355	7.21934542114537	16.59967829930253
H	6.15409509818957	7.89527562371149	15.89550199751521
H	4.62578511328328	7.02157945822663	16.20207948291796
H	6.19176925356971	6.26384435144430	16.60357454570439
C	6.24286533406323	7.47877491377849	22.28017217136868
C	7.41061735380088	6.71003510382241	22.20317907227699
C	8.65714303264147	7.34041294540995	22.05270758505285
H	9.70381632927420	9.23288744930450	21.87239681699281
H	9.56825333042345	6.73872879563558	21.97410080266469
H	5.26367951827864	6.99553720098317	22.36738020074191
H	7.34724005102608	5.61798760764004	22.24340390631680
C	4.76908036094482	9.55038211445590	26.40663313429167
C	3.60158467780952	10.24565754907037	26.75367046615600
C	2.80172906193992	10.81898185993377	25.75000971723851
H	2.54246961387897	11.13073612687061	23.61968806335748
H	3.31252940409490	10.34162681000626	27.80513187236339
H	1.89066755538340	11.36429561098291	26.01635132326976
H	6.06068316854383	8.89287887534363	24.79095407005008
H	5.39561826719488	9.10460764528062	27.18596095208986
H	-0.09904256125040	13.99364363404759	17.74968628834337
H	-0.93165804949722	12.74976656538726	18.73930658664000
H	1.24106238669629	14.72807978016934	19.65199892704108
H	-0.47004645220968	14.75777120436260	20.13959141794573

(chair/ax)-TS14

Pd	3.45089594530585	9.74505597823256	20.63386633834878
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O	2.92833000566141	12.52615134343600	16.37771795869359
O	2.82417754017071	10.42200623863249	15.32962204817616
O	2.31233340675614	9.64995568668569	18.89531814958828
N	5.01463084295829	10.72897717083825	19.56300141761102
C	5.55983756572875	11.56013198311678	22.46495717514802
C	5.79710560705990	12.15670517726489	23.71632723023936
H	5.50957469518248	11.61897776165374	24.62380002063729
C	6.39579905627959	13.42143466121183	23.81951226999165
H	6.56282305163660	13.86304599278119	24.80709440527876
C	6.78128318014881	14.10778467419313	22.66066475900245
H	7.25041897683256	15.09394055530647	22.72923534350442
C	6.56354349297952	13.52736286295328	21.40596572957143
H	6.86005312991091	14.05036480342064	20.49408529686376
C	5.95069603369728	12.26212097331807	21.28689557835697
C	4.18741734004809	9.56826190054149	24.07175260931518
C	4.73536513686631	8.57681597883305	24.90631470851350
C	3.05805421837092	10.29880057414373	24.50154082518039
C	6.26854375074275	8.77566724746199	22.19594742101133
C	8.66514938621503	8.36481924824890	22.12122135307489
C	7.58960817548007	9.23646694474103	22.35025451332715
H	7.77746572241924	10.27580497951331	22.63562501624948
C	2.71008495018008	11.40997678759971	15.99388433124940
C	0.74396128992808	10.59147418764698	17.39371492728004
C	-0.25712370506549	11.68488816919569	17.05331493318494
C	0.01702354789297	13.03809131132867	17.72925874554256
C	0.39297309177624	12.83558354665686	19.20300883370330
H	0.55375520990433	13.80704582681705	19.70686706821176
H	-0.44160296848931	12.33317126052192	19.73134108932999
C	1.65422228593862	11.96663148254564	19.31538095431897
H	1.86038804792356	11.69488361943090	20.37054218797062

H	2.53902014719519	12.53557470278653	18.96481656301525
C	1.56066810513052	10.67583776103369	18.51395080221885
C	0.51654253597943	9.25886851340229	16.72484574939099
H	-0.44723040552062	8.81514344827709	17.05218295691377
H	1.31907173491311	8.54984953060596	16.97617058495842
H	0.47143213730505	9.35657802666012	15.62524850365040
C	1.88268472477129	8.79274520640885	21.58082056498848
H	1.80405025368980	9.07496422533844	22.64225721179401
H	1.00654323590346	9.13314512009536	21.00670533667724
C	2.18870166129400	7.36256189001962	21.38086089564083
H	2.07568802320809	6.99143825709201	20.35206406252069
C	2.61596459119128	6.50740727436096	22.34314147075121
H	2.73473821535784	6.83471171374337	23.38327588815862
H	2.84221517862083	5.45849714590260	22.12368561594926
O	6.43220630445891	12.36815762503852	18.93345443647261
C	5.75982140320142	11.72919818162339	19.92707476294533
C	5.19690430779786	10.49877683446005	18.11067230281966
C	5.94725657857249	11.77968957753565	17.67662631522231
H	5.28102966294235	12.51607149333229	17.20060428418213
H	6.83026562404078	11.60281676335808	17.04689452051381
C	5.92479310317614	9.15164030500884	17.81423236518475
H	4.19273224774788	10.43511527214455	17.66733033353520
C	7.29983463098068	9.10152191296978	18.50466599312115
H	7.80465711544694	8.14679455055600	18.27645056080763
H	7.19779815481410	9.16855027056191	19.60003756211237
H	7.96619761462321	9.91691060662817	18.16805520712453
C	5.04754669042944	7.98503907107142	18.30970767943752
H	5.51933601577235	7.02006061340418	18.05065952844759
H	4.04149982865802	8.02713566466450	17.86091554939191
H	4.92012952884305	8.01934606471768	19.40618362884545
C	6.07857316245151	9.03404914969679	16.28266426256557

H	6.75765030363844	9.80098664160559	15.86779632879778
H	5.10178227228202	9.13161353086099	15.77773307806726
H	6.50356717574174	8.04855926507106	16.02316727466916
C	6.02890574013840	7.43600029350461	21.82381480696854
C	7.10772289487520	6.56918071847050	21.60819586791979
C	8.42614530458890	7.03351833024734	21.74801199325364
H	9.69164007376374	8.72976336036047	22.23018243939278
H	9.26761307481785	6.35782660492308	21.56326080841471
H	4.99617092163607	7.08456620043501	21.70694865081128
H	6.91772252913543	5.53135004903381	21.31599520483423
C	4.16068321553856	8.32185370331842	26.16129978604498
C	3.04600437199928	9.05742237986185	26.59006136769457
C	2.49839338883182	10.05104530860539	25.76044150254296
H	2.62220737426445	11.05682401303980	23.84109687635429
H	2.59866951203197	8.85429115066635	27.56835182912638
H	1.62446852432122	10.62242669791463	26.08914250192260
H	5.60549194075958	8.00466884492306	24.57183287276343
H	4.58764452394373	7.54576554457622	26.80474375178884
H	-0.31193057109297	11.81891929719799	15.95352110028349
H	-1.27261844753843	11.33215715334695	17.34673823155651
H	0.85052787446638	13.54721834648497	17.21425221459626
H	-0.87113940764426	13.69084239818605	17.63841437150531

(boat/ax)-TS14

Pd	3.62960200372559	9.94263960189564	20.58894443662359
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O	3.55939807800790	10.73958424611661	15.57802337841891
O	2.43226266734111	10.01436569080127	18.85234037100118
N	5.30565617821885	10.66088715938721	19.48439088163210
C	5.89943516357669	11.60726401114116	22.33878675740136

C	6.17990630855425	12.25129668337604	23.55732470604726
H	5.82922302922915	11.80163445122119	24.49004693690233
C	6.90089485968370	13.45456544751362	23.59560936933424
H	7.09916881153160	13.93665472241397	24.55810748798802
C	7.36606265129740	14.02802869018412	22.40527024885209
H	7.92933674940345	14.96588825511727	22.42369782954557
C	7.10772837607263	13.39625810522421	21.18322779443664
H	7.46566214467351	13.82957972976819	20.24666806861806
C	6.37415793312346	12.19289564880456	21.12888843391057
C	4.30119696602048	9.86914054891357	24.03212376336891
C	4.70211543807436	8.85573749600840	24.92198613608709
C	3.27177100054150	10.76098546989093	24.40499498888182
C	6.31498239913564	8.74659897079019	22.25616397211047
C	8.65358971911212	8.08011220537570	22.28346900649694
C	7.67346428115017	9.07390307510168	22.42532734661734
H	7.96492175574462	10.10357719157398	22.65258199017748
C	3.17169095034064	11.72047961965986	16.20766927823847
C	1.46075960466999	11.25016540251271	17.08110255516029
C	0.52703211904174	12.44273623954417	16.78840564546682
C	0.21519436080521	13.29882008811736	18.02614078717970
C	1.51822772225058	13.66329541622844	18.74722971522481
H	2.19356723484063	14.16378688854522	18.03436452735355
H	1.33387730264882	14.35632404589856	19.58852377244876
C	2.19890100288681	12.38545578418665	19.26863810343527
H	1.81342801202137	12.10814090401059	20.27055128075312
H	3.28640977780251	12.54113982228926	19.39936100989063
C	2.01310886442956	11.15290832757342	18.39900499545233
C	1.04751812644553	9.94004439823370	16.43135248519340
H	0.11061748142515	9.56342654075692	16.88687004073265
H	1.82601609712554	9.17488899845961	16.55273850498975
H	0.87421680601419	10.08344084486380	15.35205263936837

C	1.96535006544932	9.22087968636081	21.58109405961987
H	1.90459688496461	9.59035672932469	22.61630002280667
H	1.13205369000983	9.60549406611452	20.97107897908429
C	2.11595268686302	7.75391178572867	21.49730767928708
H	1.97735713876035	7.31278436194354	20.49945064370526
C	2.43154894867628	6.93627790086564	22.53201364421789
H	2.56952126219208	7.32921448570917	23.54638440716499
H	2.54477461250277	5.85524796758947	22.39818852031539
O	6.91423026707791	12.08026829023168	18.79007659331671
C	6.15462661908551	11.59440567612208	19.80022532877006
C	5.50169746739368	10.30354631964846	18.05706079781950
C	6.37754439556282	11.47284689986765	17.55555150733942
H	5.78270173952171	12.24270078824834	17.03767843491870
H	7.24326431277642	11.17569131878198	16.94843891626522
C	6.09204610975645	8.87220542862277	17.88263709028601
H	4.52400509929535	10.30769720567362	17.56007463532103
C	7.43063760687697	8.72045737814070	18.62595610383185
H	7.84005371642039	7.70679196466823	18.47206615360490
H	7.30589054444978	8.86634444325236	19.71102215930154
H	8.18653720506298	9.44156891560915	18.26473810925514
C	5.07000454445058	7.85018921526542	18.41903723019978
H	5.44716792345024	6.82124400434745	18.27834073527603
H	4.10396755577679	7.94753164276576	17.89514550791753
H	4.88149964380954	7.99860403952555	19.49790250941733
C	6.27744193613277	8.63346882114096	16.36827266755041
H	7.08199938658258	9.26097265341895	15.94451687741623
H	5.34787779551414	8.85789194186261	15.81801301302558
H	6.55395236556340	7.57999608674989	16.18511843467545
C	5.94083026199253	7.41978136318788	21.95675952871859
C	6.92477864003317	6.43148783307095	21.82743203536213
C	8.28141959728942	6.76117396291371	21.98225708073014

H	9.71037065098528	8.33987267754570	22.40277139279546
H	9.04933667921052	5.98975465082347	21.86475687516984
H	4.87978752357627	7.17327618751201	21.83010076115917
H	6.63164790260818	5.40357779819629	21.59105905233085
C	4.08063788567869	8.73837003510847	26.17517060602519
C	3.06580509928664	9.63232774130203	26.54666037264848
C	2.66590449224500	10.64853917603920	25.66171150264494
H	2.95024005899065	11.53880182293958	23.70333174517300
H	2.58155005464403	9.53643628287602	27.52369519728719
H	1.87066185451258	11.34478989869658	25.94631052752882
H	5.49427849577010	8.15955249278082	24.63232361968093
H	4.39294947771240	7.94508685648459	26.86192768749845
H	0.97151314305325	13.09256709080053	16.01312301091720
H	-0.41401553965730	12.04345315447677	16.36491230213734
H	-0.33638646509802	14.20945882496803	17.72830650921364
H	-0.44405919432572	12.73224074674543	18.71552494023071

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O	2.71576858183699	10.14109541913982	15.35967176161166
O	2.30496179011666	9.64787323592486	18.87251038979214
N	5.01687187827910	10.74232603123324	19.55673565566355
C	5.53556002223060	11.56447864841079	22.46969538862157
C	5.75633335705652	12.15723574763854	23.72565790189272
H	5.47411001736441	11.61345916701192	24.63086982424418
C	6.33583327968647	13.43111692521619	23.83856763266994
H	6.49069746292212	13.86906491675455	24.82928160712618
C	6.71718372092904	14.12963219763956	22.68518223813938
H	7.17012924615099	15.12242181001679	22.76096152242182

C	6.51757475962152	13.55128944447034	21.42552313823829
H	6.81347962792964	14.08824830945120	20.52157469799102
C	5.92556662435984	12.27661904756734	21.29714585281947
C	4.17087467978877	9.53993187785814	24.05165316897509
C	4.69663062251303	8.51832997222771	24.86453661811581
C	3.05271523079570	10.28174666229296	24.49296866733976
C	6.28094208345863	8.78711568736875	22.18560106791445
C	8.68312123605363	8.40393352930594	22.13330340953060
C	7.59514312189558	9.26257638256385	22.35679574152206
H	7.77105163734213	10.30088848393819	22.65295489704311
C	2.66250811499319	11.20982580633253	15.88671241847679
C	0.63949078929910	10.58420606849956	17.46929389283358
C	-0.30660494245492	11.71966069533171	17.11506076587721
C	0.08536892340962	13.08494231646587	17.70421562514423
C	0.53517008270048	12.93041632478466	19.16296504424812
H	0.77511945037618	13.91350904474231	19.60924761853640
H	-0.29377359098583	12.49979906626715	19.75961358524307
C	1.75329257629402	11.99940882916625	19.24689313307068
H	1.99736717424487	11.75588297756142	20.30148329365850
H	2.65091056346245	12.50676781464704	18.83885785609071
C	1.55417585724808	10.68196509692211	18.50770102101315
C	0.31105419039489	9.24001142067724	16.86953295216692
H	-0.69197660057892	8.89262859786164	17.19827293438351
H	1.05340534857957	8.48784993096222	17.17710249553846
H	0.28666498242975	9.27361136227124	15.76394543574532
C	1.90103200153470	8.78090922462158	21.56742654364488
H	1.82145130083481	9.06963731519981	22.62723923405664
H	1.02321827059498	9.11744847818292	20.99157298613334
C	2.20571699337737	7.34803798690408	21.37759327281134
H	2.10233474477486	6.97201853343242	20.34879209799638
C	2.62765977580595	6.49316423397518	22.34302607375740

H	2.75167064347668	6.82526821238784	23.38121373502672
H	2.86939407593639	5.44760296463290	22.12286648021304
O	6.44862566244565	12.37680116027743	18.95222004848395
C	5.75737077532427	11.74206616115636	19.93521743147804
C	5.22595273945111	10.51174003383633	18.10776715826575
C	5.98497459783692	11.79075845490424	17.68574339828581
H	5.33126471374339	12.53197510993414	17.20007451174779
H	6.87699988025131	11.61611132192160	17.06933933923040
C	5.95774983695378	9.16496307034807	17.82098942467169
H	4.22854721846558	10.45066744874845	17.64789511152332
C	7.32258542091659	9.11466910836566	18.53136365697642
H	7.82636414288615	8.15663857994553	18.31499194287099
H	7.20370569928161	9.18767290883882	19.62457624262731
H	7.99374285269212	9.92689062452444	18.19755302074764
C	5.07220432967507	7.99846079318297	18.30108608636673
H	5.54296221399258	7.03322711315100	18.04121821117822
H	4.07086421016377	8.05078244651726	17.84144324463205
H	4.93321380798745	8.02884702034424	19.39644106961712
C	6.13857592904328	9.04755196514811	16.29235831346472
H	6.80886480709278	9.82674553706349	15.88777253456904
H	5.16703767281568	9.12605187477875	15.77280084649748
H	6.58274960583142	8.06795554453239	16.04262501864680
C	6.06063529601832	7.44703571220405	21.80219475848174
C	7.15091237861025	6.59279949398409	21.59103833064665
C	8.46299115748745	7.07187691021416	21.74813350071947
H	9.70377080066671	8.77963071582649	22.25775507406353
H	9.31378210367964	6.40667773475850	21.56895527064725
H	5.03391569268366	7.08354682475852	21.67472900509087
H	6.97616759669638	5.55446487697992	21.29146941388266
C	4.11027425563433	8.24338873882232	26.11075702214060
C	3.00611260721998	8.98926368869491	26.55153212033273

C	2.48129600594109	10.01368819057981	25.74318315908260
H	2.63572770110654	11.06886530590633	23.85476055802092
H	2.55135811845890	8.77285856367230	27.52341152141465
H	1.61925798150784	10.59634969724841	26.08295088183505
H	5.55934103103831	7.93831540049193	24.52478823341113
H	4.52122761901831	7.44556183627818	26.73752292781799
H	-0.40346871810385	11.80247761524387	16.01224895168625
H	-1.32965592880366	11.45331738086542	17.46915379653302
H	0.91694474321685	13.51585794649309	17.11842938933760
H	-0.76572527708915	13.78705136057879	17.62748649703896

(chair/ax)-TS14_diast2

Pd	2.42840692658436	4.55005383347162	16.06966701267764
P	2.02218823069277	5.13266308508481	18.17174508447816
O	1.91003843522130	8.07649566579140	14.38186341815788
O	3.72621553216335	7.59169179261566	12.96545576120433
O	2.92281499668311	4.16236851516827	14.09754552212631
N	3.97484277182706	6.03530688321441	16.12893142294110
C	1.98527338284567	6.97517625285166	18.27310345341808
C	1.04381986078255	7.61206636790315	19.10093548520759
H	0.33323700679569	7.00253672305327	19.66538450254684
C	1.00094865801813	9.01013720305124	19.21251205143453
H	0.25108052705985	9.47909743231530	19.85756303447685
C	1.91730804629794	9.79633746301199	18.50253783356166
H	1.89032108962594	10.88743227949547	18.58006474760808
C	2.87211934629904	9.18069086441813	17.68546101876206
H	3.59126245700302	9.78000062043018	17.12318234398152
C	2.91679082161981	7.77797125319196	17.55441607426766
C	0.46612841415649	4.60426304480435	18.97002353799179
C	0.44432332169384	3.88671431076648	20.17977316539072
C	-0.74170036134605	4.85694784248308	18.28306660280431

C	3.35373890147452	4.66874096182874	19.34625932664634
C	5.02820958084159	5.20417093652920	21.02833065873101
C	3.95893718596293	5.60057054942312	20.21053565568964
H	3.60455946957438	6.63535199541539	20.23434345126065
C	2.72211167478041	7.64860380146934	13.61778048682871
C	1.33470623384696	5.60121881859682	12.91726710131257
C	0.87765459929243	6.12069970635537	11.55775914167373
C	1.95787481315107	6.12470011010500	10.46697142494534
C	2.71566549789756	4.79279828541928	10.47679604589778
H	3.46680421479794	4.75395148929057	9.66569081308753
H	2.00382122209447	3.96323687153349	10.29474804077165
C	3.39542747557883	4.59331448911343	11.83742723550321
H	3.82420802054022	3.57941206934805	11.92832500954067
H	4.23986707579857	5.30475115222440	11.94027772535071
C	2.46378018795919	4.79946164462038	13.02934932461586
C	0.27330325649283	5.70844626346514	13.98408793258883
H	-0.23386837945718	6.68817480468718	13.92897450110844
H	-0.50240875543610	4.92285370290574	13.86804593797992
H	0.68876089370820	5.60816975740053	15.00640486945513
C	1.03970473651839	3.01907717146421	15.95521738294079
H	0.11108919821488	3.27166384752692	16.49040747018278
H	0.86801524452161	2.95139576786542	14.86999684410586
C	1.72271138247378	1.83325805585387	16.50771013395800
H	2.54486605051557	1.42884754165547	15.89863426930415
C	1.43459972762880	1.23260274356907	17.68880644458459
H	0.61996855293215	1.59360818632959	18.32759789487424
H	1.99276196287238	0.35895795827523	18.04262409524634
O	4.98942074030872	8.03784574248454	16.36787874742004
C	3.95046978611847	7.21573415078321	16.66915017589669
C	5.23564671582695	5.88210577284852	15.36323651623498
C	5.79657491914910	7.32690803734297	15.36771826130759

H	5.65176019363380	7.84070513045844	14.40626850671672
H	6.84424185344619	7.40702338024950	15.69112006842251
C	6.18202517499620	4.80579588983256	15.97997205311689
H	4.95823220537438	5.55622237949232	14.34808471218755
C	6.56142794643400	5.16699430945391	17.42789354059017
H	7.21367138469377	4.38616491878174	17.85574734888128
H	5.66649497909226	5.23625227062512	18.06632137267339
H	7.10788880128989	6.12549245109856	17.49313342934700
C	5.48852011890948	3.42965817096342	15.95343310983086
H	6.18697894605013	2.64704280361215	16.30124052964167
H	5.13862079743366	3.17933229025987	14.93822355081939
H	4.60250756387880	3.41690097529455	16.61381253638004
C	7.44336090754415	4.73435282517215	15.09313896217641
H	8.01085772370639	5.68262756524604	15.08650468612129
H	7.17987726619992	4.48567682992298	14.04928962270609
H	8.12320035312044	3.94874065650562	15.46685159167138
C	3.81594807249996	3.33595155691300	19.31407294016833
C	4.87468358801405	2.94473294736185	20.14307384930594
C	5.48795881717067	3.87899163574151	20.99449124810491
H	5.50446745890760	5.93483316240394	21.69025369902594
H	6.32602602879460	3.57429432539948	21.62983023673434
H	3.33672758360746	2.61648280283206	18.63933551288791
H	5.23119085172963	1.90991403060444	20.11397468693631
C	-0.77620232391980	3.42768088112341	20.69947460571760
C	-1.97534758896490	3.68847572904301	20.02016309191874
C	-1.95719956181882	4.40953883040890	18.81369931835350
H	-0.71916814282766	5.40089452999803	17.33215588679717
H	-2.92526303125050	3.32666701544082	20.42671017332098
H	-2.89049618717079	4.61007176850058	18.27796770542322
H	1.38003927520281	3.68359565742515	20.70848813173521
H	-0.78753004943169	2.86458858924629	21.63836501589898

H	0.46040461087392	7.14155300326195	11.67835565431557
H	0.01814417097617	5.50240842152435	11.20989326596650
H	1.49664398280058	6.31203251232242	9.47934926137614
H	2.67345457899968	6.94677593462733	10.65328510264862

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Pd	3.42684413884050	8.63050198541674	20.84011072013584
P	4.73109854732399	9.69898512600671	22.35071938756460
O	1.94149578315135	10.05277770090060	18.91028265335003
N	4.59453647734034	9.67664383955632	19.40874452567051
C	4.85291367205046	11.47616891835193	21.90638936810509
C	4.92743663052682	12.44910848891869	22.92035070879696
H	4.94351392307049	12.12688798552398	23.96529161950001
C	4.94583536843334	13.81594835609095	22.61323300341692
H	4.98653344117036	14.55429244973647	23.41986807027582
C	4.88692989900230	14.22844647801851	21.27272335872647
H	4.87417224912596	15.29274334272673	21.02002919492238
C	4.85123767510073	13.27534475274218	20.25036868184595
H	4.81830735111073	13.58860635687352	19.20510052017674
C	4.84181572815195	11.89303830028651	20.54125648386467
C	4.30335106959519	9.69867982078670	24.12821013020435
C	5.25900468508680	9.44055728428209	25.12933337215149
C	2.96494979725082	9.96885624886645	24.48612326894816
C	6.46102030253805	9.09514246275753	22.26698027499653
C	8.85591128162997	9.46049734015768	22.03304135749825
C	7.55604798732554	9.97347510821259	22.16205828193013
H	7.38813382797707	11.05469288720301	22.16896578316431
C	1.09103971569898	11.93978991499992	20.13536957604273
C	1.05123275110952	13.46643680977831	20.12362648845492
C	0.77362721332651	14.10632800726979	18.75661216912812
C	1.65721877170196	13.47739428674579	17.67306074008579

H	1.48572462467048	13.95649384303852	16.69053017837613
H	2.72797697850188	13.63036549709278	17.92030264203567
C	1.36571679462299	11.97270795808564	17.59553946567661
H	2.00057758635210	11.45796689543923	16.85284050925945
H	0.31656946013339	11.82404421514966	17.27116242513614
C	1.54296372540409	11.24981597133747	18.93823928533627
C	1.47067782450891	11.38395273293863	21.49077469691315
H	2.45839732859036	11.76283113171017	21.81744426888940
H	1.51242758142504	10.28591725545704	21.46265687114960
H	0.73846322039168	11.68669656336007	22.26203071191832
C	2.13996143908602	7.42875987395630	22.03155066182354
H	2.70912583500341	6.50464589834145	22.20435018135343
H	1.72245545943101	7.88748602107275	22.93360121831302
C	1.49295562634884	7.64139652468309	20.76922918806969
H	0.68474748685228	8.38166531775191	20.66933386277649
C	2.16247743148282	7.21157012577004	19.61084457278822
H	2.81563689029637	6.33053047363076	19.63347144552952
H	1.83259561949273	7.58268292303917	18.63774480053319
O	5.10132394279059	11.51274350023535	18.19832926836744
C	4.82947912009520	10.96063681166710	19.41115370537523
C	4.77434979375197	9.15969396890901	18.03331970769504
C	4.90540016739117	10.46046493216511	17.20540760488046
H	3.98496071246173	10.69679533058742	16.65070724141286
H	5.77340853606343	10.49233650727246	16.53078746106274
C	5.98477756536541	8.18090270230909	17.93881952852625
H	3.84914224970574	8.62836768761151	17.75933704193055
C	7.27202301803293	8.85573972050733	18.45009377852900
H	8.13096362371088	8.17100892206663	18.34108595729940
H	7.18408615139935	9.11734550356358	19.51690733247053
H	7.50882219958323	9.77727106397240	17.88799051506915
C	5.69294395301329	6.92830442329659	18.78723458641858

H	6.56086162548935	6.24507452996411	18.77252892617575
H	4.81904115703464	6.37938015249596	18.39421087067672
H	5.48404906432254	7.19704048652483	19.83701427908787
C	6.15000751161663	7.74853897433565	16.46700864915682
H	6.44082218909156	8.58778016325092	15.81066494602860
H	5.21413695768798	7.31363044631637	16.07103173805063
H	6.93940225306521	6.98096423441040	16.38457369851850
C	6.67917441302803	7.70197159816864	22.25054096490523
C	7.97892042971821	7.19449865153265	22.13195217178659
C	9.06850764074587	8.07376867303639	22.01617369947713
H	9.70316942688691	10.14757012895976	21.94024669279747
H	10.08295913060661	7.67670916074105	21.90820106424078
H	5.82111880442343	7.02386090573004	22.31490194575582
H	8.14108984345625	6.11203775798605	22.11588062396152
C	4.87643961379760	9.45121607883721	26.47962721764431
C	3.54713235223567	9.72603412000083	26.83392582203783
C	2.59319257716683	9.98864776506617	25.83579200042141
H	2.22549898064521	10.17208782984550	23.70536882566644
H	3.25211803504502	9.73412552133242	27.88815529366748
H	1.55520411742361	10.20404034342636	26.10844006861357
H	6.29677466530893	9.23240624777722	24.85184977238956
H	5.62117874823175	9.24582463426776	27.25546781418100
H	0.29352221413227	13.80940646030843	20.85248575535257
H	2.03438866300774	13.83369046089923	20.49995697209948
H	-0.28772441396673	13.94065969232975	18.50294694131315
H	0.93735244167785	15.19913198491851	18.81389220585272
O	-1.52855146613326	12.19614667443189	19.71988759617024
C	-0.79273341506918	11.26333130659616	20.01715567011697
O	-0.80223379427583	10.07372046828146	20.31804731998264

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Pd	3.35678465886014	8.56277040816999	20.81805586452820
P	4.65047785066719	9.66523318011915	22.31658049691421
O	1.92988145602026	10.05734674666577	18.89454607206737
N	4.55896800966625	9.55867440554145	19.38236800762730
C	4.74453536879023	11.43419325154667	21.82298942852871
C	4.77457099056995	12.43785098581841	22.80876567262215
H	4.78900177947522	12.14758255492781	23.86293652281281
C	4.74436897890790	13.79485960953932	22.46060383581079
H	4.74704761896050	14.55711556713188	23.24584025996218
C	4.68690947518021	14.16728370998904	21.10889432973820
H	4.63492449102384	15.22248703988289	20.82560339199190
C	4.69824403953105	13.18393202948610	20.11489938731429
H	4.66251070787718	13.46358948465298	19.06034022430632
C	4.73247682327218	11.81288876165312	20.44864209873460
C	4.22590288825942	9.70841369657971	24.09417480005996
C	5.19201636684728	9.51832941534390	25.10073246785378
C	2.87974269704681	9.94472873872208	24.44633622214027
C	6.39003924970374	9.08874313056361	22.24784903421333
C	8.77866856747069	9.48566503981937	22.00030879936983
C	7.47040569204405	9.98098349968148	22.11260586289298
H	7.28510873755865	11.05902922095389	22.08418782507677
C	0.93599781143564	11.87027412232930	20.12256464699826
C	0.79959261985516	13.39777736403263	20.14958603131245
C	1.12959719098360	14.10725028109434	18.82468510657621
C	0.59066912636477	13.29679824663030	17.64103147792436
H	-0.48577766066044	13.10590724813787	17.79610916251552
H	0.70546778547300	13.84561790231937	16.68726541726015
C	1.34886536066636	11.96556355513722	17.58548760315918
H	2.38807581386678	12.14758067292095	17.23826513646048
H	0.90085776321040	11.25749436202693	16.86403280256801
C	1.46765767843981	11.23105278383610	18.92958700603559

C	1.32556014211840	11.30097615438583	21.47239962181940
H	2.31908837042360	11.67394627583928	21.78599960494394
H	1.36015274944342	10.20351849069040	21.43946389963580
H	0.60240885501591	11.60656029150654	22.25131564459708
C	2.03638908624524	7.38023561058146	21.99636549488580
H	2.60159895430034	6.45661664774137	22.18452030822987
H	1.60405201046754	7.84562486425921	22.88794207949862
C	1.41480237834592	7.59115210294393	20.72202952158758
H	0.61057433746092	8.33457400870356	20.60067081554946
C	2.10816152473270	7.15773161975638	19.57790824798744
H	2.75463613890702	6.27157458539417	19.61002695126266
H	1.79461584555430	7.52907981095096	18.59902280112012
O	5.01314899350028	11.36910235160971	18.11657009540048
C	4.75718463288335	10.84643147261195	19.34393323644607
C	4.73382711572704	9.00859332754307	18.01847922353748
C	4.79777545543377	10.28893796371734	17.15439394439114
H	3.84120244236868	10.49012025286848	16.64831355015429
H	5.63130779599945	10.32770168279391	16.43862678587610
C	5.97078001183061	8.06428015095920	17.93622267756048
H	3.82455164326806	8.43707584908767	17.77502423822802
C	7.24492163342560	8.79246442645447	18.40522547070814
H	8.12212435227653	8.12997498651056	18.30437597229228
H	7.16532031122920	9.08556392548936	19.46466786897933
H	7.44469191498131	9.70158795895145	17.80957752941020
C	5.72328070007823	6.83475615502066	18.83186655580526
H	6.60712810275960	6.17220851108524	18.82663556734095
H	4.85690258357865	6.25143512077669	18.47256452715244
H	5.52439012006012	7.13503130507208	19.87448517133450
C	6.12764730153822	7.58857695808341	16.47719857092180
H	6.38525360445361	8.41413571824620	15.79033791336664
H	5.19923087813649	7.11497908911170	16.10902900128172

H	6.93729153977130	6.84109719116775	16.40786741024933
C	6.63133932300493	7.69968883005138	22.27862157638835
C	7.93941367965666	7.21018945782070	22.17648530082434
C	9.01427304174123	8.10288001627490	22.03038496864106
H	9.61439534911619	10.18323471396105	21.88427265379321
H	10.03519668887371	7.71928492261850	21.93575016516954
H	5.78505018104348	7.00960715566872	22.36736302776995
H	8.11947170742903	6.13065510387324	22.19714533740817
C	4.81183229473464	9.56312155776889	26.45086424379760
C	3.47440358723281	9.80470145556707	26.79930799121351
C	2.51011595527311	9.99938243755943	25.79570720808384
H	2.13268385264690	10.09512937766187	23.66101212171048
H	3.18130520397990	9.83952934066015	27.85352509179749
H	1.46589452948564	10.18862252105049	26.06384434677002
H	6.23571935935122	9.33572732873783	24.82747974828227
H	5.56443505833550	9.41016482766550	27.23119829410714
H	-0.24180461116299	13.63695354524776	20.43274715255640
H	1.45639936984860	13.79883483446770	20.94824954704650
H	0.71438601424487	15.13210317378938	18.83331455029624
H	2.22961393425290	14.21104658433710	18.71417854554133
O	-1.67419573595768	11.98876680126321	19.67830553045244
C	-0.86748474733412	11.10067669401985	19.93959755184720
O	-0.82626549947982	9.89375744476756	20.17958974957207

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Pd	3.46532757359886	8.49396585542160	20.81978164198864
P	4.84499690435096	9.54011257472582	22.29770487754956
O	2.42727148056154	10.84045180048166	19.25273050488695
N	4.70603088212059	9.38065607557174	19.39789983230119
C	4.82047039708451	11.29963943188350	21.80137020098137
C	4.80856293270551	12.29749461104989	22.78807150493755

H	4.90770598970540	12.01345540583215	23.83947399904625
C	4.63204739961030	13.65091545308048	22.45083849254841
H	4.61258360957838	14.41109639681863	23.23788590543448
C	4.47619411162133	14.01024592460646	21.10453916196433
H	4.31751167650718	15.05670125873451	20.82582067278995
C	4.51421098504618	13.03041601806668	20.10644074108117
H	4.40491148874292	13.31279589176255	19.05783777797341
C	4.69398699377864	11.66529232801669	20.42470408697982
C	4.42400502146611	9.55062857817242	24.07911542901522
C	5.37267817869488	9.28102897162794	25.08335012246594
C	3.08881621060073	9.84090290740050	24.43589379373287
C	6.59219220694877	9.00642285220991	22.21456006432067
C	8.96201882684283	9.48499289642515	21.93627059924827
C	7.63686238935467	9.93478657309877	22.04545195592917
H	7.40950665643812	11.00384237285997	21.98947654034195
C	1.30913836138674	12.64370149082361	20.32377618816634
C	0.60271001953049	13.97721138824375	20.24794534917092
C	0.27225509691822	14.41997950795518	18.81356602083166
C	1.48089931728386	14.18625376654775	17.89720260388487
H	1.29750761268550	14.59095170699545	16.88338899752090
H	2.35261036039322	14.73455883850491	18.30811584689517
C	1.80163643947054	12.68608121886059	17.83634804429014
H	2.78029363317233	12.50664927052449	17.35282279949301
H	1.04997258599429	12.16416426450191	17.20857364899251
C	1.84742323280627	12.00560763677462	19.20992217668053
C	1.43847913192739	12.03087501853233	21.68721365773540
H	2.08188371905297	12.64591346048931	22.35132629007119
H	1.90048638406257	11.03203903617210	21.59996695904432
H	0.45457668997590	11.93747814718538	22.19201013375879
C	2.12158280659623	7.34275873738420	22.02801451731787
H	2.59522073602126	6.35198597088493	22.04975647536966

H	1.81913898985458	7.74100344153687	23.00152509813493
C	1.44445916683458	7.78535090895949	20.84917184531294
H	0.73022505971148	8.61418825830231	20.92416120907256
C	1.96227126907609	7.43778422694496	19.57934392267715
H	2.46262630392610	6.47376396448645	19.42349615866517
H	1.59844716622682	7.96178442080727	18.69184584565088
O	5.07890599359505	11.19863324535996	18.10639752370273
C	4.72479306274368	10.69957536389629	19.32574884589292
C	4.91024142672559	8.82066505313889	18.04672330318241
C	4.96478680477657	10.09326529404526	17.16273495167731
H	4.03484288650606	10.23969912208841	16.59099387419383
H	5.83299106461137	10.15217740881334	16.49022103168696
C	6.15073911895092	7.88313229704170	17.98558750053691
H	4.02374481937556	8.21997003066432	17.77524959984864
C	7.41754112399824	8.62693170896475	18.44613797871397
H	8.29296239760927	7.95490487678017	18.40774818515682
H	7.30435988702241	8.98052233569321	19.48348379725127
H	7.63628382999496	9.49891080980046	17.80291879399662
C	5.89025689185658	6.68065037528213	18.91440175283913
H	6.75605502318597	5.99412819427102	18.91355439468432
H	4.99955559384084	6.11357746031784	18.58589430983811
H	5.71915763069559	7.01631094827838	19.95095361740255
C	6.31790402712985	7.37233860398407	16.54035377817405
H	6.55734420131222	8.18927354677150	15.83629826937449
H	5.39639403835075	6.87459777262092	16.18543864074462
H	7.14157228407310	6.63818010733682	16.48812795608769
C	6.88230401790665	7.62801695639472	22.28071888016486
C	8.20738507217054	7.18379684332724	22.17900373249921
C	9.24787846721377	8.11178728216831	22.00069583234938
H	9.77091030463506	10.20929121221091	21.79635920626090
H	10.28148588831932	7.76308171183941	21.90856645126156

H	6.06658005058093	6.90680081459441	22.40234497073759
H	8.42719380400611	6.11255292366425	22.22670981523336
C	4.98692156308288	9.29836813078944	26.43414249605108
C	3.66047279313691	9.59275173263764	26.78607906632640
C	2.71204031981771	9.86895464571489	25.78435895554805
H	2.35463145400653	10.05668675610316	23.65245785785759
H	3.36340840515893	9.60706506350873	27.83961531445786
H	1.67701494154203	10.10132334472758	26.05471971828523
H	6.40935580899177	9.06076178425625	24.81167191736361
H	5.72785603144004	9.08502368833039	27.21136244147079
H	-0.32993640799604	13.93866561417666	20.85150669352966
H	1.22727120978037	14.76009937494869	20.73852620632329
H	-0.58429244015416	13.82756610768505	18.43289458025489
H	-0.04126967691541	15.48094532599930	18.80081131977456
O	-0.60817229354607	10.29832692629781	18.45831679316504
C	-0.98672353222783	10.75481830333590	19.48119705738172
O	-1.46778388557048	11.14110204287453	20.49140089446399

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Pd	3.52668449999001	8.31978219782851	20.44804627983453
P	4.65125262489240	9.50205746266063	22.02885681263273
O	1.93700590880949	10.33705912459520	21.23960646745764
N	4.64415519172645	9.39457713844040	19.03465464398200
C	4.67713933711055	11.26297895839932	21.51524436280866
C	4.64498066533287	12.27056970183244	22.49482150485963
H	4.56549707776908	11.98358720039838	23.54696539369310
C	4.69130594063637	13.62633990299528	22.14336709491401
H	4.64628708614725	14.39043700386937	22.92561686079013
C	4.77617592722624	13.99821099474280	20.79318891695934
H	4.79733786705579	15.05399403851587	20.50793241134578
C	4.82660639752522	13.01069911398854	19.80619999473427

H	4.88999276171322	13.28733419056327	18.75209205499753
C	4.78265963784403	11.64018921247189	20.14608614327901
C	4.11914390828735	9.51117294712928	23.77938766366201
C	5.02851570981260	9.27526547030554	24.82900519516830
C	2.75296039161155	9.74163417908107	24.05693132328790
C	6.43448028299331	9.05604683340342	22.08452819863103
C	8.80455584635291	9.61348230281590	22.00714826156020
C	7.46116286063091	10.01874981682213	22.03925403244266
H	7.20768860713414	11.08289306263704	22.01779493652463
C	1.20743614796723	11.73305601101972	19.43810874988798
C	0.90713301214680	13.15016338199211	18.98634962256756
C	0.27818856925900	14.03884614777706	20.06835366550057
C	1.07842744587606	13.94267239704074	21.37151324262089
H	2.11461540031599	14.28615553334389	21.18744207465087
H	0.65607924845047	14.60690907041282	22.14992407824836
C	1.11290372027888	12.49189183995615	21.86933480705493
H	0.12173517590286	12.20912755502431	22.27904385865050
H	1.83186438962970	12.37131194835088	22.69956986352800
C	1.48605872267432	11.45680062118794	20.79814140409675
C	1.71004647194170	10.82214851318849	18.33756267520754
H	2.60122037088304	11.25850908218675	17.83652804791512
H	0.95210579143418	10.68459610328264	17.54274253929326
H	1.98217809146519	9.83540382558729	18.73990254444269
C	2.33153052268450	7.04308254428499	21.66247362369499
H	2.91758090008064	6.11783973903904	21.74967482785145
H	1.97496265882794	7.46852043516825	22.60522571307093
C	1.61645872580567	7.32902980353870	20.45723464637785
H	0.81591191652097	8.08052315496789	20.46986191759485
C	2.20835315288632	6.97524710867756	19.22494170691107
H	2.85180957580494	6.09055317423230	19.14262377800373
H	1.77570155316501	7.35521157782769	18.29401307655012

O	5.33269155213895	11.19292225526904	17.86410003565720
C	4.89804901296643	10.67497063812313	19.04563068095438
C	5.03220465825842	8.83924453054852	17.71566148303781
C	5.23743740451606	10.12262046139977	16.87609033156627
H	4.37722603231699	10.34866651820833	16.22533550489813
H	6.16613132471664	10.14468166060724	16.28860580308731
C	6.27760356064690	7.90199821166526	17.81394745928711
H	4.18181682105855	8.24949436531165	17.33280293328545
C	7.46722933786404	8.64456488649715	18.45121094081597
H	8.34938754933551	7.98295034873879	18.49271633273082
H	7.23612541778585	8.95553115448437	19.48205736940523
H	7.75305489081731	9.54292625423645	17.87484060570912
C	5.92218812313840	6.66761310279939	18.66496101105385
H	6.80827118162306	6.01921275627389	18.78438761683565
H	5.12416568642526	6.07223814769945	18.18587665118571
H	5.56637999920893	6.96101691543994	19.66902381214575
C	6.64042518482683	7.42649036135073	16.39123615859683
H	6.98341946391175	8.25185366211667	15.74242524282793
H	5.77872184950261	6.93927605802938	15.89908372486774
H	7.46009046209191	6.68864016264379	16.43976777325744
C	6.76944307186086	7.68583538338464	22.10785842731572
C	8.11094376247192	7.28490816776305	22.08877614639193
C	9.13113323163947	8.24923584176454	22.03062060848183
H	9.59732913574954	10.36726866640317	21.96049984897074
H	10.17977164666996	7.93615242606337	21.99958124418857
H	5.96721090904195	6.93978791966489	22.12548472624478
H	8.36124555956244	6.21921807578107	22.10521128699175
C	4.57202496401401	9.26878466416781	26.15607819815246
C	3.21708914579189	9.50183714049659	26.43666057995656
C	2.31360564392407	9.74175653612507	25.38714599872310
H	2.07910635459146	9.94490243050115	23.20982309742745

H	2.86509755054173	9.49633920233795	27.47374868685845
H	1.25647782062969	9.92779486826646	25.60451360362452
H	6.08642853872235	9.09974924525368	24.61192063847875
H	5.27954025138107	9.08395923603911	26.97123690789016
H	1.85597898245809	13.62090784166063	18.63316958786877
H	0.23769539131896	13.11410416650142	18.10588750376201
H	0.22731714594098	15.08638998894453	19.71569985678634
H	-0.75921004931305	13.70162131445414	20.24170261940504
C	-0.83776514707128	10.76024088495393	19.57234917020676
O	-0.65907698165292	9.63049431262749	19.96557919789188
O	-1.57294653602684	11.61606881381885	19.13668557589128

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O	-0.64786619808312	11.08582003401714	20.61191104913627
O	1.54965573026328	10.41051304672881	20.36730689359177
O	2.17107651373272	9.92497116455657	18.03490410004003
C	0.41817084156462	10.86964593237595	20.06424348803383
C	0.44700165856465	11.52693278809816	18.33687825587469
C	-0.96130486752946	11.95523219791087	17.92553392545968
C	-1.79992381299754	10.80758525608624	17.35006199803886
C	-1.05669236983499	10.15764029558407	16.17397454492219
H	-1.66775331984263	9.37686894106596	15.68867256652228
H	-0.84958055408330	10.92547598279557	15.40425497038555
C	0.26369442717950	9.54216352416794	16.66251395879205
H	0.96220857859848	9.31388368478244	15.83524242866413
H	0.07957924207964	8.56743725442938	17.15914796326696
C	1.00123232640474	10.39101756238262	17.66111008378631
C	1.38765974258353	12.72853228089181	18.56973150582149
H	1.46341363909252	13.31665670690822	17.63753293578891
H	2.39824275999382	12.42166511839191	18.87473511582071
H	0.97453770316540	13.38498852175901	19.35315219503054

H	-1.45182235937898	12.38466832674943	18.81512663113319
H	-0.87977777023229	12.76411905842244	17.17205530473261
H	-1.98788849973401	10.05850629392910	18.14305170623970
H	-2.78482963475650	11.18706604270020	17.02657497429382
H	2.22077622324991	10.19566998526589	19.07221340462463

(boat/ax)-TS16

O	-0.71278617403765	11.61607743379007	20.49786878016437
O	1.38959517262413	10.66008291476351	20.34726974005645
O	1.99708262793110	10.03542527753584	18.03131391911575
C	0.33783744319947	11.25181250074715	20.00645538864336
C	0.52413358770054	11.88757475450455	18.24181849926330
C	-0.79489136509304	12.51819995952496	17.77200852583073
C	-1.22910391547453	12.07778457655434	16.36583153262074
C	-1.23210551001929	10.54627308536763	16.26988533524997
H	-1.90330966984146	10.13300062507160	17.04598039694949
H	-1.61785136258460	10.20238738908694	15.29445578744288
C	0.18936701618343	10.00167256481365	16.48029000348582
H	0.79628947026246	10.17478672475108	15.56600494078063
H	0.21047182817994	8.91049021625486	16.64974713249906
C	0.93298994398154	10.67730463557057	17.59865178697712
C	1.63302296745108	12.92638808697829	18.51911421520035
H	1.80607957123101	13.51455814743260	17.59919892919483
H	2.58333345394585	12.46518152916555	18.82398736825419
H	1.31588715914093	13.62321377494415	19.31205570516364
H	-1.57625263873249	12.25362870087146	18.50710932076986
H	-0.69848036808082	13.61738858700149	17.81249017278371
H	-0.54126209990045	12.49368683224568	15.60250861224618
H	-2.23280999483754	12.48084631779544	16.14238906650696
H	2.06094285677041	10.31226536522852	19.05484484080066

TS17

Pd	3.39064050297018	10.59940553854215	20.17689569088060
P	4.87922285154830	10.16120076597504	21.85179833698755
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N	5.90897464649820	10.79864491581933	19.26249966891450
C	6.13676147733202	11.47176978287428	22.17267098447532
C	6.43237280156961	11.85180973790380	23.49824044080794
H	5.96077549135952	11.31196778072147	24.32322669199166
C	7.31768977040399	12.90011178636764	23.77951087210561
H	7.53329386524902	13.16168481383696	24.82072414610706
C	7.92478592880741	13.60610124732020	22.72982263378757
H	8.61221721764791	14.43158337248891	22.93986356295946
C	7.65103489276786	13.24643588010409	21.40761201685131
H	8.11716937581440	13.78102109868255	20.57674260822834
C	6.77258384151532	12.18135427003614	21.11074955962393
C	4.14632114629733	9.89796281077366	23.51788028931163
C	3.22196928665462	10.86812690134156	23.96599617560982
C	4.35989444175578	8.74427136863432	24.29558080793133
C	5.86818992509777	8.63922810168281	21.57444901329497
C	5.87206242825998	6.27092865498498	20.99894140319697
C	5.16945452727568	7.45428819635513	21.26249280149099
H	4.07485467930649	7.47533573376020	21.22482397240507
C	1.32333593773368	11.42910207416013	19.22374308920224
C	-0.02417012737899	11.01852671454558	18.60492228198944
C	-0.04561944946032	9.67927803012912	17.85913745263153
C	1.06020030496920	9.64101831702792	16.79728143053720
H	1.06332797434278	8.67344158383863	16.26248102347125
H	0.86533315386785	10.42589097537802	16.04024929798098
C	2.43594114073478	9.89808150525438	17.44034682600406
H	3.22244753251132	9.97489916997582	16.67194168572376
H	2.69815643723162	9.04021914106549	18.09456692733770

C	2.46183415044099	11.20216319588371	18.26556896971264
C	1.26898446127806	12.83903180726040	19.79615357939029
H	0.97531877698486	13.55499588355485	19.00515185485180
H	2.24979719164059	13.15535388996658	20.18195373471325
H	0.52293372842491	12.90138274198882	20.60866508561969
C	1.26842908214910	10.28108655099468	20.95070064891724
H	1.58648495042281	10.77534215488244	21.88477340586180
H	0.19629185429057	10.50623850179129	20.84048354044648
C	1.46597891903769	8.79890113415047	20.99769402990457
H	1.36866082645424	8.25666480932361	20.04819188559225
C	1.65937591347735	8.08040288712030	22.12689532137798
H	1.74952200625478	8.55619578446446	23.10777543097517
H	1.73877326464473	6.98846040654659	22.09618100949711
O	7.13772420417800	12.66280709272786	18.77998289628221
C	6.56059635113476	11.82980425169131	19.70338048981373
C	6.05114742674143	10.78643272780807	17.78978080719343
C	6.71346823911515	12.15409572773563	17.47784722941105
H	5.99028412060991	12.87180636642272	17.05962246220402
H	7.60916555751829	12.10266850621157	16.83882668921880
C	6.82528604644135	9.52136332599155	17.31973607604745
H	5.04054352216451	10.77332551764011	17.35502428602610
C	8.23315220279990	9.47434792394277	17.94269194102840
H	8.77837372938996	8.57942851851938	17.59332708570035
H	8.16671165947020	9.42150117119555	19.04204745455517
H	8.83706509898539	10.35948800036000	17.67182157235673
C	6.02979503472934	8.27799719825763	17.76269831402489
H	6.54766852985814	7.35301631906596	17.45116815417146
H	5.02117233801317	8.27331198698096	17.31146625694560
H	5.91204583556297	8.25968321918512	18.85617525930623
C	6.91916239916103	9.54703825418600	15.78137476161649
H	7.51271866343046	10.40324994594784	15.41270089062151

H	5.91460894125959	9.60846555558920	15.32358783163626
H	7.40381810209348	8.62614722653680	15.41083910891505
C	7.27377611989863	8.62677077431382	21.60676088572998
C	7.97423462654728	7.44521853090881	21.31882070149977
C	7.27660062196410	6.26585449683185	21.01700372452274
H	5.32199207988860	5.35454558333046	20.75989054424586
H	7.82570530996590	5.34540187344378	20.79293371560775
H	7.81935700539552	9.54448410081952	21.84693291273873
H	9.06929996566359	7.44782334604011	21.33141131918317
C	2.52733640169624	10.68799380412973	25.16838889429776
C	2.73368909341064	9.52511326675675	25.93065300958270
C	3.65229557902897	8.55857728996227	25.49336290640580
H	5.07172552620635	7.98649696940532	23.95591522942764
H	2.17874816902032	9.37421082948460	26.86236406143181
H	3.81964045685573	7.65337561930912	26.08680303879670
H	3.05575224469122	11.76688112749268	23.36003457748375
H	1.81444283455381	11.44775423233221	25.50566285734256
H	-0.82418250974022	11.05376213171860	19.37180411661456
H	-0.26931024784318	11.82243008615607	17.87759590151318
H	0.08483684728067	8.84362703489581	18.56995706239169
H	-1.03685500531056	9.53907083070241	17.39001613525964

(Si)-TS19

Pd	3.46556416613259	9.86917211729575	21.36660816010463
P	5.15481258267155	9.94636072645745	22.83469882288139
O	1.67513987166454	9.87814720093637	19.09963648824638
N	4.90114094813866	10.60528259949404	19.90962466942768
C	6.01247095926268	11.57017998822747	22.63671755033744
C	6.45267857197857	12.27859491668984	23.77098151488342
H	6.27769092315744	11.84974819075060	24.76133948097428
C	7.11895105965345	13.50731306522726	23.65916953803746

H	7.44642069614717	14.03056206044016	24.56361704052236
C	7.37268659500189	14.05079520367259	22.39274781353210
H	7.90073839989540	15.00393777047674	22.29061852856152
C	6.93943734412973	13.36926019054684	21.25035389334733
H	7.12105447364532	13.78683986317848	20.25758653560122
C	6.24735031849919	12.14175221587362	21.34578841571823
C	5.02756664806931	9.72750046689596	24.65383166926349
C	6.08370144279577	9.24763767484060	25.45595372467557
C	3.78305789589902	10.02644453685287	25.24388450078085
C	6.48346575866006	8.75769547816723	22.36692182278957
C	8.77704627901358	8.18861209060672	21.76603819885326
C	7.82741866434305	9.13578529926069	22.18091875640546
H	8.12940508946404	10.17366373945502	22.35093196234572
C	-0.23724438367597	9.51392042525947	20.44591313539068
C	-1.46002795080627	10.09252157350108	21.12729135531506
C	-1.39398295379762	11.61155497551419	21.34635208524866
C	-0.97057081030796	12.32488319381730	20.05518484411476
H	-1.69747689633620	12.08805923055424	19.25318677165718
H	-0.98671642563408	13.42284973484348	20.18404657568564
C	0.43070402956574	11.85680332613572	19.63740888721912
H	0.71893964909662	12.23944108606958	18.64212870062548
H	1.19253444168228	12.25975880156528	20.34315904701791
C	0.61512379950476	10.34230760821870	19.62430319689779
C	-0.30792630487102	8.03351635014949	20.14067117207304
H	-0.50242732683861	7.44027496082697	21.05257555618396
H	0.62846484455015	7.68797323873331	19.67341288892584
H	-1.13504259478441	7.82325887231065	19.43349305147612
C	1.36989503818999	9.51444740906849	21.94345928327481
H	1.37017370079469	10.61382424619906	21.93871340844636
H	1.77716602298060	8.89826929404757	21.11026841078488
C	0.90601747497701	8.84915331335647	23.14499858313639

H	1.04522637979266	7.76038468462799	23.18465347084166
C	0.29304358653330	9.46597026113644	24.18662364466902
H	0.12671837346565	10.54976428198830	24.18676805960002
H	-0.04143562040802	8.91230141425005	25.06881883854570
O	6.32204576559318	12.07738091634973	18.94024762168884
C	5.78292747691791	11.54287859310661	20.08042812101187
C	4.75906085768705	10.33406712244063	18.46273485506145
C	5.59681285955745	11.47312218370007	17.82382585312644
H	4.97317490974247	12.26048907429117	17.36769527759508
H	6.34925784417668	11.13600632806310	17.09490864019018
C	5.21443336125807	8.88543330418773	18.10306690586264
H	3.68486089018484	10.42416350706356	18.22528144254731
C	6.68317444593687	8.65488216436869	18.50398860994461
H	6.98787802858413	7.62234586286315	18.25945880731748
H	6.82146433337469	8.79518466282617	19.58807587118103
H	7.37468886403044	9.33672971663671	17.97545171221942
C	4.31203092587749	7.87553577584723	18.84040967092898
H	4.56882730010794	6.84420698591142	18.53622013667235
H	3.24724253986825	8.06504175045853	18.62410336601787
H	4.44650707387344	7.95564383524122	19.93468197805928
C	5.02941099269748	8.69442201114395	16.58353669251220
H	5.67006192439180	9.37389369030903	15.99187922382445
H	3.97888957464538	8.86843724312178	16.28871039545292
H	5.29546892133268	7.66182013435473	16.29616776865103
C	6.10769410752178	7.41654878583665	22.14047706781393
C	7.05911938068072	6.47125400522584	21.73882463073077
C	8.39601995456590	6.85700213123355	21.54403925242734
H	9.81741125534619	8.49513929155223	21.61376032420148
H	9.13702976959097	6.12171737946526	21.21370563651873
H	5.05759738899687	7.12963114454654	22.26389374190414
H	6.75420566749567	5.43483880609295	21.56045513062544

C	5.89719326813054	9.08606431316822	26.83604233370579
C	4.66029131949061	9.40297404488380	27.42277035841471
C	3.60403489026503	9.87249260166026	26.62558456666259
H	2.95437428915114	10.34754425353997	24.60409948503471
H	4.51762822356582	9.27214810683652	28.50071053294958
H	2.63283683030897	10.10233329027063	27.07605254968037
H	7.04559741995657	8.99969212341502	24.99508476650604
H	6.71825634362600	8.71058716353901	27.45622574506062
H	-1.60169577183284	9.57496952659777	22.09854419013704
H	-2.36184755397435	9.84763315804320	20.52377272647696
H	-0.65877386804047	11.84003853195139	22.14330804630709
H	-2.37176656657981	11.98259280233566	21.70389591055783

(Re)-TS19

Pd	1.64615960673236	5.22024495102225	16.47970994305601
P	2.10561083903519	5.38332613118839	18.66686047773832
O	1.59730641597839	5.29127869032438	13.95590465737618
N	3.68541939610469	6.00882165364830	16.20217138744504
C	2.77128605796676	7.08487160771406	18.94772275117305
C	2.35922715602860	7.82367235958705	20.07385333675649
H	1.64984875034854	7.37068577974335	20.77138362479124
C	2.84585369960156	9.11362161755133	20.32742201913937
H	2.50361523649960	9.65697689718132	21.21440884270167
C	3.77469263814597	9.69449777513814	19.45280904302736
H	4.16839484038179	10.69772874039425	19.64337355281686
C	4.19476311733126	8.98454466079420	18.32361670547315
H	4.90984095242966	9.42850727986356	17.62751945713081
C	3.70117276906442	7.69075501014646	18.04368931979280
C	0.90971455239849	5.15961311566230	20.04453097932583
C	1.27623272813876	4.70951682925991	21.32957609127454
C	-0.44268442149275	5.44252994795104	19.76474347612488

C	3.52587970505210	4.33248153516949	19.19277114247510
C	5.71694780298012	3.99130358192569	20.20806852070003
C	4.64833638848189	4.83916692958466	19.87678962441294
H	4.68919584511685	5.89987115660636	20.14251300364292
C	-0.70903661113652	4.88021287025167	13.60907013844828
C	-1.79850583562818	3.91676833454118	13.17378596155772
C	-1.37885417995501	2.44214926022170	13.23771903699931
C	-0.03822887830948	2.24823176261363	12.51545651136112
H	0.24573640917202	1.18032428281498	12.48059558037882
H	-0.14139543601866	2.58468003655497	11.46489004787638
C	1.05664253575535	3.06528871145166	13.21670517657589
H	1.99919303191209	3.06991638444637	12.63972749828499
H	1.30766503011716	2.59200654241088	14.19235508117320
C	0.68150259866484	4.51488652211123	13.51366760479453
C	-1.08526638182158	6.34026482390678	13.50832014776054
H	-1.96235073128779	6.57062150385628	14.14258826950123
H	-1.36238423156744	6.59470210275152	12.46622655164832
H	-0.23897562884024	6.98169605255771	13.80284413131746
C	-0.50574093475245	4.73398721348546	15.75983331371861
H	-0.09009908698074	5.74252465167352	15.58195749266038
H	0.08610199501056	3.81268470280943	15.69294507411516
C	-1.78231780596130	4.65170511170659	16.44425031768333
H	-2.14417802413561	3.64382377800152	16.69178938344503
C	-2.57906870894177	5.71344414276322	16.73063003723504
H	-2.25572809489744	6.73911707106540	16.51936803624492
H	-3.55914735001561	5.58794424096176	17.20055597570668
O	5.23036146992726	7.66655701188681	16.18303217493419
C	4.16917691211475	7.05552923363119	16.80049849496236
C	4.50731528020813	5.72224780339332	15.00732861231549
C	5.38816298796575	6.99197320304023	14.89580953929637
H	5.03960945552103	7.68513847410619	14.11124218941294

H	6.46306413447177	6.79803770052365	14.76238375611996
C	5.28501577126587	4.37915716891944	15.17142816586255
H	3.81532533766676	5.61825629662467	14.15476824067279
C	6.19271295676795	4.41267341967694	16.41446934689255
H	6.73787596037827	3.45793491122028	16.51527089528396
H	5.59961034210940	4.55550699246821	17.33145926449596
H	6.94551192257155	5.22024715335974	16.35950100421413
C	4.26253419751432	3.23519137437364	15.30701960922280
H	4.78073283333749	2.26786012893285	15.43788682432390
H	3.62293643035441	3.17596699879117	14.41143671010653
H	3.60262971707658	3.39893704551154	16.17655040627854
C	6.12353404879638	4.14704698978277	13.89791607867714
H	6.91059862304736	4.91180757857582	13.76694273189917
H	5.48542739817838	4.15444573498453	12.99544019160749
H	6.62691945860810	3.16527286578168	13.94839354997154
C	3.48662645147991	2.96339143163973	18.85563834644796
C	4.54883207997077	2.11691573642541	19.19643374832051
C	5.67041211940063	2.63089514580687	19.86831016553818
H	6.58940601391729	4.39747084233934	20.73091159983253
H	6.50803721728130	1.97274807349613	20.12156319595959
H	2.62076165517650	2.57449219410370	18.30827880980106
H	4.50880456242813	1.05701775686977	18.92425762528454
C	0.29897861716533	4.55530401866921	22.32352829118785
C	-1.04505471677114	4.85432271463535	22.04506027321229
C	-1.41376574224003	5.29908174270439	20.76484788066454
H	-0.72780630810837	5.74913770560022	18.75275752785278
H	-1.80534285919296	4.73119074505978	22.82370100881086
H	-2.46205856337624	5.51951704220406	20.53734469664913
H	2.32465421539120	4.48047700007426	21.54624920428641
H	0.58722991455842	4.20119820470478	23.31921475569565
H	-2.69704285463053	4.09761174439967	13.79666981046726

H	-2.10400946912433	4.16328317937551	12.13319452422398
H	-1.27206701621520	2.13091940461615	14.29608838082101
H	-2.16496831169863	1.80370087827700	12.79507304353185

(Si/chair/ax)-TS20

Pd	3.84257460521667	10.46200030588772	20.67075436643298
P	5.15074034163713	10.15540810514023	22.44989358148340
O	3.10449122326373	11.10540713618474	18.73383187122506
N	5.84104531506366	10.78626216728257	19.66415109109233
C	6.40986318662365	11.49163600998721	22.59047962762167
C	6.71682422964359	12.04545318851498	23.84936121116300
H	6.20191758410556	11.66365854261842	24.73492008858182
C	7.67509072661005	13.05776618909766	23.99055088860824
H	7.89438558298250	13.46131444642498	24.98454035117295
C	8.35744999100930	13.53799269390182	22.86256948398570
H	9.11203179215067	14.32442565264521	22.96182636562786
C	8.06577304234885	13.00824271948597	21.60222109516002
H	8.58223739357375	13.37829443471840	20.71372535693700
C	7.09404141793846	11.99557597485309	21.44104759074771
C	4.47514479813729	10.01649408498777	24.14915082829500
C	4.90739045080366	9.04920912519858	25.07773803637211
C	3.44234466375550	10.90972550080610	24.50663230633511
C	6.19029542302571	8.64574104111240	22.27853065557956
C	8.32212207053690	7.46608060877630	22.31920856089274
C	7.57839807602744	8.64027827139748	22.51455931926415
H	8.07733357196175	9.55767031783308	22.84136153335676
C	0.88636924621206	10.92433996852201	17.97358995934897
C	-0.35250497908573	11.67131799174944	17.49039565174745
C	-0.65337466383279	12.96706441495538	18.26385197996850
C	0.61409879139738	13.81639296880220	18.43802216049653
H	1.00255549452595	14.10471944398356	17.44117647855183

H	0.38461961013094	14.75587126803808	18.97421913413459
C	1.69022936022627	13.01569230648428	19.19003126954549
H	2.65114576969032	13.55754838041684	19.24166668484575
H	1.36966394196727	12.85589376641623	20.24273678516854
C	1.95194401964328	11.65649774255665	18.56198722310843
C	1.24369971788827	9.68062124272109	17.18569062379161
H	0.34785135653868	9.06384708940188	16.98870009423725
H	1.97977754912762	9.07570288425797	17.73671398114214
H	1.68764089912940	9.94423269215636	16.20571411840790
C	1.97995551424616	9.99043034672134	21.56835818584344
H	2.27504508408442	9.33148410062073	22.39883360717235
H	1.57104379778184	10.94641581615323	21.94185872745719
C	1.20753320361223	9.36862043951070	20.53106867229126
H	1.43547267909753	8.32307376391354	20.28400190467620
C	0.22286470620963	10.03201990852669	19.77898145302082
H	-0.20639528570615	10.94379297084639	20.21273301917761
H	-0.49507347432973	9.42165325119865	19.21830890218480
O	7.70735402531856	11.95524235298889	19.11611308360739
C	6.82458843816749	11.52867208669833	20.07380180945096
C	6.00170237925380	10.55066214014787	18.21280281103999
C	7.15565812499212	11.51510437144334	17.83698124274905
H	6.80683245334326	12.41245487571676	17.29844119185316
H	7.97769986227431	11.04789514174991	17.27374738516654
C	6.25997159415831	9.04286903872788	17.90763591380394
H	5.05350058107962	10.84098597742140	17.73124894497424
C	7.49998144665082	8.53204749400017	18.66392303280958
H	7.67519822345439	7.46604056528939	18.43635155343050
H	7.36214836253402	8.62341059270417	19.75291686086506
H	8.41523401893656	9.08554073829311	18.38378840056377
C	5.01874592008928	8.23644334593780	18.33502313167518
H	5.17039827794867	7.16041938571676	18.13366252912862

H	4.12302877614314	8.57772334224015	17.78952498466234
H	4.81413185620666	8.36689778224057	19.41158947170407
C	6.45205590061290	8.88219978223940	16.38547314945966
H	7.35738938507715	9.39791225610909	16.01676639824987
H	5.58168142946780	9.27880830319676	15.83155730512140
H	6.55728026995629	7.81347868903979	16.12772874347014
C	5.55551924218644	7.45855655031138	21.85765497066307
C	6.29785227830335	6.28496713831961	21.67608903859047
C	7.68469808580988	6.28865019089804	21.89943948632574
H	9.40334170633804	7.47349295584421	22.49300312790627
H	8.26807865874872	5.37561151820832	21.74161781951342
H	4.47882059562402	7.47216971085428	21.65635776451643
H	5.79633528111831	5.37028095240347	21.34351483996044
C	4.32162749818138	8.98589598305703	26.35063244758296
C	3.30538648461203	9.88696100052709	26.70625692807196
C	2.86842497231517	10.85126943140725	25.78309331379914
H	3.09636306714269	11.64514044448267	23.77203228602484
H	2.84903740792217	9.83366078032276	27.70019750765648
H	2.06985055518909	11.54981724844311	26.05378061296737
H	5.70408672893973	8.35136333434521	24.80241273274088
H	4.66229480830661	8.23184365038084	27.06813086331798
H	-1.22988158897917	10.99493691410892	17.52676898919124
H	-0.21370820011031	11.91466999070673	16.41462979114665
H	-1.05964475087292	12.72013348770468	19.26364707405090
H	-1.44082198141107	13.53971118096474	17.73992763593413

(Si/boat/ax)-TS20

Pd	3.76869537525428	10.27319818716468	20.64439814301653
P	5.11978872630579	10.05401310882865	22.41819867835826
O	2.97838551614558	10.48197399659644	18.54482319759419
N	5.77485852510456	10.71710713504038	19.61276609970989

C	6.25892629611481	11.50467556028682	22.53317357245155
C	6.53017525352799	12.08800614943564	23.78705440517035
H	6.06088992909580	11.66555564198550	24.67910475775591
C	7.39428831698654	13.18337401711339	23.91827783050221
H	7.58364343198725	13.60747351668726	24.90988878508611
C	8.02084102399408	13.72029863579018	22.78436748197058
H	8.70135786995868	14.57264123778296	22.87456601304301
C	7.77172249789041	13.15701368523697	21.52940372592120
H	8.25170206151234	13.56303921073674	20.63618600975213
C	6.89428439806343	12.06020349767682	21.37978918799655
C	4.45547745263040	9.91115408513791	24.11997464076119
C	4.80593179029328	8.87158083349988	25.00400225204298
C	3.47626075766294	10.85220954500574	24.51424167092435
C	6.29309458020006	8.64298150467809	22.28827070141134
C	8.52385551815821	7.66391459609970	22.36334019046537
C	7.67449581776910	8.76772383144708	22.53391328065257
H	8.08524706119302	9.73119325336250	22.85031686366611
C	0.80258254197707	11.29248089765533	18.09027832513407
C	0.01092154740104	12.49174600695100	17.56202532628815
C	0.45886836314928	13.83345061821096	18.15958585268406
C	1.97424929596174	14.01789916063923	17.99582173400571
H	2.30040467188244	14.98697504884486	18.41667658967954
H	2.22614044253991	14.03876092414379	16.91697791541377
C	2.72224864799469	12.86276966876082	18.67781927025053
H	3.81114297949520	12.89553738085934	18.49683231475390
H	2.59890528591919	12.93106882813653	19.78647292168731
C	2.21084057016619	11.48262705223343	18.32494709895360
C	0.41447743362790	9.96963139316230	17.44445855186219
H	-0.66247369451079	9.76068917619246	17.57836311128309
H	1.00136401109072	9.14504822097716	17.87801632432027
H	0.61451840726999	9.99467309735664	16.35612350476063

C	1.85974044578169	10.01123094175865	21.54296149914493
H	1.56924929310350	9.01630971433542	21.15924757917581
H	2.08537031058119	10.00018671319497	22.61876762957162
C	1.06747939203665	11.09971029119650	21.07566617509504
H	1.17819293086548	12.06626601650494	21.58805588942757
C	0.18018454262636	11.03297712950621	19.95842459844542
H	-0.60461976957079	11.80144827995450	19.94005791977186
H	-0.20884988629736	10.02454548506809	19.76431062312445
O	7.54371117771319	12.03017751443384	19.06283893587714
C	6.68217220618794	11.55064442958448	20.01618678696289
C	5.98452488933169	10.45518030926084	18.17340596636465
C	7.06984455741747	11.49412166099165	17.78883586173763
H	6.67027031379727	12.33799758605587	17.20095354855752
H	7.94357479071932	11.07126706910230	17.26972265535413
C	6.35637745387368	8.96261837822868	17.91689091343847
H	5.02572552364290	10.65487016680667	17.66749112992749
C	7.62343168864114	8.56917238746027	18.69800392746182
H	7.87445663125713	7.51038335901303	18.51165621669669
H	7.47088607679976	8.69030844513371	19.78203245102719
H	8.50043381059189	9.17420224494946	18.40225687200304
C	5.17387392442681	8.07959409111499	18.36235824809887
H	5.40651018004336	7.01301761850377	18.19005136792996
H	4.25392464085700	8.34035246598980	17.81297984335090
H	4.96193608629487	8.22179524806859	19.43627783597091
C	6.57625670047919	8.77216666897685	16.40219987293358
H	7.44008030247795	9.34985291442712	16.02525473109969
H	5.68208022908742	9.07871615857564	15.82937754518553
H	6.77190755670103	7.70856392634661	16.17833539202048
C	5.77412615205207	7.39516255235262	21.88292837850841
C	6.62179670152323	6.29084369082463	21.72932729324559
C	8.00061730881164	6.42539946180884	21.96123413226875

H	9.59835614137625	7.77338927789768	22.54458559939009
H	8.66649944563902	5.56717443782996	21.82366208836471
H	4.70250540473672	7.30708273434019	21.67294691718699
H	6.20845816470079	5.32853408741872	21.41012408220724
C	4.19565184079683	8.78145175289799	26.26366522490287
C	3.23511280488528	9.72768852046665	26.65511387678221
C	2.88002830276856	10.76657007591665	25.77889815042247
H	3.19767864001387	11.65743243990262	23.82467792343534
H	2.76074469436789	9.65387120934768	27.63915553919178
H	2.12784061490932	11.50467279768127	26.07633344908101
H	5.56121007540278	8.13836939802239	24.70546566973286
H	4.47713506098202	7.97149173176049	26.94506364116355
H	-1.06795013342348	12.32539327615485	17.75030160766938
H	0.11811600508708	12.53151041669169	16.45719802602602
H	0.20724564614465	13.86063788329527	19.23805944877611
H	-0.09253157405542	14.66423833712910	17.68224060655954

(Si/chair/eq)-TS20

Pd	3.81254152170841	10.45397295902255	20.70394067169945
P	5.14419424991107	10.13497059393073	22.46526215438384
O	3.10503758114228	11.33013509736117	18.79638310016697
N	5.79616194962513	10.73672794211603	19.66797880030888
C	6.39894882359945	11.47769645550886	22.57662777372864
C	6.71727716024658	12.04877732546332	23.82513737909934
H	6.21644492994868	11.67302760441915	24.72138495127216
C	7.66968968612490	13.06943803441526	23.94283238873579
H	7.89871714108096	13.48554582567102	24.92946219850553
C	8.33458738516469	13.54196930899504	22.80099623025529
H	9.08467792257930	14.33476687186333	22.88210461768816
C	8.03029286902716	12.99672338115317	21.55034453273175
H	8.53177391060709	13.36149056685706	20.65109286649833

C	7.06413496843898	11.97528825458336	21.41242622423443
C	4.49374200260464	10.00313391029924	24.17519584365045
C	4.96225616827021	9.06269774316547	25.11407192095504
C	3.44117123835215	10.87368444031034	24.53073097711859
C	6.19018051741421	8.62959692565986	22.29342587994615
C	8.32883649971475	7.46117712874260	22.32222563404649
C	7.58092684409758	8.63323290816509	22.51441674797542
H	8.07834862109326	9.55630528794948	22.82728056724692
C	0.92037191864094	10.99395371131276	17.98871138514417
C	-0.33698675598462	11.68938771012111	17.45457334856903
C	-0.34877751826562	13.21055617866549	17.69288548726078
C	0.09327082608121	13.53796867750277	19.12582469918027
H	-0.00606183564817	14.61881845752389	19.33461767784727
H	-0.57907657091317	13.02154796608179	19.83776486048747
C	1.54879581568841	13.08556073699306	19.34283015182051
H	2.25307159299704	13.86314124121898	18.98762772092044
H	1.77515222705322	12.95024086206461	20.41887007503007
C	1.91991164112978	11.78799280629678	18.63455163383822
C	1.41374098563397	9.81634550518630	17.16958706303115
H	0.57731870785311	9.14904639169543	16.89336232099576
H	2.15961281197428	9.23974072675914	17.73738488639480
H	1.89184282830025	10.16061358170564	16.23222271942563
C	1.94278398843058	9.97366147742411	21.57073767803397
H	2.22348737162242	9.30012046614036	22.39411982185092
H	1.50156609393157	10.91351213960504	21.94711192056092
C	1.25762190705422	9.37604616944019	20.46556488961019
H	1.51643853500362	8.34284107956522	20.19976058380685
C	0.28381219985567	10.04615077558392	19.68315329919726
H	-0.21338296053782	10.90470170525018	20.15391064766241
H	-0.40706403538644	9.41694389182594	19.10705207014940
O	7.63792578019060	11.92236436590813	19.07593388560737

C	6.77771106017851	11.49461883020019	20.05392781250936
C	5.93724177892913	10.48539756755026	18.21754815431341
C	7.06227517571965	11.47127590744204	17.81112042784969
H	6.67965659927377	12.36095981949052	17.28290332398177
H	7.87897531798394	11.02144487027496	17.22650141445267
C	6.22892793149321	8.97940616979025	17.93240030221785
H	4.97516830776791	10.74928807973365	17.74776266065972
C	7.48908406312749	8.51171552408572	18.68352835755298
H	7.69558830511716	7.45016076682300	18.46146078610121
H	7.35611985851426	8.60617446884443	19.77268140300956
H	8.38428616792003	9.09193185306266	18.39331673124952
C	5.01338453747351	8.14939288924694	18.38777385125679
H	5.21093509393368	7.07030174577551	18.25471819532317
H	4.11631602753830	8.41420242141807	17.80246770800739
H	4.78160352118363	8.33622340477473	19.45045231489363
C	6.40955271641723	8.79609808771353	16.41146898991615
H	7.30504000001638	9.31688565521097	16.02653191006403
H	5.52953013105279	9.17282231737982	15.85877364692218
H	6.52601392563664	7.72465280901188	16.17017110590958
C	5.55777815027946	7.43509765202702	21.89058256901798
C	6.30424997501543	6.26369981812123	21.71172653284318
C	7.69336354050111	6.27649518219943	21.92022284331193
H	9.41177903903941	7.47586827959293	22.48460900707499
H	8.27983721060347	5.36500701943296	21.76481780433751
H	4.47881171028382	7.44097204275614	21.70131911463254
H	5.80399495006456	5.34322670558561	21.39338000532138
C	4.39263328782290	9.00405540032209	26.39441027136516
C	3.35650542107974	9.88332781897624	26.74776608594900
C	2.88346186539022	10.82067013494516	25.81469876579504
H	3.06743722620434	11.58672183554890	23.78758326152001
H	2.91291438771420	9.83365311768104	27.74767482002492

H	2.06951953989534	11.50196192834698	26.08377139833523
H	5.77444994579007	8.38216577272566	24.84047075953048
H	4.76138798513300	8.27094538603333	27.11974181358308
H	-1.24166085491268	11.23939501641513	17.91354035637984
H	-0.42310169365214	11.48539911479901	16.36938813579335
H	-1.35561299043410	13.61756226665066	17.48598394699619
H	0.34677323944805	13.70003713048820	16.98279312532470

(Si/boat/eq)-TS20

Pd	3.96549297738227	11.26125830786814	20.96653476464072
P	5.17754523730177	10.30181252618874	22.56396341662964
O	3.32364734683133	11.68026878411266	18.81155895438335
N	6.09864474380148	11.21717084571306	19.92420630204229
C	6.75193843180013	11.19484128215419	22.92139494391649
C	7.21778588584019	11.29439706267455	24.24770215301646
H	6.64236258224856	10.82050961829430	25.04699022294013
C	8.40059171170668	11.97607528491892	24.56319023834351
H	8.73523692251383	12.02786587655297	25.60445463021081
C	9.15121495472300	12.57872143659632	23.54347476602800
H	10.07641785829111	13.11526923946920	23.77584429986356
C	8.71360680987319	12.48797218019319	22.21921773718545
H	9.29085638844708	12.94827770676529	21.41470536252446
C	7.52323289206190	11.80341364975142	21.88437137673311
C	4.45617494156906	10.02166651583792	24.22689798637180
C	4.24681396801748	8.73539155359724	24.76237202634741
C	3.99555748926115	11.14875041974229	24.94532975527921
C	5.76741974893315	8.63505713802320	22.05248372103367
C	7.50814259564765	6.96121837410877	21.72619787978470
C	7.10778199911268	8.22519208122874	22.18598574820636
H	7.83913879394938	8.89853289703266	22.64288383944915
C	1.18070176787813	10.67766848190986	18.62605666067529

C	-0.05016893281923	10.50438771944954	17.73244380910818
C	-0.07963368749963	11.45488848943164	16.52226703646898
C	0.31563180209485	12.87723670833983	16.94023116641056
H	0.20671400179070	13.58346942884048	16.09689950136307
H	-0.37514149367253	13.22911192942303	17.73015257856806
C	1.76397838106222	12.88639642684283	17.45889333070090
H	2.47463469083252	12.95254894832627	16.61163982737535
H	1.96458460065821	13.77769769747592	18.08554656493935
C	2.15943311736106	11.66571289732031	18.28543646943873
C	1.66299377757619	9.40568518948993	19.29339104185885
H	0.81682008681033	8.84678415585322	19.73305069386907
H	2.39943773975540	9.62779757387124	20.09104359026108
H	2.16333659317926	8.74244805804432	18.56298980570969
C	2.21708764430060	11.68253746001963	22.08146942930248
H	1.83947177932411	10.71656980247585	22.45465512557599
H	2.62577870711302	12.30738902845006	22.88936597081260
C	1.43082333847147	12.34759530195070	21.09870921961474
H	1.66887494031311	13.39992656997728	20.89288968614539
C	0.45905815819383	11.72052801735596	20.28212476953341
H	-0.24088396014246	12.37072986131815	19.74502232763953
H	-0.00764620057362	10.80523075495030	20.67127328844735
O	8.06696441452881	12.31198053730450	19.60230604423731
C	7.15686339748840	11.74698942115463	20.46073326542354
C	6.24545957186807	11.30066982162942	18.45220543751519
C	7.44955941762437	12.25838137671331	18.28081479227442
H	7.14474702174906	13.28488248479819	18.01300345611870
H	8.21987007847363	11.91028556418399	17.57620188971573
C	6.42915586532358	9.88111717298686	17.82992445957586
H	5.31503472952998	11.73413710025503	18.05196403939519
C	7.65163673331702	9.16554774387350	18.43510043539861
H	7.78234713694598	8.17325572916602	17.96829226519271

H	7.51677052753461	9.00939818809328	19.51816992503718
H	8.58793290439343	9.73228840762915	18.27923318374472
C	5.16005918854813	9.05467318530994	18.10807955934942
H	5.26171165588376	8.04068539579252	17.67995864286691
H	4.27240610215330	9.54112749222292	17.67285995229843
H	4.98783225432507	8.95912993854752	19.19059012327780
C	6.59710457065900	10.03705119769282	16.30460321799850
H	7.52237651257261	10.57684493100719	16.03257713608601
H	5.74124669406679	10.58171091255367	15.86569705752912
H	6.64601949896900	9.04316568077660	15.82532948774856
C	4.83288493177779	7.75781860960444	21.46272617555673
C	5.23106168184634	6.48844000191847	21.02405860893588
C	6.57247278627155	6.09085138686327	21.14669638378875
H	8.55576196102018	6.65674025269115	21.82189605925749
H	6.88835269415945	5.10635974815843	20.78633794356853
H	3.79672478881786	8.08937693893433	21.33428893279950
H	4.49722499098569	5.81755135105159	20.56560934962004
C	3.59173829270166	8.58034057215153	25.99312037382697
C	3.14564862142023	9.70431356125002	26.70518917281495
C	3.35455752087485	10.99044060443642	26.17995193934760
H	4.15904509030427	12.15195766935388	24.53695369183374
H	2.63541175247768	9.57990272482212	27.66589111807594
H	3.00905218115339	11.87225833260277	26.72960356665450
H	4.60051057729717	7.85635741592950	24.21563977327927
H	3.43618441324566	7.57546663869879	26.40003135157723
H	-0.97406273010156	10.63945309446047	18.33312682374718
H	-0.08326520469397	9.45628674575876	17.37567745832255
H	-1.08151227614261	11.44200107072555	16.05521500441635
H	0.63528851930910	11.09572771695703	15.75570988304371

(Re/chair/ax)-TS20

Pd	2.34452071384657	4.78801334207330	16.25591422665224
P	2.14500505482831	5.26814777886733	18.43914554275776
O	3.17782550270889	4.40861760736970	14.26407130459803
N	4.10919860017617	6.21202666442933	16.45899457541355
C	2.19711251344383	7.09913475484243	18.67906234712807
C	1.32776583434737	7.71346929952222	19.60236261609159
H	0.63521949354608	7.08909675286807	20.17249950224478
C	1.33860746198362	9.09867225209913	19.81426476751889
H	0.65051260494761	9.54023710791400	20.54262415361113
C	2.23635674427813	9.90814408429235	19.10327836940111
H	2.25646930402200	10.99077053410183	19.26205671499544
C	3.11269805966046	9.32226177800739	18.18512204302198
H	3.81814837768448	9.93864340238405	17.62358884569600
C	3.10742392937445	7.92870527592326	17.95396947445706
C	0.67603765547052	4.76092911784785	19.40945707175941
C	0.75900509650557	4.02055306597296	20.60541943934939
C	-0.59636788583575	5.06038380817863	18.86997698639956
C	3.56533075586309	4.69719945796609	19.45913374993427
C	5.35986504952096	5.05689600424373	21.06864256954388
C	4.24669075039017	5.53674800101424	20.36191336613284
H	3.91009151712231	6.56790346216796	20.50490877491158
C	1.71499897348486	5.38447596626345	12.67305010339055
C	1.33289042389042	5.41142684470593	11.19397558025802
C	1.21237736432684	4.02080891639756	10.54801558206902
C	2.43184634835855	3.15050326409896	10.88523240691314
H	2.35209531763043	2.15929421471672	10.40189866196474
H	3.34552159317395	3.62935309113676	10.48071083719428
C	2.57543675207063	2.99412305387321	12.40892424015160
H	3.50709042413722	2.46922998210946	12.68243051212560
H	1.74244661319989	2.36677866556363	12.79769130584446
C	2.55555682827235	4.32743264747851	13.14039144159152

C	1.89387963283909	6.74317120685201	13.31822609340553
H	1.90476151591589	6.65455154933970	14.41940734666361
H	1.07988768247280	7.43062032185403	13.02484736667888
H	2.85316671633122	7.20445425786309	13.01115432784069
C	0.51370194454720	3.81296931849349	15.86086349623625
H	0.77269889875683	2.84604736022842	15.39618870479840
H	0.04821679477822	3.69342679738385	16.84955220620771
C	-0.05397370298995	4.79196117182426	14.98400271650247
H	-0.45808624887757	5.70683805881591	15.43965967852616
C	-0.03829767779716	4.71030380131909	13.57349465918458
H	-0.67266274473764	5.41788930129101	13.02415036659512
H	-0.02831638925304	3.70495242290993	13.13501797826892
O	4.98963407754436	8.30334614905990	16.50348287242819
C	4.05740539889260	7.40833758223784	16.95924418526863
C	5.26831031409973	6.13704533923107	15.54347957972317
C	5.71112437310620	7.61736055195025	15.43341281284786
H	5.41228360177738	8.08498706582477	14.47976574559821
H	6.78464310873818	7.78890173544295	15.60440776407096
C	6.34684023415977	5.14671401410646	16.08006707106736
H	4.89512509841517	5.74845227087206	14.58218187073456
C	6.83093727731166	5.56448884580351	17.48107122480416
H	7.59520628962899	4.85698202369247	17.84763171960750
H	5.99799099643659	5.55832724406542	18.20253197099504
H	7.28443047737038	6.57291949220343	17.48360071613112
C	5.72913459189671	3.73628180996896	16.14605030207821
H	6.48012394137423	3.00645956085084	16.49946595903669
H	5.35103199426381	3.42057905640612	15.15981006891384
H	4.87369653503549	3.71913201460063	16.84101772334841
C	7.52474445107197	5.12974187278224	15.08462944089906
H	8.03848196266096	6.10646018196067	15.02107315592984
H	7.18268920393642	4.85561255421770	14.06998777307950

H	8.27677314010613	4.38493520307868	15.39984880528502
C	4.00614964653718	3.36834610887534	19.28506932593437
C	5.10726993094843	2.88695208952531	20.00459394108100
C	5.79212441400925	3.73360080928849	20.89176402823907
H	5.89126612508414	5.72071972953174	21.75879728328385
H	6.66432077730343	3.36335498952676	21.44044905707971
H	3.48711424060439	2.72470478041098	18.56605240182442
H	5.44316305659494	1.85523342297657	19.85807849963956
C	-0.40957044147316	3.59479104814399	21.25373403906099
C	-1.67006632224565	3.90619442877717	20.71964950653912
C	-1.76075910932556	4.64431570221205	19.52802057295873
H	-0.66548945521635	5.63402217952236	17.93893963484984
H	-2.58005207828340	3.57193050262779	21.22854311407923
H	-2.74051016101344	4.88728544480843	19.10374001086799
H	1.73960357972210	3.78396700350649	21.02908807930223
H	-0.33429055329362	3.02266357077420	22.18461398050211
H	0.38786897044769	5.97553476583105	11.06355162298711
H	2.10391142420666	5.99692054983783	10.64789028792429
H	0.29581300503790	3.51768060805493	10.91089098917065
H	1.09881168811256	4.12641193080762	9.45330080879850

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Pd	2.32398592005340	5.06052641930654	16.27857514494454
P	2.12014638135394	5.53842091160195	18.43508967297818
O	2.95043860610861	5.28317599317048	14.15520303320822
N	4.21880193781758	6.32548961526115	16.52311115498875
C	2.40426630695724	7.32462369856692	18.78111102366464
C	1.57870302159045	8.00635241708804	19.69771267683709
H	0.77819359526021	7.45665461944335	20.19965429957702
C	1.77233623403216	9.36268728257806	19.99024933020917
H	1.11720870672669	9.85969942833554	20.71323281328702

C	2.81101935899951	10.07151758221268	19.36797901524912
H	2.97441364668853	11.13018616809366	19.59210924396716
C	3.64060251273438	9.41763474709151	18.45227981453430
H	4.44885745948248	9.95782655374880	17.95424222957024
C	3.45249708361139	8.05334277774618	18.13832605170386
C	0.57202392825792	5.16105818027747	19.34206305681558
C	0.54536422708043	4.47476927669382	20.57136147667988
C	-0.64358392667679	5.54437334807671	18.73449663287751
C	3.42834412275808	4.72147082295798	19.43985866983319
C	5.21239335027516	4.74351013380576	21.09928633428533
C	4.19016454403324	5.40828412585105	20.40439269858275
H	3.98962260030196	6.46545361138572	20.60277276513375
C	1.00319687060236	5.29164802559874	12.80366402316288
C	0.42963159301902	5.16134431359641	11.40021444135488
C	1.16528860891157	4.15236396552177	10.50168372911045
C	2.68687943027396	4.32356991922753	10.60758546773804
H	3.20876500421161	3.61291823279564	9.94019975883140
H	2.96598726144068	5.34153028520292	10.27066700714981
C	3.14100818263837	4.12988990168305	12.06264003251944
H	4.21656404037816	4.34833198527447	12.18746688672288
H	3.00397535684007	3.06821510422819	12.36557597457134
C	2.36633243875589	4.99573900515859	13.04517048087660
C	0.32586425588860	6.31215654729901	13.69110678562564
H	0.60338909881025	6.16689401109130	14.75237726105298
H	-0.77432565653419	6.25484051557178	13.59808116178768
H	0.63116135986190	7.34059468367777	13.41407622825226
C	0.74253340921125	3.66418278494787	16.19259069183150
H	0.95067488200933	3.01935244904859	17.06205317637301
H	-0.20281606096611	4.21519564605761	16.32355109033424
C	0.93490680147035	3.05896047385001	14.90724888111356
H	1.74016933258800	2.31732176371266	14.81317358732951

C	0.25581577701703	3.44796265956066	13.74804608355071
H	-0.70605734209859	3.96285473510927	13.85827825775876
H	0.34402632362616	2.82303697701126	12.85372704329855
O	5.44345648704669	8.21631440253047	16.79885947538760
C	4.35101890353356	7.46036210410177	17.13722950934450
C	5.37540483602498	6.13780108638759	15.62315028277659
C	6.09975647420803	7.50748873819443	15.70264866048781
H	5.97283262407724	8.11449614361821	14.79052715602729
H	7.17019745499671	7.44508556259605	15.95253704998406
C	6.22722416813712	4.89876224732406	16.03729022867672
H	4.96579021351170	5.94640300376159	14.61761935007721
C	6.72776622530836	5.03253659517890	17.48717711764078
H	7.32012611953241	4.14550032230521	17.77222336620735
H	5.88221274073740	5.11015166881868	18.18904440815864
H	7.37341383746921	5.91951530450405	17.62471103675400
C	5.35676958810942	3.63373965352345	15.90169037056370
H	5.94713168159419	2.73275336617387	16.14980633712480
H	4.96058861715070	3.53382470832634	14.87691478601076
H	4.48676751191650	3.68028370348868	16.58066094138474
C	7.41752177879366	4.78635216709517	15.06264213460839
H	8.10438724063594	5.64934204679588	15.13473106011526
H	7.06774270756610	4.71360327171040	14.01657513277138
H	8.00709805086048	3.87941827762879	15.28525502340806
C	3.69381264652542	3.35853911906084	19.19120533478605
C	4.70396922850762	2.69354253425926	19.89721496085492
C	5.47114751596078	3.38762420386823	20.84746690732082
H	5.80937212661895	5.28870320170521	21.83795508136482
H	6.27285246916089	2.87284313688244	21.38702209912590
H	3.11389844811768	2.83268771101539	18.42525610574081
H	4.90489528660648	1.63682587383774	19.69289975240419
C	-0.68117076142323	4.18166858941514	21.18662804089857

C	-1.88581167228279	4.57727466784582	20.58515189670149
C	-1.86488400773042	5.26394496984850	19.35942372635049
H	-0.61804040867608	6.06504634814608	17.77067567741048
H	-2.84128501357792	4.34654137982140	21.06759766866064
H	-2.80271885717270	5.56929312063806	18.88383542040545
H	1.48474225064723	4.17427421244400	21.04522960940523
H	-0.69452790615825	3.64558686492760	22.14152947125929
H	-0.64566694666652	4.89665479109418	11.46461664006928
H	0.45428923514264	6.16282788056422	10.91717080375866
H	0.90122395591157	3.12010423603765	10.80278834751069
H	0.82773456387592	4.26836108600611	9.45526383918876

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Pd	2.14206334577778	5.06781302995360	16.29796780948247
P	2.06867316928344	5.40491038821191	18.51711345122051
O	2.92574608046495	4.66841482230981	14.25444391530394
N	4.02282125481153	6.31392347611547	16.49671440614190
C	2.29677848249869	7.20655873713805	18.86822271873905
C	1.53121398391623	7.83007265989307	19.87330895136770
H	0.81132373651858	7.23130845586528	20.43702248835736
C	1.67792608816458	9.19133866318898	20.17331853755234
H	1.06634719547901	9.64066176665063	20.96267535657416
C	2.61269871699570	9.96528001854075	19.47130866875803
H	2.73885414664855	11.02847301576927	19.69806322361349
C	3.39038745971534	9.36829885849459	18.47446982215687
H	4.12473894069513	9.95661156688483	17.91993470066576
C	3.24666898633788	8.00008887167000	18.15443945133742
C	0.58607533557363	4.97429135457705	19.50266373031785
C	0.62482443408612	4.11488466119766	20.61883323961178
C	-0.66343521794220	5.45653047401708	19.04719394922128
C	3.45894835959039	4.64943099881639	19.45627113029385

C	5.32745362836051	4.74979393018927	21.01843458727637
C	4.24053971556590	5.36821513224690	20.38207574666954
H	4.00236708128808	6.41386420511948	20.59855538418725
C	1.54582619794691	5.76011112117355	12.67150213408296
C	1.16487307161060	5.78629678580097	11.18452865375435
C	1.61931694535526	4.53597883395009	10.41007088916073
C	1.27750962641524	3.26399564467293	11.19768406601760
H	0.18774424319566	3.24439075501579	11.39118054153161
H	1.50383718892051	2.35674992096019	10.60848654975018
C	2.05842337802747	3.24465873189461	12.52537115908593
H	3.06569334535973	2.81046849575517	12.37529482853919
H	1.56492596132010	2.59240762859232	13.27397009316159
C	2.25427048703552	4.61452072402508	13.16497726563923
C	1.92996838137416	7.09883019603128	13.27235834680160
H	1.95508912372123	7.03965867656367	14.37444763319108
H	1.21396907277803	7.88532729863605	12.97271060786416
H	2.93588344977277	7.40894885371488	12.92788560395899
C	0.20314789700834	4.33847753002852	15.89385062942224
H	0.31439956357602	3.35234164337208	15.41111013533001
H	-0.27589733746332	4.27197095401514	16.88095637296032
C	-0.18955553996547	5.41427334331612	15.03799249441055
H	-0.45235300118411	6.36999770254119	15.51194662044877
C	-0.20592015893791	5.35605256879165	13.61826203043821
H	-0.75218980598613	6.15928264615963	13.10641558692136
H	-0.38733166815507	4.37176720547404	13.16758177391952
O	5.11109203875297	8.29774909226437	16.66315041794027
C	4.10651784774569	7.46690131100973	17.08601487743511
C	5.15239235183105	6.19094092080770	15.54930854066058
C	5.71603055688954	7.63202423612840	15.51059036902293
H	5.40855113945298	8.18768142839656	14.60797567000644
H	6.80729470165402	7.70311130318561	15.63131729907648

C	6.15567344428999	5.08752418554994	16.00808724074486
H	4.72832599647708	5.88782798346859	14.57861195792637
C	6.71092059527797	5.39413579933851	17.41173865211376
H	7.42399490817510	4.60919841421780	17.71903258553908
H	5.90133741059098	5.41769947247927	18.15907006243526
H	7.24565380491819	6.36110210180167	17.44892778698520
C	5.42506232652026	3.73084090750456	16.02823279503524
H	6.12093319068637	2.92797512223188	16.33272511320805
H	5.00176261690793	3.49095227604946	15.03928021834405
H	4.58517716190651	3.75256300182755	16.74161501494472
C	7.30192886622332	5.02117751164305	14.97814220570866
H	7.89585585000202	5.95288963668285	14.94518890901548
H	6.91149917444223	4.82736380648243	13.96245134202756
H	7.99514515536627	4.20085966318516	15.23538491235742
C	3.77418786864799	3.30051857457227	19.18797169586099
C	4.84857444270589	2.68042492529299	19.83835880131188
C	5.63361129063307	3.40714471966832	20.74866015528040
H	5.93715404260205	5.32048109630066	21.72695830398873
H	6.48550921871547	2.92859072639084	21.24277248602767
H	3.17871408120221	2.75119263284301	18.45012797390478
H	5.08576731043682	1.63421616136188	19.61932458639433
C	-0.56227946489491	3.75102925589131	21.27094108662126
C	-1.79806537873601	4.24294250648644	20.82130133937294
C	-1.84497616799790	5.10103292173791	19.71023997723298
H	-0.69947278457742	6.12627192135273	18.18055136879822
H	-2.72263779700558	3.95675894233989	21.33317861816999
H	-2.80531221396910	5.48656966137400	19.35222019131295
H	1.58668607341167	3.73703907198334	20.97821309157436
H	-0.52011864994862	3.08552142400942	22.13980139194825
H	0.06749805032926	5.90388381114277	11.07035263010392
H	1.61031780855954	6.68835749427395	10.72172975552823

H	2.71494638506097	4.57757890407183	10.25021438738574
H	1.14987140115873	4.52021472731621	9.40933090341591

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Pd	2.23666039766097	5.34699513524838	16.31565547199435
P	2.11255854251032	5.73295845299891	18.49684388415117
O	2.86987025831257	5.74949407546947	14.15656642989168
N	4.26105648125475	6.40716522757900	16.59272738174846
C	2.57510611998604	7.46220625341664	18.92792885046936
C	1.82620791325401	8.17762838499319	19.88393922098695
H	0.97906421989580	7.68547459281343	20.36886589003212
C	2.15403824799997	9.49316983183677	20.23681121989032
H	1.55560996756850	10.01729552046690	20.98925441015260
C	3.25359702449248	10.12532771747460	19.63701154583584
H	3.52202556422481	11.15100009568933	19.90846081010691
C	4.00856942032370	9.43748118371324	18.68232226036051
H	4.86249310599904	9.91913376678506	18.20071506289435
C	3.68477741293256	8.11490798432998	18.30674838283091
C	0.55046013009944	5.45946173179352	19.41815317392956
C	0.48331283119452	4.75296028459901	20.63459719166141
C	-0.63705596878412	5.95407707519542	18.83640057281248
C	3.34936650587613	4.74213517261760	19.43354541606779
C	5.15280644245620	4.50300053268981	21.05492574639390
C	4.19137668075891	5.30012738334103	20.41446712910277
H	4.10067921263723	6.36055630887507	20.66839634048100
C	0.87236296360818	5.93007638492859	12.90039033785780
C	0.26833147870617	5.98833206774771	11.49783080418396
C	1.26726348876958	5.63848535881917	10.38007015219981
C	2.09218733729186	4.40032109482243	10.75632258666004
H	1.40705539289322	3.55139260598223	10.94299449042863
H	2.74702216712557	4.09153272346418	9.92091113890656

C	2.93151995456773	4.69012849131574	12.01318284548004
H	3.87523379239437	5.20062682688364	11.73745290931362
H	3.23596587843757	3.75210434386997	12.51914287308531
C	2.23596639757292	5.55172633109640	13.06325488768497
C	0.29369619065454	6.91011283574394	13.89904917228883
H	0.58550315231088	6.65165794324678	14.93489908272724
H	-0.80945373137252	6.93752902736756	13.83336662240236
H	0.66834360421673	7.93357611819565	13.70259487219629
C	0.55361548871433	4.08365381151072	16.15670330692204
H	0.71913228025844	3.36783934432056	16.97782457912711
H	-0.35826085536274	4.68034066225011	16.31851395745363
C	0.75882440528711	3.58941940519821	14.83135298020723
H	1.52761582314927	2.81747351657417	14.69167119813198
C	0.11724428293386	4.10106343317833	13.68469309262333
H	-0.85334764337975	4.59459114111586	13.82491230061713
H	0.18873190450352	3.52211687666561	12.75760870152635
O	5.67392297602475	8.14644167245688	16.95564404583652
C	4.51202761794584	7.48704036768551	17.26544630968102
C	5.38368301498659	6.15651932844972	15.66591327552271
C	6.25209092597127	7.43356834982669	15.81934638431023
H	6.19393020524925	8.10056826674443	14.94291728480994
H	7.30914330058335	7.24194744240791	16.06116080191978
C	6.10103668789051	4.80968955052186	15.98709525744491
H	4.94646411745503	6.07531009932604	14.65688136328979
C	6.62328353450658	4.79357378816293	17.43524011481601
H	7.11797637275860	3.83125530403800	17.65482831544918
H	5.79642745598304	4.91680785005361	18.15246845131323
H	7.36246152380682	5.59491017927329	17.61954178127014
C	5.09800788336791	3.65739626765531	15.78153065556358
H	5.58663357198353	2.68335242237294	15.96681057819653
H	4.69324062979564	3.66585967864626	14.75487100411140

H	4.23840550139933	3.75540313119446	16.46893364852637
C	7.26544675828981	4.63488621758356	14.99065893662908
H	8.04165940293589	5.41277215438980	15.10954550956002
H	6.90279248677167	4.66974103476757	13.94707423752765
H	7.75560617674791	3.65736368710757	15.14554141184713
C	3.47349916924880	3.37382139792662	19.11361866464428
C	4.42277042264433	2.57700962437380	19.76542895785283
C	5.27046724641180	3.14253241739493	20.73241473379132
H	5.81284113177654	4.94835332084046	21.80680449796408
H	6.02489100789534	2.52414026500505	21.22970987833258
H	2.83213090547634	2.94767339052649	18.33482890782496
H	4.51360544170130	1.51718531727929	19.50588804996121
C	-0.75493750276130	4.54983296850124	21.26242156793267
C	-1.93057772381177	5.05602364936391	20.68671997153993
C	-1.86910990751161	5.76319516988141	19.47409894675291
H	-0.58021668001721	6.48868362993945	17.88155344041290
H	-2.89537780765296	4.89525664560002	21.17894834842365
H	-2.78473755800686	6.15451696060267	19.01854185084714
H	1.40094105522346	4.36644246243512	21.08843948382204
H	-0.80019485782524	3.99722220215422	22.20690311412961
H	-0.61148170453128	5.31356833552831	11.43442134041020
H	-0.13184889015819	7.00708002988422	11.32639822881395
H	1.95530972180549	6.49254996045449	10.22285010054402
H	0.72987212170495	5.48138840341985	9.42678126455568

(Si/chair/ax)-TS20_[des-*t*-Bu]

Pd	3.77726341166022	11.13947603769249	20.96181065602216
P	5.14490392907383	10.38692000407568	22.56722654686595
O	3.00495702677183	12.07643037635980	19.16381810166962
N	5.72553724142902	11.21500035595590	19.84414586916806
C	6.64291004528538	11.43767843925343	22.74599534735242

C	7.14081808829936	11.76686388071261	24.02279171387375
H	6.62182055046926	11.38761499878103	24.90722673511651
C	8.29119579443777	12.55067277603232	24.17924599284654
H	8.65714862302919	12.78027358578953	25.18541782496343
C	8.97643541354271	13.02485564773769	23.04930198216462
H	9.87909205345387	13.63335740783256	23.16140604944125
C	8.49636556829501	12.71989720369148	21.77285506378454
H	9.01187861038225	13.09095537847733	20.88407947723758
C	7.33223625761755	11.93870727704128	21.59742734992666
C	4.59411111615936	10.11053015400699	24.29235722031097
C	4.81993108488260	8.91404854512222	25.00065357279543
C	3.84377462420983	11.14358061228647	24.89742446350366
C	5.86996369491302	8.77368050340554	22.05553974734638
C	7.66699256744281	7.12964591867375	22.03059813302250
C	7.16099866714425	8.36957897208962	22.44815733342861
H	7.76919761902126	9.03064657986503	23.07437474496595
C	1.29185104708956	10.77431933305395	18.17418897050957
C	0.06319172130543	10.79269461573234	17.27187486951292
C	-0.89058454195797	11.97210317994145	17.52864315642622
C	-0.11729462870117	13.29476931262491	17.63126254867861
H	0.40380628780581	13.48876184497560	16.67284777575756
H	-0.80976256849825	14.14147224023960	17.79331000944286
C	0.92027708815435	13.22458666204293	18.76482096056963
H	1.56685068215675	14.11895989439305	18.78420367770785
H	0.39810000935082	13.20016805960350	19.74701823490669
C	1.81658401029976	12.00000131119217	18.66249825961660
C	2.25978392034687	9.63528277927873	17.94674113442590
H	1.72298445389697	8.67741050763898	17.82033569602859
H	2.95565512401727	9.54455466722938	18.79962284371830
H	2.86709220530327	9.80046808179310	17.03481751114774
C	1.92384259114286	10.89843800643912	21.93308220866446

H	2.17128067034776	10.58398377224939	22.95697377117379
H	1.42429696229644	11.88258193447061	21.91158521766905
C	1.34905082832590	9.89761916468562	21.07614770610111
H	1.70683466468569	8.86552924398085	21.19518564588697
C	0.42048268587624	10.16326549143832	20.05935501873106
H	-0.20281915543081	11.05838040728702	20.16138948342403
H	-0.08389911394215	9.31470162180521	19.58245082795649
O	7.73674273737623	12.07032078575441	19.22558629277441
C	6.86929146287325	11.70527944489691	20.22543122065438
C	5.73608630709035	11.13888674506944	18.37091074209703
C	6.97173304015850	11.97219142336197	17.98039758969586
H	6.71341968954446	12.99942935484308	17.66746686687915
H	7.62509743246884	11.50761186221887	17.22716728627212
H	4.78095416397234	11.53506128629869	17.99594190677388
C	5.09562970244529	7.92931739041401	21.23542417237439
C	5.60198343372915	6.68900537156926	20.82324736561139
C	6.88817622004705	6.28828127614984	21.21982109982851
H	8.67268624385419	6.82147027653954	22.33571616367436
H	7.28678175621616	5.32232447116642	20.89212235420063
H	4.10567779781266	8.27145724016225	20.91196922742489
H	4.99563276954622	6.03833498054481	20.18430972633979
C	4.31963780483899	8.76240769945213	26.30230501300813
C	3.59330372811142	9.80056645089011	26.90679590435254
C	3.35802554608467	10.99309192036742	26.20273724692323
H	3.64751624389637	12.06263228060809	24.33302493542498
H	3.20326311877542	9.67779508874122	27.92251921398667
H	2.78289639858608	11.80147277126742	26.66606444712298
H	5.39022817711557	8.10590476394402	24.53296630764622
H	4.50029239475964	7.82973910592788	26.84720770661669
H	-0.48490234748309	9.83362723162589	17.36480224987926
H	0.40893396470484	10.83115888498864	16.21565488888694

H	-1.44715590901675	11.80427312844947	18.47035735269803
H	-1.64681438505785	12.02263186427883	16.72358976427028
H	5.82356557615823	10.07584011349078	18.07715350072062

(Re/chair/ax)-TS20_[des-*t*-Bu]

Pd	2.19064953466682	4.83534195740050	16.21542871685454
P	2.06378364648871	5.31148294707797	18.39422245731392
O	3.07785252550368	4.44312776344476	14.25532200068484
N	3.87739959101435	6.35158015019458	16.33668223859273
C	2.11119295018585	7.13153518268150	18.71755524706772
C	1.27669857489287	7.71319165921945	19.69140449992296
H	0.58708170244491	7.07379368402376	20.24878731794104
C	1.31894549423552	9.08707363162847	19.96811655750338
H	0.65740929145781	9.50512781762975	20.73409968216297
C	2.21399052238721	9.91445586144789	19.27548926795804
H	2.25880310896909	10.98717466939002	19.48728078766795
C	3.05601598804100	9.35909252747327	18.30671804717928
H	3.75968067156913	9.98937467691364	17.75810452159276
C	3.01488190740473	7.98000640827040	18.00842360832690
C	0.69432467343506	4.71431158407063	19.45024809428974
C	0.88761957954738	3.81400668192981	20.51705129848256
C	-0.62366878545342	5.06929169444354	19.07887387216403
C	3.59297175297027	4.76608255821372	19.26854869881083
C	5.17965864241444	4.89433517403543	21.11209614986306
C	4.00111639013452	5.33327802275696	20.49208045364296
H	3.39783685143331	6.12268223489265	20.95283935215611
C	2.16774349290312	3.02526157644265	12.60950856123139
C	2.36169889750862	1.74873993274533	11.79520107289835
C	2.92697444210918	0.56497698150388	12.59901197718432
C	4.13727925248525	0.99522106806630	13.44074071041956
H	4.55225930428943	0.13477831246776	13.99797991372840

H	4.94038648336846	1.35812955397594	12.76910921079969
C	3.73652656345766	2.12178448044266	14.40735987951640
H	4.60754310551599	2.53144010379229	14.95023707269814
H	3.04833048743889	1.72172122559574	15.18461143740724
C	3.03377674409999	3.27644968434171	13.71040472380671
C	1.68931960644826	4.22718281282308	11.81833984433891
H	1.43185061515722	5.05409146963073	12.49745390860512
H	0.80723637531782	3.97422176585835	11.20200348988298
H	2.48113885021791	4.58573637739930	11.13172361643648
C	0.48550428929852	3.59033029977270	16.04941804883656
H	0.82101698095299	2.60982541191660	16.43363942944532
H	-0.21828537020367	4.07326091381586	16.74409374392535
C	0.09696485412829	3.60355013571500	14.67098631633325
H	-0.47328571803224	4.47050662130854	14.31162505173941
C	0.45756986768727	2.61278362034845	13.73845695061203
H	-0.13700619876260	2.53470320916581	12.81986648233624
H	0.77605306456006	1.64376457196721	14.14476322591542
O	4.94282199709871	8.33850603151003	16.60784514461967
C	3.92567252363189	7.48705405568761	16.96284910550045
C	5.04291296784727	6.28295986586913	15.43680666764267
C	5.57786741390529	7.72862633408989	15.43673832634245
H	5.26035246580369	8.30417168942621	14.54905638815649
H	6.66627873970748	7.81971037691988	15.56696084042175
H	4.71720794336218	5.90920072046247	14.45578192728689
C	4.38071774755081	3.76443030238872	18.66874024942813
C	5.55839567791179	3.32614672632899	19.29114060532977
C	5.95848434240034	3.89055458592530	20.51277591438140
H	5.49395163600092	5.33935477178725	22.06218405701700
H	6.88085734216294	3.55255269684015	20.99694139321972
H	4.05803188559762	3.35426532431633	17.70367582325018
H	6.16707827543651	2.54745841693624	18.81939109973331

C	-0.21509921343755	3.29478033840502	21.21097354170923
C	-1.51947709474442	3.66784315553257	20.85088029252626
C	-1.72095970797546	4.55920195725826	19.78408687843739
H	-0.78080400490171	5.75916291576249	18.24174194797147
H	-2.37772208785746	3.26078623123871	21.39531365968638
H	-2.73599305535479	4.84896331749992	19.49299427964149
H	1.90256657358661	3.52453067119332	20.80494650497430
H	-0.05303758966249	2.59844357465991	22.04064293895412
H	1.40060651906750	1.46273300203057	11.32310722001867
H	3.04835079100435	1.97503055458891	10.95099059289612
H	2.14591506689949	0.16255602888965	13.27236074979426
H	3.20042997468512	-0.25666366926135	11.91150547206252
H	5.76276226658368	5.55693300747920	15.85998084072197

(Si/chair/ax)-³TS20

Pd	3.95175004860422	10.21650056965823	20.46108233447719
P	5.16095978715724	10.17835956493851	22.34649131334572
O	2.88206069334796	10.40325203886559	18.55675761325373
N	5.77634326924770	10.72658516209045	19.55988654318050
C	6.24532702544647	11.60529858102105	22.46855532248183
C	6.50183150162623	12.21267800251195	23.71908417294051
H	5.98041563109490	11.83612468542099	24.60419897896879
C	7.41856584449240	13.25598397902914	23.85318014127378
H	7.60259614074734	13.69986947426537	24.83622095755899
C	8.12336356447320	13.71591332949539	22.70816650304605
H	8.85355822645482	14.52650870920291	22.80319750402183
C	7.89014552384781	13.14654733237517	21.46598589328498
H	8.42425338413922	13.50646636966700	20.58305716050896
C	6.94212700721271	12.08984050734798	21.29092783799182
C	4.28880298942784	10.05423084887479	23.94667832356003
C	4.41591433139598	8.93943101592569	24.79666284505254

C	3.39303325226735	11.09146432654517	24.29013328017701
C	6.25537260477079	8.70402385110545	22.27726009531749
C	8.46417572067458	7.69454644607318	22.42513757407309
C	7.63327413367854	8.81999168954988	22.53776569270850
H	8.04733743343474	9.79449022469444	22.81419010337840
C	0.66533832888282	10.97869312136870	18.04754965749222
C	-0.39948788406216	12.04788382039356	17.91943811357477
C	-0.19817146424397	13.26301658962462	18.83998620828500
C	1.26014235268042	13.73930223316423	18.80058755883094
H	1.52299150885691	14.03273725111708	17.76518154884944
H	1.39926194722040	14.63656571962569	19.42994474294915
C	2.19951007385861	12.61609695277900	19.26786099514862
H	3.26333728388923	12.88065359980973	19.13406647907955
H	2.07453593665882	12.43535360529844	20.35738480771534
C	1.95709338421312	11.29486471669141	18.55885310891522
C	0.51264363439430	9.76056906308279	17.17335765814016
H	-0.50889935066265	9.34374224963174	17.23209559545882
H	1.24258261178968	8.98739996128032	17.45465753603065
H	0.69206138315976	10.02529691604807	16.11176259613055
C	2.16110071299558	9.47252550930460	21.49623461002076
H	2.54882346000866	8.59900334017467	22.04159129814026
H	1.91299446913357	10.29681917918482	22.18370349957899
C	1.14924411525187	9.16337712653015	20.52310821666983
H	1.21943011169013	8.18350527626967	20.03008084836534
C	0.13129419926025	10.01840970132311	20.09730120209688
H	-0.04914068030446	10.94768665164981	20.64873137988962
H	-0.72710036603871	9.60944669369282	19.55767459602130
O	7.55099836267234	12.01781596109445	18.97011928057943
C	6.71316000254079	11.57865002856093	19.97629930847912
C	5.98458038634724	10.42968488743021	18.13018559108101
C	6.98989957479338	11.53527091238546	17.72406551229929

H	6.48777543997116	12.38003462674180	17.21687380712832
H	7.82747638461500	11.18731949441689	17.10047947810780
C	6.45609615772352	8.96210182513150	17.88118279251531
H	5.02182442222294	10.56248275396056	17.60584630771744
C	7.73334240775929	8.65629687810585	18.68365046940621
H	8.06312787890386	7.61781755166384	18.50349581255468
H	7.55086118732627	8.77082065363927	19.76396526132229
H	8.56625142274011	9.32660254461621	18.40398967055907
C	5.32867549788580	8.00299871378166	18.31067663214240
H	5.62885971666138	6.95300062929521	18.14020410202302
H	4.40090341823412	8.20214457035896	17.74599691361750
H	5.09746763094586	8.12577890786655	19.38300565421180
C	6.70619636172289	8.77348515483894	16.37058297792091
H	7.55229035168772	9.38191524295730	16.00387463932423
H	5.80991262607325	9.04338617588336	15.78172494198750
H	6.94525328604503	7.71732612411074	16.15320655627476
C	5.71665811375339	7.45526392557550	21.90632187967107
C	6.54657869594765	6.33058652076691	21.81109696777487
C	7.92324044315546	6.45119691226551	22.06390685198383
H	9.53813513588554	7.79211584453040	22.61495747986248
H	8.57478323324507	5.57584338773987	21.97256154930420
H	4.64845797210555	7.37706575905287	21.67676585719792
H	6.12212147212751	5.36283032426870	21.52429519175285
C	3.66635669074443	8.86916772152288	25.98059685001087
C	2.78820893430546	9.90824713502853	26.32472972746771
C	2.65660837238827	11.02256215763797	25.47855198636866
H	3.29028298131224	11.95445929398117	23.62281223985427
H	2.20439985068237	9.85014380775094	27.24914720923467
H	1.97158208196959	11.83516078230355	25.74210436401790
H	5.10690811309367	8.13295705646829	24.53422030086207
H	3.77474688138962	8.00098114010756	26.63914541350011

H	-1.39783024539658	11.59679313211943	18.08524586120986
H	-0.41037399286721	12.39204503636254	16.86103853211677
H	-0.46232967706857	12.99231083095600	19.88010175439121
H	-0.88638145581968	14.07408960801811	18.54116182618109

(Si)-TS21

Pd	3.34691054258442	8.66207409685199	20.56775318153323
P	4.63295132224564	9.70815344300554	22.04141194950066
O	1.69696935396556	9.61352238202612	19.16750792284658
N	4.54687239874108	9.59076274483560	19.09964236039351
C	4.70356400000331	11.47632766232928	21.53000482719263
C	4.77446001830440	12.48254021853765	22.51128698360713
H	4.72486819656692	12.19694587641411	23.56608636743767
C	4.91799377638443	13.83375226795785	22.16557769716199
H	4.96522241081779	14.59560760450871	22.94971785019788
C	5.01261826626987	14.19531476875725	20.81031038898402
H	5.13613550410353	15.24475007716558	20.52521898375146
C	4.94046820600850	13.21631604099938	19.81882916715641
H	5.01462397197677	13.48996438819628	18.76457822560749
C	4.75445079056577	11.85019307664109	20.14696248380400
C	4.19577581674109	9.75844991482283	23.82244184663922
C	5.16489447315778	9.58317874440760	24.83064752474191
C	2.85062626162931	9.97945411145279	24.18744518653092
C	6.40323485605210	9.20423968423552	22.05238476204153
C	8.78278961262409	9.69173105403420	21.88698657167686
C	7.45196176723748	10.13558645381248	21.93143644110484
H	7.22333212853982	11.20333890309534	21.86126272679759
C	1.87105354842702	11.93386445257248	18.66050598810433
C	1.70405794072949	13.37690308953145	19.06411696680711
C	1.44900851386461	13.61163783379855	20.56219095965714
C	0.51062904621625	12.54108817128179	21.12800117755158

H	0.29046748538303	12.73504294525424	22.19521532917227
H	-0.45717772553655	12.56144737557903	20.58929033065086
C	1.17015941221388	11.16760212491503	20.95555023504302
H	0.50386425215636	10.34709540510933	21.28003020699757
H	2.07085316624588	11.12175444060919	21.60316789694473
C	1.60246850662128	10.86937213426149	19.52067382772150
C	2.13950355152527	11.68520706007354	17.20504341740020
H	3.06802462297549	12.18725202253318	16.86470072326393
H	1.32106142699095	12.08471443520425	16.56932673029824
H	2.21644369996173	10.60146887528393	17.02067343991217
C	2.09817537890796	7.60332739151587	21.84315785275549
H	2.70191055368064	6.98109738826258	22.51984953877326
H	1.36391454189160	8.22376266454482	22.37042604094608
C	1.67962236034292	7.02913906966528	20.57307619208767
H	0.81689953190176	7.48636349258468	20.07582193507765
C	2.45937681270153	6.14842143786627	19.86344646690971
H	3.32951008344527	5.66308465597459	20.31866006025416
H	2.20577354849731	5.86737541915751	18.83716815797614
O	5.21225405659471	11.35071737616391	17.84456132426952
C	4.77517197943854	10.87955513658713	19.05129621849179
C	4.89465028562773	8.98611808461385	17.79638523846770
C	5.15832020909970	10.23116893826881	16.91153090151795
H	4.34700880495655	10.42632776740706	16.19535452688793
H	6.12311715185807	10.21134024039567	16.38322237552049
C	6.10535168195011	8.00486930028709	17.89368274153066
H	4.01337972112644	8.42627517342028	17.43711617374306
C	7.34449038656992	8.72185253701481	18.46073192553473
H	8.19130857662617	8.01792494036519	18.53584718758421
H	7.14447596617547	9.11293167940537	19.47000959086402
H	7.66907464951301	9.56385386616249	17.82329697136617
C	5.73326879236083	6.82639466422045	18.80975333537127

H	6.58700878870055	6.13192231311594	18.90848922550703
H	4.87455073495209	6.26485323910636	18.40167211813128
H	5.45273331716838	7.18203421458522	19.81553045739645
C	6.39924305702577	7.45563810273650	16.48188055419006
H	6.73045837895171	8.24359194202276	15.78203174816060
H	5.50613815334151	6.96839426429984	16.04920759767156
H	7.20441435939652	6.70141361326710	16.52951967138576
C	6.70033826397587	7.82849696433317	22.13468056271854
C	8.02951630284318	7.39003859788027	22.10251267643270
C	9.07346021980164	8.32178514156883	21.97127884449194
H	9.59386652874271	10.41970693159157	21.78074894739544
H	10.11212778230561	7.97810146179096	21.92858296195152
H	5.87781513759545	7.10818072982094	22.20843755224208
H	8.25201694919507	6.31983316634695	22.16546195025951
C	4.79099715488506	9.62643369473778	26.18250926670905
C	3.45348227961892	9.85228973842763	26.53913870190123
C	2.48462812750376	10.03228014716542	25.53748975761889
H	2.09777840653313	10.11660334526629	23.40680202019872
H	3.16474131533361	9.88708974223527	27.59468943582824
H	1.43865355817655	10.20906243041073	25.80852967012502
H	6.21047086235520	9.41556998552997	24.55711395858690
H	5.55104160944841	9.48640772396040	26.95832284869693
H	2.60803838361786	13.95162071993392	18.75766647765776
H	0.87504460762216	13.82771597034826	18.47122203733139
H	2.40582804961747	13.56202158603106	21.11215511967979
H	1.04287147573117	14.62808912950847	20.72085040357035

(Re)-TS21

Pd	3.33407118412520	8.78733699473262	20.75919452205932
P	4.66221183876787	9.70607668218595	22.27081046085963
O	1.68029420741475	9.63823236112423	19.27150894632712

N	4.49988073403770	9.85490261240162	19.34560028026575
C	4.74037333869129	11.50952686291124	21.93697201811089
C	4.87397120145891	12.41509766753227	23.00601892373755
H	4.90464468700635	12.02523610389240	24.02778934468090
C	4.96312915169100	13.79668165457161	22.78664608271773
H	5.06255955499814	14.47933686740952	23.63609554794277
C	4.92203575834461	14.29131192335951	21.47184655516694
H	4.98891332031906	15.36761043651294	21.28391897024909
C	4.80380661843693	13.41179569569493	20.39382720716040
H	4.79946336024199	13.79154563799278	19.37020202586294
C	4.70239426281789	12.01079011758831	20.59446383061063
C	4.28225867546215	9.57823946347955	24.05864871840456
C	5.25831315688440	9.21618548067394	25.00734048197906
C	2.96331522715416	9.84485531666211	24.48455868803847
C	6.41425422914832	9.16150346770256	22.14834255305169
C	8.79674404713347	9.61515427022937	21.93777749316628
C	7.48033017330768	10.07863183814757	22.08686311253568
H	7.27537340603573	11.15196123766052	22.14337191490922
C	1.56645348644157	11.89434081671323	20.09259060336309
C	1.49540418615768	13.37276329474844	19.80302473117164
C	1.12962346103727	13.72494938683583	18.35154225695875
C	1.88069621053682	12.81783463171361	17.36919472442203
H	1.66652757528622	13.10609789613366	16.32216628299723
H	2.97050565773461	12.93718365686003	17.52289665594161
C	1.48489043056574	11.35673511140515	17.61858451407609
H	2.08310763126922	10.65556701273276	17.00952404325973
H	0.43342503137764	11.19745900069021	17.30115983685374
C	1.60252426618664	10.92512184657996	19.08516081898894
C	1.44735742541066	11.49347853100746	21.53041734901866
H	2.34308477430601	11.76741714883408	22.12906509233743
H	1.30619582956023	10.40390051208331	21.61604246305652

H	0.58813030328467	12.00408772949045	22.01256329995813
C	2.18630732230469	7.59294883718620	22.01567171218554
H	2.85165794335105	6.92442956658257	22.58208731063519
H	1.49174594584067	8.14606764252066	22.65952015571600
C	1.67498405104078	7.12402379824140	20.73714226673473
H	0.76604510361649	7.59893806896508	20.35112736033001
C	2.41250946416358	6.33883792025051	19.88595929820959
H	3.32660130194406	5.83707496629668	20.22192320324016
H	2.08352895083177	6.15343274806103	18.85969065491049
O	5.01389176044100	11.75825829624350	18.23483993044312
C	4.68195977257543	11.15071143680464	19.41557873363089
C	4.74790331193731	9.40032909944347	17.96081475309835
C	4.95030437540613	10.73662327873450	17.19868802782355
H	4.11240530359470	10.98629503292026	16.53060758070905
H	5.89518103670721	10.79260654448370	16.63694971340528
C	5.95560634300093	8.41775164168902	17.86751761253026
H	3.83855750663365	8.88147089705192	17.61137829384287
C	7.23034641463237	9.06275672886277	18.44218764648684
H	8.07691440470716	8.35699087967350	18.38102206273219
H	7.09111311612002	9.32963478265233	19.50134144542949
H	7.52072075191904	9.97623021136692	17.89222733556586
C	5.62517619470407	7.14284758709754	18.66332938216150
H	6.47393580856972	6.43610722640224	18.62983656569005
H	4.73552078512839	6.63755665992387	18.24785796626704
H	5.41188585087223	7.38314392927422	19.71833931772158
C	6.16181358999641	8.03640953982887	16.38695150969238
H	6.45869200863617	8.90064795883289	15.76599708474692
H	5.24007076686341	7.60589257797689	15.95419824201674
H	6.96127122319275	7.27982294270043	16.29770413376574
C	6.67954293633962	7.77920446808813	22.06783629152291
C	7.99519687810164	7.31969777243792	21.93206897322187

C	9.05587399279589	8.23855025289882	21.85946997511989
H	9.62090511719575	10.33353918060220	21.87730032083745
H	10.08308960430528	7.88033055819646	21.73591639265302
H	5.84274797829541	7.07245160606458	22.09599438684960
H	8.19297036468335	6.24478341070102	21.86761683060913
C	4.91701110682030	9.12082881862748	26.36540923724638
C	3.60665139560692	9.39273699611371	26.78505490917765
C	2.63145132385276	9.75879610227916	25.84167816812918
H	2.20727567711026	10.12729706655971	23.74673792815537
H	3.34340227480154	9.31858815172183	27.84524693338012
H	1.60707345224227	9.97252593652386	26.16375665594284
H	6.28303768220841	9.01229221852086	24.68360392774297
H	5.68097163282790	8.83651329590779	27.09660120946416
H	0.77127341401991	13.85214555851143	20.49492263223106
H	2.47401456228565	13.84939911456535	20.05762360122383
H	0.04062416982529	13.58693982132501	18.20136547301712
H	1.34696162531807	14.79125960199330	18.15206650351413

(exo/Si/t-N)-TS22

Pd	3.00339600148483	8.78150247554201	19.63617605364680
P	3.96240907637686	9.23732420353416	21.66202196365462
O	2.43692674627325	5.43996550869067	22.70987345101942
N	4.65832928553101	9.72486105237653	18.76409112341469
C	4.66752856687023	10.92502536465580	21.63667593290230
C	4.67299571766400	11.69216498241020	22.81814268071112
H	4.22960011511450	11.26539083270374	23.72239943357461
C	5.23479770320760	12.97400321927675	22.85794162436820
H	5.22464288691501	13.54403817910130	23.79224520246944
C	5.82018217936119	13.51425131165794	21.69889128961756
H	6.26726851522106	14.51297947297421	21.71772576250970
C	5.83107184326616	12.77369232559784	20.51637211683343

H	6.28258262691395	13.18759206677431	19.61203932283950
C	5.25544581136438	11.47960395712252	20.45208797595428
C	2.83072701772918	9.18800750368298	23.09541006517624
C	2.86973592769325	8.15709495027508	24.05060420042798
C	1.76456908317108	10.11693131358957	23.11109466432351
C	5.38354299515768	8.13622919806324	22.01613854939914
C	7.77590633052725	7.76818588416026	22.27620441502416
C	6.69194731732026	8.64680701262998	22.12929076977719
H	6.86331718994686	9.72711631342039	22.09774964605748
C	0.39315192894780	5.05260559706877	21.55691656004455
C	-0.35439967839614	4.37399377294976	20.43614275982631
C	0.56319657380532	3.79505816312135	19.34798572171547
C	1.69502222707220	2.98249712715221	19.99105026736451
H	2.31458529665794	2.48260417945919	19.22234177283426
H	1.25067624319452	2.17886096143745	20.61133562413715
C	2.56018970612906	3.89329129138526	20.87426578403847
H	3.24867413334782	3.30821799365917	21.51143163019796
H	3.21821872370463	4.52444529070337	20.23566887956450
C	1.77060970170557	4.82906844065183	21.80393020462241
C	-0.41213182694209	5.85422207202435	22.54074157177476
H	0.25759404812350	6.33661686098442	23.27122968341304
H	-1.12568051169309	5.21268962025366	23.10199110101127
H	-1.02642703431284	6.63245788732650	22.04361168461416
C	1.59537018557503	7.27481051900265	20.39195301769722
H	2.19839764695781	6.41136495905201	20.10750070280998
H	1.35256792499379	7.37920756218684	21.44726421468854
C	0.99389444748192	8.08818595613720	19.38796656583135
H	0.23463103557406	8.82506545148266	19.67936385940535
C	1.55998897429993	8.13016306941948	18.08167633451617
H	2.03132009082253	7.23081842921148	17.66641540776510
H	1.17156037388580	8.84353271887856	17.34731836045949

O	6.17325835640240	11.32145729691553	18.24146138722087
C	5.31571420120961	10.78674844824047	19.16672494404357
C	5.18845237728766	9.31420954740457	17.44358032914521
C	5.95802096269745	10.58201339556235	17.00433594623942
H	5.36804668802641	11.22217298702936	16.32537248595674
H	6.94716248759630	10.39259878412173	16.56346488318809
C	6.05392824811221	8.01468828734463	17.53587428498751
H	4.33387931097396	9.11265761256400	16.77541789786968
C	7.25134444524848	8.21806950352816	18.48301070138675
H	7.85973811561309	7.29816598057477	18.52527772363917
H	6.91265435635334	8.43311208050030	19.50919261423645
H	7.91261679713411	9.03966821486284	18.15419213088147
C	5.19389204937404	6.84656451641527	18.05759339145339
H	5.79499429287143	5.92073225482121	18.09183881479354
H	4.32372425247889	6.66396994423748	17.40220010489267
H	4.81939334364613	7.04321868717903	19.07806256990293
C	6.54386811808112	7.66793711287852	16.11407551895431
H	7.21364578660351	8.44129327520795	15.69707500027792
H	5.69466691236965	7.53959735430615	15.41785867568078
H	7.11017016732270	6.72062296714884	16.13107586127037
C	5.16038503304616	6.74283350459072	22.06593548510435
C	6.25109468566080	5.87759283172209	22.22808598549396
C	7.55843541508994	6.38245015963920	22.32001943786252
H	8.79138584305981	8.17018057314665	22.35743236217859
H	8.40627729757668	5.69853493262814	22.43436340807764
H	4.14215018378663	6.31913147923054	22.03520328786547
H	6.06679066516649	4.79959432464187	22.28324165725734
C	1.86150723006956	8.06984926888763	25.02376271346943
C	0.81965280374318	9.00542138535308	25.05343376458731
C	0.77403427087723	10.03414896337065	24.09483028937527
H	1.71714756729172	10.90088763678757	22.34667448605108

H	0.03274202005547	8.92785701629841	25.81071144073873
H	-0.04295226004305	10.76320943932541	24.10688006612623
H	3.66121306924480	7.40694644680457	24.02509417468485
H	1.88962816811416	7.24976113340718	25.74739614348005
H	-1.07081822699553	5.09166276730616	19.98304653656890
H	-0.99432717803252	3.55405507448190	20.84172007488778
H	0.99973688892483	4.62587297752836	18.75793125331075
H	-0.02157789408347	3.17378678221901	18.64426421482539

(endo/Si/t-N)-TS22

Pd	3.26969125107253	10.21846177927695	21.51214535215530
P	4.65851814569447	10.31864757173167	23.31712045723942
N	4.90919791017853	11.03157245641126	20.37920641035314
C	5.79829146668827	11.75175296594645	23.27822682869084
C	6.27925244742262	12.27179465416469	24.49679376842193
H	5.97410060155528	11.78810918668131	25.42917465508514
C	7.13107749314268	13.38156391862926	24.53749056130905
H	7.49054576092278	13.75701844929896	25.50082073145284
C	7.52257148404016	14.00189369416106	23.33918065169090
H	8.18781957964541	14.87071448398871	23.35533304512289
C	7.05959803523658	13.50736558014520	22.11875817689580
H	7.36005181211912	13.98512790492816	21.18404380828299
C	6.19583487079605	12.38567637839117	22.05626043549013
C	3.95181479170704	10.33001350962839	25.00478517289504
C	4.20060658765138	9.32297635432844	25.95469920462721
C	3.03470004159844	11.36096877756905	25.30536653355566
C	5.71061536722699	8.82551258267213	23.20372391655443
C	7.83366300762116	7.74148913825964	22.71117537205896
C	7.08802976358356	8.91101147253079	22.92560505348535
H	7.57517629641975	9.89023768832161	22.87679775541022
C	1.51086044491848	9.30293064608280	22.72556315706459

H	2.03839266965631	8.78444971412990	23.52493302294221
H	0.95163767476518	10.21197953396749	22.97110726802130
C	1.62606361331973	8.86359580936115	21.37263595055860
H	2.01191964066008	7.85080062988815	21.19867199154226
C	1.46299921493090	9.72428881996132	20.26248378546493
O	6.42998085676912	12.55405044746839	19.67525921556148
C	5.78281316822065	11.94281738485326	20.71968778930227
C	5.01428305665694	10.80881780505197	18.91990211955832
C	5.80241646281383	12.05688263643571	18.45753377463094
H	5.14513601331731	12.85299013104489	18.06636943060152
H	6.60717749311674	11.85703229614268	17.73519543224554
C	5.69476582749858	9.43772641706276	18.60141670015991
H	3.99665588158473	10.79609067490976	18.49510773790605
C	7.12114406459244	9.38413253522516	19.18153879487086
H	7.59285163192953	8.41812074719078	18.93076941027769
H	7.10002517404279	9.46290545872891	20.28088855811461
H	7.76938531749463	10.18482578311218	18.78293657177062
C	4.86363688062596	8.29077086252978	19.21075532941465
H	5.32066066233725	7.31792643645362	18.95610673292328
H	3.82964366661553	8.29503494195787	18.82244663692824
H	4.81257931533016	8.36869948796453	20.31031986812629
C	5.73179897431096	9.26862802995885	17.06836694975531
H	6.35243391505553	10.03726811162135	16.57340025880088
H	4.71560324059929	9.31986517084376	16.63604476606910
H	6.15900391564201	8.28498946119636	16.80655733723200
C	5.07954652489986	7.56188673196958	23.27932174421140
C	5.83960673994024	6.40182721493195	23.07996961078217
C	7.21143743174304	6.48625955507188	22.78621738197824
H	8.90374831644465	7.81439757804878	22.48965672141308
H	7.79551233088883	5.57464091164952	22.62134697653818
H	4.00808572077038	7.46093582902772	23.51118186392916

H	5.34552656423640	5.42758670534641	23.15302337586428
C	3.55082677829205	9.35828039672859	27.19795825234226
C	2.65960286237404	10.39686079875830	27.50219642252648
C	2.40390389570086	11.40164806329324	26.55316521389230
H	2.81690372362439	12.12543632135670	24.55053644269376
H	2.14941365608122	10.41588456781701	28.47056444556327
H	1.69639980047440	12.20577224084766	26.78009043965949
H	4.88688853753763	8.50578594644455	25.71866745561746
H	3.73754872922586	8.56250070405003	27.92584809074935
H	0.87326269390559	10.64502098209668	20.35577081140578
H	1.57489395531509	9.32663965708799	19.24875722926918
C	0.71710460617329	5.67823980571600	22.74947324272598
C	-0.75766441113517	5.53041348271227	22.34690926069057
C	0.99245517189769	6.78173479900714	23.78217699538232
H	1.33154906478736	5.89010673531180	21.84913294370248
H	1.12351991754234	4.73843234324655	23.16600789427107
C	0.00167374679467	7.78667698672085	24.01659418885042
C	-1.34106868929598	7.77181433501825	23.32416624038010
C	-1.36335860085120	6.90964101538954	22.05308449598157
H	-1.64704652544250	8.81209507378981	23.08347908221334
H	-2.12551361579229	7.40079765992723	24.02615805480512
H	-0.85588811086357	4.85695078391320	21.47448906163893
H	-1.32364487264770	5.05930216786801	23.17518603200869
H	-2.39798369927243	6.81613037662803	21.67352282758133
H	-0.77232172023258	7.40769275800252	21.25971050332684
O	2.14570895682248	6.80527043880476	24.32458716612097
C	0.12358178164060	8.64170370848384	25.25092283686481
H	1.15150769026848	8.59811378085450	25.64429356290706
H	-0.55899439498893	8.28336961403107	26.05117538192581
H	-0.14352004798711	9.70087140983926	25.06603126956525

(endo/Si/t-P)-TS22

Pd	3.18971573106307	9.63370126028518	22.46387958941686
P	4.94565757658574	10.28688733756475	23.73989667864031
N	4.27878779494251	10.48709899261935	20.81275360655620
C	5.43783109548172	11.99534270011779	23.29570448514057
C	5.84236654282761	12.90193713730921	24.29415202110096
H	5.86224790761628	12.56915238382792	25.33560138658164
C	6.22845507887652	14.21101659026268	23.97648342865252
H	6.54026553111065	14.89357174643583	24.77353433851136
C	6.22202772584341	14.63460459930842	22.63907381279386
H	6.52556381577919	15.65270730615901	22.37714831897942
C	5.81911530840074	13.75008557669400	21.63316907320771
H	5.80388623900118	14.07220074277857	20.58996492573643
C	5.41272632569415	12.43134369630608	21.93557330729165
C	4.90340948568935	10.27844057560364	25.56970056464641
C	6.03059052350216	9.96094007793115	26.35321168439789
C	3.68444164147403	10.60617443974931	26.19728998932925
C	6.42410909838530	9.28898080919582	23.30729163399286
C	8.75708025795623	9.06292351258859	22.64999138589195
C	7.67442159197145	9.87229273812462	23.02701402767349
H	7.79552081088949	10.95797396658425	23.09085871505373
C	1.65450757450123	8.78239956469112	23.68807251339567
H	1.93586263108264	8.09896270742345	24.49697262508914
H	1.07515359092737	9.66026020474645	24.00701131992676
C	1.48793026576362	8.27360428767335	22.36188930178097
H	1.79749815532385	7.24255056730747	22.14664029719582
C	1.26542108763137	9.14056634288520	21.26715940027329
O	5.32115652534200	12.07018392817458	19.57878825918750
C	4.97395037896878	11.59170769348395	20.80432796372792
C	4.14111190386638	10.00537704418170	19.40568127409815
C	4.63573133342952	11.22335564517153	18.59830338471789

H	3.80842838640138	11.81493638929534	18.17177696015880
H	5.36620583761646	10.98915842866744	17.81125642159985
C	4.92744747593428	8.68182426487508	19.15319503757777
H	3.07826747118507	9.80328796048058	19.17883186730879
C	6.41917755620007	8.84107389329167	19.49568848841955
H	6.96092230648904	7.90120435415766	19.29006862994497
H	6.56118402429738	9.08093058906756	20.56205025738207
H	6.90017778700969	9.63651121850445	18.89699882956948
C	4.30607159296963	7.55572460509863	20.00272842784608
H	4.85700008612104	6.61124938078568	19.84234810064795
H	3.25290765195095	7.40249009550223	19.71146707627473
H	4.34640224521221	7.79497237306554	21.08144951279487
C	4.73102906777688	8.31202043048669	17.66601393629911
H	5.23068016238153	9.02608654446935	16.98592900685030
H	3.65513280748100	8.28182443465942	17.42132489930928
H	5.16795598481465	7.31696278103308	17.46768642965223
C	6.27036106269058	7.89013595665831	23.21319003559014
C	7.35580310929529	7.08555675960077	22.84596317374014
C	8.59940886608937	7.67176883454070	22.55821025607999
H	9.72411054692213	9.52264971015678	22.42152976599787
H	9.44342062137793	7.04400812282588	22.25492441949001
H	5.28943132424352	7.44405741572190	23.40921304076932
H	7.22667262384346	6.00151042471630	22.76661644162483
C	5.93756030567529	9.98096288277737	27.75246076665244
C	4.72530925019008	10.32117002389632	28.37398894591895
C	3.59929209994036	10.63569711228185	27.59548120817969
H	2.80844000498767	10.82891037073084	25.57862092965800
H	4.65575857874765	10.33392136408813	29.46654308993664
H	2.65108564065847	10.89270429913419	28.07865185235911
H	6.97439775182468	9.69781999044062	25.86522633420862
H	6.81396036866466	9.72982980443269	28.35889044659566

H	0.80443905009463	10.12609485589614	21.40125044616794
H	1.55482407668688	8.83858220320647	20.26041847312589
C	-0.17109231806028	10.62238856256386	18.25017195300022
C	-1.66978977870575	10.92301103059687	18.39372317889099
C	0.23050035028688	9.18917181164784	18.61713264210919
H	0.41483071965251	11.30626621808739	18.90369314424752
H	0.18768508014372	10.81469201038021	17.22197052991975
C	-0.64108496331210	8.39988044090443	19.40000587471786
C	-2.01181128679646	8.87764822777058	19.81958702705691
C	-2.17953020418097	10.40300459603669	19.74457996433725
H	-2.22825713666126	8.52386552535799	20.84976457777114
H	-2.79626004233810	8.39867469581043	19.18584105735771
H	-1.86335221435325	12.00727971874611	18.28448905384376
H	-2.22851672833791	10.41733255504753	17.58106972469408
H	-1.59445189496013	10.87755948576407	20.55846304122957
H	-3.23797471866315	10.68194704029939	19.90489256443487
O	1.42984923891350	8.83248303745048	18.30804481057088
C	-0.33120133543744	6.94675169093252	19.63440598829029
H	0.67741666427393	6.71127847334744	19.25663779016228
H	-1.05552095737205	6.28693604125415	19.10979421827643
H	-0.38615772979338	6.67134678827126	20.70833003837077

(exo/Re/t-N)-TS22

Pd	3.11541446867386	8.82499302285520	19.84354685173129
P	4.16988278683207	9.43616953063761	21.78212309811077
O	3.53383393151494	4.89117810139959	21.58036847855484
N	4.67514280795856	9.85804611275416	18.86607709219387
C	4.65040018051867	11.19441661506862	21.67177543946586
C	4.56231705561321	12.02449906314504	22.80552478010531
H	4.19166144137988	11.59751053242729	23.74221507163600
C	4.95021301405299	13.36933487498514	22.75807214821321

H	4.87226141261915	13.99038168903785	23.65603549574798
C	5.45052040227915	13.90918561673045	21.55974970929094
H	5.76508284535442	14.95630956208298	21.51288966505095
C	5.54198414662498	13.10733689254504	20.42059452409601
H	5.92190571304747	13.52179692948583	19.48402887718475
C	5.13597110283603	11.75041037323075	20.44267798541951
C	3.28981148869406	9.24914350101552	23.37636825117693
C	3.91576241394861	8.74092810238326	24.53035501451264
C	1.90635762934893	9.52643846872646	23.39852811980272
C	5.74186244462477	8.52519285691505	22.01741493075610
C	8.15530418641952	8.45069022899170	22.31738939204223
C	6.96992583174061	9.19181020304958	22.19638282549806
H	6.99811216847360	10.28543188815505	22.23281174785518
C	1.15915289860227	4.78207432178571	21.53539536768161
C	-0.15634912488310	4.91297452983804	22.26575020113447
C	-0.05550646754117	5.67478602060056	23.59769780035637
C	1.12188262966847	5.14554878981751	24.42665281240909
H	1.16413697538436	5.64333377275281	25.41412595282108
H	0.97156284579483	4.06451364350257	24.61888301316541
C	2.43644904619937	5.36264788744592	23.66520066182141
H	3.28211142996555	4.83749899865849	24.14548861103777
H	2.70411477455454	6.43966386883050	23.69310003942545
C	2.40975828390613	4.94140734363383	22.19156574625553
C	1.11572852809686	4.23044501255216	20.13768096025872
H	0.49293456970564	4.85130883322313	19.46183633896946
H	0.67664313122902	3.20975550318215	20.11671497925236
H	2.13785039006663	4.17032549597545	19.72937288365824
C	1.84838303732623	7.24504045960037	20.73031557821339
H	2.58975399588690	6.46377703051506	20.53617533009980
H	1.58354602192250	7.44379144212050	21.76846746484655
C	1.17000096096391	7.92264443674302	19.67586891137864

H	0.33718271594778	8.59678283968642	19.91578903848474
C	1.72459478210591	7.93182412157823	18.36572810458691
H	2.29279154833253	7.06399300865361	18.01206720341144
H	1.26243289243809	8.55009817958698	17.58897225050167
O	6.01044896778484	11.56662900953012	18.21732255724132
C	5.23710392929115	10.99715449707372	19.19284461036994
C	5.19121911396219	9.43946173474680	17.54149279333330
C	5.84117222528877	10.74601201876122	17.02457609201847
H	5.18959081540301	11.29771807145570	16.32487397386058
H	6.83663610324815	10.61844015162132	16.57577276295461
C	6.15780664977913	8.21466624073446	17.64368061852141
H	4.33151947197216	9.14661497994500	16.91474692203904
C	7.35499866946322	8.53657764959751	18.55732906669480
H	8.03607242311812	7.66977315655067	18.60681160882464
H	7.02270208712778	8.75159752449968	19.58490809733049
H	7.94068020175424	9.39984433610817	18.19279438658311
C	5.40075308906232	6.99708314767013	18.20779762397785
H	6.07689206287905	6.12717874701342	18.27695513459751
H	4.55261770283852	6.71637792187725	17.55829221778494
H	5.00557021400166	7.19147397478513	19.21993017412926
C	6.64481228201783	7.87161589362501	16.21969557483744
H	7.25399265806700	8.67807521996363	15.77325047629786
H	5.79426945356254	7.66987302652572	15.54270030652770
H	7.27357800466204	6.96483846121266	16.24677451396556
C	5.69730518814201	7.11527565929341	21.97575603687286
C	6.88710296772243	6.38651373077118	22.10819639661354
C	8.11558453169742	7.04811410014785	22.26923831500450
H	9.10983503758841	8.97150014258439	22.44795261232709
H	9.04280188432932	6.47211836155583	22.36028237066133
H	4.75734426378994	6.55379771415589	21.84658254811939
H	6.83777481621893	5.29350448120756	22.07676986343124

C	3.16393145877282	8.51360096817221	25.69337528106212
C	1.78881241271698	8.79129071063982	25.71098351741324
C	1.16102002791830	9.30453107499070	24.56323583849862
H	1.42153547012730	9.89886755422976	22.48868821786015
H	1.20224876390887	8.59784930025796	26.61469499816541
H	0.08659528488693	9.51378424445900	24.57156140981563
H	4.98318975407191	8.50269526662338	24.50756584942633
H	3.65310244639769	8.10535862107962	26.58353554275811
H	-0.89947260527664	5.40463228405772	21.60269318947411
H	-0.58344091869125	3.90073095653515	22.46343839914432
H	0.10398441917861	6.75392992189088	23.40096513746055
H	-1.00596466701272	5.59055943814549	24.15762621578702

(endo/Re/t-N)-TS22

Pd	3.25211260785692	9.92693052307006	21.69351425890745
P	4.73014905519070	10.31843039230776	23.38549523076346
N	4.79903795283794	10.77368336622353	20.42641581213863
C	5.68245766835739	11.86836965866128	23.19718443140576
C	6.12434233603408	12.55529302481100	24.34547621107839
H	5.91813050865099	12.12196560652999	25.32847017171414
C	6.81892665904367	13.76725267279966	24.25401389455977
H	7.15314912580953	14.27313552139762	25.16542496493475
C	7.08721447889880	14.32222763884154	22.99155444640623
H	7.63092707157299	15.26803984018944	22.90527272270215
C	6.65487735598835	13.66442590628289	21.83846519938424
H	6.85718545757369	14.09173633671917	20.85417189062631
C	5.94728796127860	12.43942778076705	21.90937268642055
C	4.22153971930804	10.26830842128428	25.14543962203057
C	4.93238763270610	9.54801591569666	26.12523821435539
C	3.01171143140099	10.90576180860106	25.49212641630741
C	5.93907982747007	8.94916670919932	23.23736270778110

C	8.16674191115688	8.07844984415530	22.78981542741486
C	7.30510872453480	9.17026107097983	22.98279697443149
H	7.69154200784846	10.19352102403969	22.93273045752326
C	1.54968988791199	8.94693518014153	23.01373751007888
H	2.10693592970904	8.72566120053582	23.91609194812621
H	0.78521025931846	9.72939522964536	23.08595744939383
C	1.85187559448450	8.32881884544456	21.76604731576648
H	2.38869350436770	7.36989010612787	21.80959653679705
C	1.58207873061876	8.96507359481020	20.53331558471344
O	6.03669411399023	12.43767645969819	19.51253598635474
C	5.54101579645451	11.82994548033918	20.63839204137474
C	4.86066525808201	10.44748649019077	18.98339619238892
C	5.43007672422674	11.75241793259524	18.37805637264130
H	4.64315321108200	12.40930042310798	17.96801090541464
H	6.21854198968136	11.60934147502689	17.62490644907347
C	5.71867486190206	9.16644865340558	18.72806222643394
H	3.83566207812046	10.25298974639557	18.62639678644917
C	7.16362981568874	9.36619079508896	19.22428479576681
H	7.75929418756903	8.45923239284009	19.02134922505150
H	7.18351835659755	9.53470455677631	20.31344365140778
H	7.66756191067206	10.21417720923550	18.72678586933754
C	5.09318603153250	7.96917693285303	19.47067248297894
H	5.68041844892830	7.05457404904545	19.27457318164082
H	4.05674908603943	7.78681445922138	19.13657654940516
H	5.07217610352009	8.13427713254304	20.56000084724047
C	5.70725562147965	8.87752478847586	17.21260694340777
H	6.18694524133676	9.68099120461267	16.62475885041005
H	4.67498295161778	8.74969914675755	16.83818600811347
H	6.25844282090236	7.94451086337276	17.00214392435999
C	5.43774399455019	7.62933677049347	23.31064924997210
C	6.30844878011539	6.54764392293845	23.13058083036746

C	7.67037941528969	6.76797482463375	22.86197510065578
H	9.22780967676547	8.25539928634502	22.58409482583074
H	8.34466669797923	5.91861636637093	22.70940794815956
H	4.37561919310785	7.41551553311161	23.49561614710471
H	5.90388259679353	5.53248855207470	23.19037512306923
C	4.44010734310721	9.47415413630465	27.43716289742100
C	3.24150093675855	10.11918069677007	27.77896532624137
C	2.52921397031097	10.83925936481458	26.80525466452946
H	2.44445001445032	11.43262438424298	24.71653725899041
H	2.85434563392173	10.05053427769111	28.80056444945873
H	1.58654713103697	11.33083078480225	27.06564710824243
H	5.85752250606855	9.03117081671615	25.85335852247448
H	4.99049058197489	8.90274655222271	28.19154943932893
H	0.84441043554711	9.77614772599371	20.47400280011470
H	1.79856312772112	8.44362246996909	19.59586932975143
C	2.15344612209705	6.89499232298424	25.74470423678284
C	1.02746821732219	7.19820458226940	26.74294496015620
C	1.68716506056915	6.50890112923144	24.33121376575481
H	2.80990092711006	6.08066941848371	26.09991185038738
H	2.81354829324795	7.78370259743943	25.65694925575033
C	0.36169633895343	6.86057891278157	23.91872411434379
C	-0.64344137858744	7.45720656397479	24.87919181698745
C	-0.00766622909371	8.13275516861145	26.10388608530714
H	-1.33867038736630	6.65907200061229	25.23395499835884
H	-1.29456187359686	8.17673227259861	24.34042232696026
H	0.52595145289212	6.25595416563451	27.04114193362664
H	1.44586887719038	7.64326882364439	27.66530706929320
H	-0.79103571693404	8.41355684681348	26.83279831604917
H	0.49595191560405	9.06988199940846	25.79657494125752
O	2.55500008733457	5.99062249650068	23.55708218859659
C	-0.18246063599167	6.28190681406528	22.64233413491634

H	-1.02957083367106	5.59435706026800	22.84848045530726
H	0.60530896824167	5.71287394355257	22.12339575570555
H	-0.56819925017348	7.05689900478569	21.94859339773416

(endo/Rel/t-P)-TS22

Pd	3.22693882553808	9.54367442398090	22.47365602960062
P	4.95098990700613	10.34166748600568	23.72016198402690
N	4.30717908941105	10.31026322027809	20.78323225379566
C	5.36328355885292	12.03704055206233	23.15315220665640
C	5.70172354025916	13.03511804855765	24.08691772738329
H	5.71246143548540	12.78367424022862	25.15104224065134
C	6.03638080799596	14.33312402471217	23.67821290034747
H	6.29760620472431	15.08735770397343	24.42738823079902
C	6.04518357382408	14.65434813241989	22.31224000718094
H	6.31047346881860	15.66263022963803	21.98016680964441
C	5.70590224441678	13.67930732286506	21.36884694897615
H	5.70116414114311	13.92020367357114	20.30364863769418
C	5.34955786651439	12.37037073800516	21.76300722408666
C	4.87995770771400	10.46806024643536	25.54500368638980
C	6.01427469629712	10.29543311898517	26.36293749576618
C	3.63011377677053	10.75123168591861	26.13179737391383
C	6.48793474729249	9.39538759635395	23.38877283845812
C	8.84108620751980	9.24494368227527	22.78356125587132
C	7.70922589655882	10.02167407599126	23.07490901114774
H	7.76941356534716	11.11386614244517	23.04570210705985
C	1.74190492159333	8.58713634698390	23.68722332023592
H	2.07190259696951	7.87245695865687	24.44906058209241
H	1.11539024954004	9.40661710231743	24.06550522481403
C	1.57830314669389	8.14868311858359	22.33265501247877
H	1.94006206579168	7.15411547641723	22.04237009308044
C	1.24925616439048	9.06811413601014	21.31285769867104

O	5.33541542360421	11.80822916396270	19.43816371957062
C	4.97006786814516	11.43010100558145	20.69363088755356
C	4.23170033637143	9.69344057884270	19.42548374557878
C	4.69604136076906	10.85689917630491	18.52357543062246
H	3.85712206999136	11.38184081395111	18.03663579109991
H	5.44724417009795	10.58212917908362	17.76991550704606
C	5.08673651375605	8.39144221317211	19.31897132209571
H	3.18788415655568	9.41462039572185	19.20094352765403
C	6.56381677304184	8.66062576250740	19.65483065686736
H	7.14860866413356	7.72792299049334	19.57149925021008
H	6.67982980021751	9.03380350045817	20.68525846998006
H	7.01974105385986	9.39741881796528	18.96800887244132
C	4.50343148118988	7.33285772204378	20.27514683089553
H	5.08134057667771	6.39374845826900	20.20208547205106
H	3.45582917024358	7.12763708894372	19.99453291031842
H	4.53809683861456	7.67398458508671	21.32614359951673
C	4.92776648227064	7.85272798851875	17.87983265526881
H	5.34389260971257	8.54182970064720	17.12189582442846
H	3.85911515076402	7.67751873938697	17.66301801403933
H	5.47156313108871	6.89603401499280	17.78047773254928
C	6.41319232531900	7.98736844048639	23.41613030146530
C	7.54738125174313	7.21641509973231	23.13411700595541
C	8.76165175352913	7.84443382557932	22.81142290378415
H	9.78530444594786	9.73690715282697	22.52835814526984
H	9.64400477217363	7.24119497926529	22.57482984213297
H	5.45581556011077	7.50489437609640	23.64016415069506
H	7.47960038499530	6.12401183469863	23.14888140226165
C	5.89701992493869	10.41578951624042	27.75520751175118
C	4.65286685481046	10.71180785215325	28.33521198184317
C	3.51987244467586	10.88109905635503	27.52260471825809
H	2.75094153080444	10.85892080929049	25.48729264844285

H	4.56456933626658	10.80302045200098	29.42268685256478
H	2.54748537928877	11.10281514203423	27.97419123104970
H	6.98259605561730	10.06580140554459	25.90703239562631
H	6.77921189888726	10.27745547652287	28.38887534580199
H	0.72883858160656	10.00200193205986	21.55810251437792
H	1.51508099649476	8.87811266608399	20.27415186004480
C	0.52512142985699	6.04375138772031	19.15272906691401
C	-0.87504632985824	5.46044926351757	19.38998150395016
C	0.55168537182352	7.55507310343861	18.89899678018014
H	1.03367219947648	5.55641765783206	18.30053600256399
H	1.16858502807694	5.84204075336721	20.03662015069681
C	-0.56768589421266	8.34290233310655	19.25096972776403
C	-1.83694189159806	7.74533595167556	19.81035290126278
C	-1.64185022107214	6.33620928360760	20.39012311874499
H	-2.62343185582451	7.70325118126130	19.01879591262897
H	-2.25608917091325	8.41941904191535	20.58683637582112
H	-1.43380914379440	5.43400130788321	18.43320182082636
H	-0.80575044964084	4.41471846792168	19.74550596388828
H	-2.61995179751725	5.88660122875745	20.64476768526746
H	-1.06085666887473	6.40583605253605	21.33126493294826
O	1.66432854934133	8.04998510609450	18.47569302564161
C	-0.61635936577653	9.78825818638775	18.83376489993570
H	-1.30396676534393	9.93986447136496	17.97334153873643
H	0.38549610519431	10.12367096631261	18.51850520674594
H	-0.98542666412657	10.45124285872264	19.64176345354990

(exo/Si/t-N)-TS23

Pd	3.36226153388985	9.55664207785957	21.46881475898684
P	4.64995504576404	10.12560034539428	23.25673973094960
N	4.80287416366553	10.56173634267935	20.28308110185569
C	5.19610470756571	11.86630395728345	23.08703283239843

C	5.28811246456664	12.69125292855547	24.22313448293690
H	5.01109001100607	12.27839368596541	25.19768206181579
C	5.73378217590075	14.01675300013859	24.12933555272954
H	5.79546813231414	14.63545521064770	25.03012461307064
C	6.10841439597531	14.53842290988034	22.87975580327265
H	6.46361477816839	15.56993886502990	22.79392486004687
C	6.02064371197907	13.73919644909870	21.73745398397815
H	6.30184746377100	14.14065832919537	20.76133134993313
C	5.55457434046610	12.40444089666623	21.80990072180460
C	3.93150551552977	10.00743912450890	24.93479386651057
C	4.61544070037143	9.43356474881750	26.02285165583172
C	2.59738848320324	10.44077875396889	25.09730505761320
C	6.22030840516367	9.18044576490108	23.33693322390113
C	8.64697197379530	9.02528803397212	23.45529978567857
C	7.47609543745396	9.79848959945019	23.48814188362720
H	7.53584917784711	10.88333898581977	23.61862068821506
C	1.86821646710718	8.40575320200566	22.41625233734884
H	2.15981517033990	7.35992134703741	22.25575690435356
H	1.65813927894131	8.65379926143571	23.46020899565351
C	1.12619157047224	9.06433155099129	21.35174805264268
H	0.59598872863580	9.99158261590399	21.58319643212871
C	1.79153406253643	8.95905245312084	20.08547439369795
O	6.18573517171406	12.17822868643258	19.50935551706941
C	5.47430600688643	11.65265562973270	20.55384293931377
C	5.14930815764286	10.12797051298041	18.90846970306800
C	5.81830536248726	11.39887583256795	18.33337768788437
H	5.12406518015613	12.00767098700545	17.72825575824904
H	6.74085369514131	11.21858209575414	17.76388419522873
C	6.05005326765875	8.84866782844987	18.89902167834952
H	4.21130400953279	9.89221372522952	18.37712336481644
C	7.34181672439348	9.08319776653141	19.70523610777386

H	7.97696720342562	8.18129261483072	19.67297616122401
H	7.11759848836706	9.29174133653536	20.76331969487246
H	7.93668752913235	9.92375999103212	19.30508511689676
C	5.27533824291750	7.66302778622200	19.50463866674168
H	5.91156804409098	6.76010949272077	19.51494077128525
H	4.36641754064950	7.43713970747966	18.91968163224941
H	4.95971511515994	7.87545812837480	20.54253295017855
C	6.38745348916824	8.50883017992214	17.43145640048537
H	7.01240508868037	9.28119599036175	16.94875836447079
H	5.46975890200488	8.38359526575739	16.82805358816797
H	6.95008882106902	7.56016848296521	17.38601903675620
C	6.14729378398231	7.78201130494013	23.16165667597221
C	7.31725337868440	7.01305761672975	23.14328674808919
C	8.56956355424802	7.63502985305830	23.28230641426414
H	9.62187882893875	9.51211808291446	23.56238114863368
H	9.48500052774073	7.03524611852301	23.25180749655577
H	5.16859684233295	7.30889725547418	23.02533115490333
H	7.25336490557384	5.92883513147286	23.00579478215311
C	3.96900531825869	9.29374552812756	27.26076578514846
C	2.64301575327298	9.72513785110755	27.41801877178219
C	1.95874669721416	10.30469733485855	26.33598589127254
H	2.06351605187223	10.87000078707880	24.24220994788189
H	2.13792778711911	9.60282845825302	28.38148081815939
H	0.92104176084662	10.63271673454624	26.45153121116786
H	5.64688054715268	9.09004316470193	25.89668087477705
H	4.50261586698340	8.84138753527232	28.10309769096255
H	1.50493438105164	9.63875251626262	19.27340188251744
H	2.09862364469239	7.95693475590996	19.75711502737582
C	-1.37931838677701	8.47604998847779	23.66143437782436
C	-1.59934379548599	7.71944943979003	24.97956295625442
C	-0.79420502257318	7.62327406809095	22.53084259710108

H	-0.68765520127056	9.33082196245922	23.83207569368036
H	-2.31854395594618	8.92610078573830	23.29002061218942
C	-0.20077859722950	6.39266004458430	22.81662678552126
C	-0.12264703587635	5.82931356765973	24.21680387531647
C	-0.35863746782529	6.88050575065358	25.31388273876234
H	0.86696509636256	5.34639469873673	24.36617267823448
H	-0.86006951460769	5.00163834693004	24.34115998193674
H	-1.83778557045189	8.42315183430070	25.80040393624476
H	-2.47246004866646	7.04460762494113	24.87786545829655
H	-0.46359340621579	6.38864104728612	26.29945243444288
H	0.52284638813001	7.54948532203785	25.38192311160184
O	-0.79039492331818	8.16386873782729	21.34517592801738
C	0.28171035859986	5.51616434995583	21.69305275090251
H	1.33738665003087	5.19749754888765	21.82569472443521
H	0.18458033478496	6.05841037883762	20.73888704360840
H	-0.30989946833757	4.57794199236030	21.62545552794876

(endo/Si/t-P)-TS23

Pd	3.34123866120351	9.59980707604570	21.73091907804416
P	4.79648133043012	10.15267542859396	23.37824592023477
N	4.71921887600736	10.58098021179770	20.42132797794027
C	5.32836332412447	11.89794596158058	23.16613021170081
C	5.51133254393921	12.72576415588851	24.28922225695481
H	5.31718233281520	12.31691447420325	25.28475321403737
C	5.94545175804230	14.05193334315858	24.15742390858173
H	6.07911517217333	14.67105499541725	25.05014579082184
C	6.21450535574767	14.57427320364065	22.88182053786622
H	6.55815337110488	15.60672467363156	22.76603797799075
C	6.03542152031430	13.77248508705900	21.75190421273698
H	6.23316846030548	14.17284167705066	20.75515780589513
C	5.58276766318360	12.43655978635777	21.86466963588386

C	4.36591386701655	10.01643690383021	25.15223649762165
C	5.30791081199194	9.65768043667137	26.13667528037800
C	3.03273900682660	10.28486824419575	25.52347624018244
C	6.37079794469207	9.21604977828038	23.22057619666182
C	8.79550139636716	9.07955418549021	23.04059064645923
C	7.63189053015359	9.84184559379043	23.22880833618625
H	7.70084875358790	10.92476310884002	23.37038328958078
C	1.76363507602669	8.56865739949381	22.67404357111701
H	2.00816796553664	7.88342494233906	23.49469376951583
H	1.04332972798472	9.35255361340173	22.94790409136279
C	1.69753871837559	8.06195937337382	21.32961694947918
H	2.16531463858361	7.10121095138346	21.10166297832375
C	1.70896522010734	9.09833801821181	20.33293513113125
O	5.96416318417422	12.23804482365118	19.50824634489077
C	5.38990937187890	11.68646470384445	20.62001641007831
C	4.88914938087294	10.17766706339957	19.00328243444849
C	5.49529437580139	11.45418221525067	18.37178406918525
H	4.74698072175642	12.05918759421670	17.83179088268816
H	6.36330234154359	11.27772509984531	17.72060916627393
C	5.75955567349820	8.88860620543233	18.85438525699852
H	3.89048557107463	9.96663537767253	18.58719033987781
C	7.14433908661013	9.08839966879442	19.49822413866994
H	7.75492548003376	8.17725420861696	19.37615549433139
H	7.05431043765609	9.28610569163343	20.57788806708741
H	7.70086648520270	9.92504273547257	19.03845935120182
C	5.04414583042967	7.70147041817521	19.52782368219677
H	5.65665918397441	6.78713314944924	19.43346597097270
H	4.06270952179619	7.50584955893659	19.06061996091551
H	4.87166309221614	7.89417387625214	20.60117502437823
C	5.90442294743865	8.57813596135027	17.34933285202270
H	6.47091114602849	9.35628484774272	16.80723316954098

H	4.91613745672081	8.47348703603360	16.86537362434239
H	6.44653444271131	7.62623601603699	17.21291490911711
C	6.28724071532839	7.82075589545868	23.03127963015303
C	7.45099467676077	7.06229551957562	22.85479809600211
C	8.70693472092556	7.69209482810641	22.85236210183019
H	9.77281557665649	9.57329404975676	23.03712836827661
H	9.61564848366333	7.10099926847318	22.69916961586338
H	5.30284782935002	7.34065388670055	23.00767179841898
H	7.37740307614932	5.98036839225250	22.70495564600378
C	4.91742156982443	9.57543428807375	27.48118547686401
C	3.59115885441611	9.85370308877926	27.84847615880764
C	2.64973673180963	10.21043535821505	26.86915143788048
H	2.30337319006953	10.54194195341430	24.74832244522723
H	3.28872004283705	9.78487350310114	28.89847725733719
H	1.61288070980641	10.41819240329147	27.15217523135685
H	6.34110573182796	9.44136902130088	25.84708227847409
H	5.65039721322044	9.29157295713516	28.24351043186506
H	1.04274629754477	9.95905733976157	20.45655728132823
H	1.96041085134243	8.85085517368814	19.29663028990468
C	-0.18509574851445	6.54909697465924	18.73554672865501
C	-0.88255161566402	6.96213441213360	17.43143106586094
C	-0.54275003873570	7.41984634695794	19.94551870224079
H	0.91833193575099	6.59055103335970	18.60133683795116
H	-0.41103551483716	5.49990232933760	19.00134607096656
C	-1.13056491591317	8.67529045578430	19.75298710273595
C	-1.48425246547552	9.21269068413585	18.38621375893111
C	-0.77183889726304	8.48048680317721	17.23795118153984
H	-1.25409817014077	10.29900065898972	18.34083777611340
H	-2.58674308999686	9.15363856542039	18.22489210248012
H	-0.45513032953547	6.41787048679443	16.56748790971946
H	-1.95451442230453	6.68526542964345	17.48162926940106

H	0.30000823603365	8.76533184900704	17.23140019582635
H	-1.19336325893202	8.79145003526770	16.26339365928417
O	-0.17699561093987	6.97142536397291	21.10660429605952
C	-1.58453506283477	9.47596149447203	20.94294695947562
H	-1.28163981813866	8.95901233228084	21.86758942811225
H	-2.68943408881697	9.59506557275418	20.95406615428967
H	-1.17096315333527	10.50685336923258	20.94947459885411

(exo/Si/t-P)-TS23

Pd	2.87802953008824	9.77911941120334	22.49655855163568
P	4.15499526655476	9.98065929403696	24.36144420939508
N	4.58133940965633	10.61326733884631	21.46094103571835
C	4.93344791477144	11.65317345964369	24.36180704485608
C	5.07192162428983	12.36208378467544	25.56869993147496
H	4.70400489034593	11.90906449228464	26.49334465043946
C	5.67492166068675	13.62784240192516	25.61054665561618
H	5.76501474502407	14.15458348662970	26.56588532058511
C	6.16431712049417	14.20643784572046	24.43055653022211
H	6.64022540823548	15.19156862083515	24.45006981690265
C	6.03904667484080	13.51957686224383	23.21919582089777
H	6.41399664737853	13.96204951773082	22.29375819879895
C	5.41971547718219	12.25062413467368	23.15791269771196
C	3.45995047401161	9.82549945506470	26.04879045023415
C	4.13733974645728	9.17724420856017	27.09981513299819
C	2.18404113120088	10.38240913716043	26.27779092777903
C	5.60865079926365	8.85715624682873	24.36302330614942
C	7.99662705223305	8.40542779445978	24.53177294465616
C	6.92130575956396	9.30371640555177	24.61090852577724
H	7.10151847087938	10.35502996175921	24.85492872434009
C	1.01953724452529	8.94199952681055	23.07819147794303
H	1.21670754591817	7.86445924033745	22.97465802128407

H	0.57346184674441	9.21968818163348	24.03957059083361
C	0.65336264688076	9.66602889414537	21.89816890185102
H	0.17516882746101	10.64265663008275	22.00201983417590
C	1.48862732793780	9.42233399949774	20.75761199258280
O	6.11218332497226	12.16875173284835	20.86297504220849
C	5.32314320622687	11.61785993752334	21.83313506727815
C	4.92445498880632	10.27034829218401	20.05964473856836
C	5.74579988161150	11.50499346039559	19.61484853118421
H	5.15500093661010	12.21982938932250	19.01724159858199
H	6.68139382254994	11.27004776548418	19.08766015784858
C	5.67699109469139	8.90445615306114	19.96123996905903
H	3.98507155828613	10.18745861170198	19.48805195120667
C	6.95794818077552	8.92382299927575	20.81640641126186
H	7.49105547828750	7.96225871066462	20.72174091712612
H	6.72205606062287	9.06834777915550	21.88234455095614
H	7.65561319222216	9.72203472918461	20.50458637427653
C	4.74964815465756	7.77364374641256	20.44639010977860
H	5.28874127326422	6.80972732414880	20.43634086917708
H	3.86293873061389	7.67749666343908	19.79571986471385
H	4.39345440994818	7.96107442089623	21.47501010883614
C	6.02404595497459	8.64975783897072	18.47920891721373
H	6.74754780049512	9.38324955669364	18.08041560699327
H	5.11909761677932	8.68002694050676	17.84538216913546
H	6.47859247378359	7.65003397086184	18.36684922266415
C	5.38525579387400	7.50010167716269	24.04735212566439
C	6.45954374056029	6.60435664256002	23.98096707527094
C	7.76844437631917	7.05750643885915	24.21569355377965
H	9.01556426629555	8.76182849365784	24.71531058539972
H	8.60988142381126	6.36033406191866	24.14869643848760
H	4.36523540208261	7.15878294286309	23.84003803921087
H	6.27694404579508	5.55420913082640	23.73143790740280

C	3.54221465287493	9.08952306937488	28.36728358657938
C	2.27726512632206	9.65402647590015	28.59384069296048
C	1.60028719957303	10.30440597218423	27.54845550469791
H	1.65660163117676	10.87071053508973	25.45119828835624
H	1.81494500331005	9.58188124301543	29.58362170013172
H	0.61031829306653	10.73901510338178	27.72009915766768
H	5.12634245711371	8.74312796216542	26.92322149782959
H	4.06941432584997	8.57928303593627	29.18015879150368
H	1.52656372512863	10.13457954473020	19.93090130284511
H	1.79480721242365	8.39685047195259	20.52702293588030
C	-0.80000592088773	6.65202735333180	20.50795126423260
C	-0.67756444241266	5.88818848379717	19.18221318539653
C	-0.98100747581182	8.16531692382015	20.35326195779142
H	0.11316112824083	6.48951003066089	21.12298824481188
H	-1.63833745871725	6.27410564962068	21.12164165118324
C	-0.65870736675786	8.78679254880100	19.14057974820087
C	-0.19338728501118	8.01524095451908	17.92681830882718
C	0.31662629798409	6.60386100142076	18.25759093325580
H	0.60274023626080	8.58898320159006	17.40356155252834
H	-1.01697093525697	7.93526531995363	17.17789226090567
H	-1.66638445026712	5.85099026043027	18.68306687730245
H	-0.37242068102634	4.83908566560639	19.35997496414426
H	0.48519133398571	6.02725971047270	17.32832904859518
H	1.29700177810653	6.67692594463870	18.77240478609662
O	-1.31344696226574	8.81129969454160	21.42614954537316
C	-1.00951415017592	10.23552123256790	18.92468035625232
H	-0.16471348141031	10.82698558985597	18.51276029407361
H	-1.33381737352421	10.68557593707892	19.87669344648433
H	-1.84031484943498	10.34655134064117	18.19429891794937

(endo/Re/t-P)-TS23

Pd	3.35664756220204	9.61166713447166	22.09518055047758
P	4.97693502589570	10.10194977606945	23.60293170485354
N	4.59113680261389	10.67509057808493	20.69606697029007
C	5.46918102634586	11.86310854451520	23.42623975449785
C	5.75957445328019	12.63708647453567	24.56511931617491
H	5.67678729699613	12.17567606215741	25.55309209725226
C	6.16158720576395	13.97545847330136	24.45717682175863
H	6.38174142395703	14.55101293375188	25.36187440794393
C	6.28850413161991	14.56578501794122	23.18950179075303
H	6.60631973887677	15.60831780242359	23.09175896578800
C	6.00021251903462	13.81842206372678	22.04471723907561
H	6.08697906864764	14.27144341831999	21.05471707622329
C	5.57777884617965	12.47132218254532	22.13536591516244
C	4.75359400135592	9.86772156916997	25.40509720700989
C	5.80820907840576	9.48859879549638	26.25924486989349
C	3.46466461348221	10.07862550789383	25.93541769986905
C	6.53094943256871	9.19680642191052	23.22118604477170
C	8.92212371320719	9.10005812789576	22.76959131597936
C	7.78095573604782	9.83711211081183	23.12312754158354
H	7.85776540229897	10.91226456024095	23.31193936015600
C	1.88567155255496	8.50714033820447	23.13338956441701
H	2.21435000574684	7.78105223445562	23.88640394941290
H	1.19290257542148	9.26803205839365	23.52115707610925
C	1.69159779007870	8.07650521836297	21.77568965443362
H	2.14035646592168	7.13683246519559	21.44661573583421
C	1.57641761909414	9.15842537138255	20.83856431447289
O	5.70373840603511	12.40320316642821	19.74410721171472
C	5.26143152224610	11.78222390849327	20.87924550594171
C	4.60615510971860	10.35138869324119	19.24801729293450
C	5.13213377326707	11.66663658316382	18.62293640921090
H	4.32773848888002	12.28530940146880	18.18984401620250

H	5.93271641119486	11.53461771601808	17.88100348405990
C	5.46069544183259	9.08153866833175	18.93529329877675
H	3.56873766942024	10.15145925320585	18.93345242803484
C	6.90602782892249	9.26143402931444	19.43580595435299
H	7.50459482332342	8.36503425898411	19.19897921405933
H	6.93215041051019	9.40006326372276	20.52799058701248
H	7.40528630626749	10.12765975791858	18.96497188227772
C	4.82683960883876	7.85323132181352	19.61672060736229
H	5.42952966868088	6.95133227062682	19.40818029279290
H	3.80175096611731	7.67305308284585	19.24761452262083
H	4.77069280684970	7.98749540824639	20.71118825985898
C	5.44262210707748	8.85401875982996	17.40879139687607
H	5.94147906158483	9.66715962499778	16.85167282766112
H	4.40810867592128	8.76288133175702	17.03024655829757
H	5.97287645894263	7.91759508091767	17.16269542688744
C	6.43708902804152	7.81175059958850	22.97071818683087
C	7.57965963817391	7.07793109007391	22.62893252645081
C	8.82325520688186	7.72276262681981	22.52127648877784
H	9.88962456343573	9.60569334733386	22.68457194655964
H	9.71375453011267	7.15163629697784	22.23941260376446
H	5.45954314603121	7.32101843761615	23.03076619917628
H	7.49752307296648	6.00411966409071	22.43242899673016
C	5.57335004684671	9.33016829119052	27.63272247158653
C	4.29056093172512	9.55207393397113	28.15888891391566
C	3.23700292929750	9.92813308178871	27.30977113563037
H	2.64705691118394	10.35033242489082	25.25960546071654
H	4.10974488574044	9.42375524067311	29.23107075246067
H	2.23385310997965	10.09140684606866	27.71648256322340
H	6.80699398797450	9.31611409495071	25.84585404701245
H	6.39367073831133	9.03089365668867	28.29341586077953
H	0.93574656308990	10.01311579198512	21.08827296783448

H	1.73308629028490	8.98352744729866	19.77199487522678
C	-1.87359492348857	8.73493538024781	22.00903066046240
C	-2.93489370297738	9.49298656388071	21.19934318715105
C	-0.94296034366538	7.86040545690113	21.16427476461046
H	-2.33241286469418	8.08857668127955	22.77971211020744
H	-1.23745840687475	9.45681692500038	22.56704570249974
C	-0.84709329201617	8.06977198725608	19.78340048089212
C	-1.67252278397478	9.10510450902526	19.05593507386870
C	-2.28126447501301	10.16699428225925	19.98521697543805
H	-2.49308975112537	8.60881150520770	18.48537934377431
H	-1.05092783525487	9.59782259635032	18.27712317383543
H	-3.70619844500596	8.78155850439337	20.84249624225161
H	-3.45668011585951	10.23475613489145	21.83365431131617
H	-3.01040129823072	10.78873391142018	19.43226293938248
H	-1.48060632772043	10.84765489300982	20.33931333766347
O	-0.19845011298869	7.02060351050278	21.81427178115814
C	-0.05950574333793	7.11073156578295	18.93200799992131
H	-0.72536237234180	6.52499751411070	18.26187213607399
H	0.48477237795646	6.40187454744959	19.57636273145847
H	0.66364620330647	7.62377983643865	18.26308693022661

TS24

Pd	2.76458009446178	4.42751037416676	15.89397756689583
P	2.23268753947741	5.04692639610614	17.96421575341422
O	3.10179809832210	4.39298420939794	13.78060922922583
N	4.31061104782970	6.00121765727465	16.08037759544802
C	2.08273956691572	6.89601930887383	17.96499152088356
C	1.02764581048774	7.50546342725881	18.66746456981669
H	0.30498464490468	6.87452382535218	19.19147344848941
C	0.88719181709914	8.90129897435981	18.71085346868254
H	0.05053635370004	9.34378105497684	19.26102246639714

C	1.81836980835763	9.71924938765562	18.05885952363769
H	1.71915872778685	10.80857022093850	18.08847770981118
C	2.88346887575284	9.13503106779679	17.36328251649002
H	3.61951113563093	9.75791286320701	16.84957550129509
C	3.02517843124476	7.73408499274440	17.29792127021201
C	0.65091065652531	4.48033026560571	18.68436255083540
C	0.55893094995338	3.91166242701157	19.96808324340493
C	-0.49639878989205	4.54563530490793	17.86409132081625
C	3.48188146905368	4.74206147126260	19.27581710163066
C	4.97626625137414	5.47821365864965	21.05124860622509
C	3.96517135004301	5.76021921622457	20.11987693039367
H	3.56034850612188	6.77352294565992	20.04174734502606
C	2.33719908304668	6.41921669583216	12.75354593815491
C	1.23877764999912	7.24305829010271	12.11386084632949
C	-0.16782144533026	6.66657506952993	12.32477280458954
C	-0.15353565899674	5.16078906372823	12.03883809421634
H	-1.17168211762236	4.73137542751404	12.09476345513507
H	0.20820026837121	4.99354814891921	11.00486443616956
C	0.77938522969833	4.45486803790000	13.03253262985950
H	0.96849423971627	3.41125543166986	12.71877269147275
H	0.28445702523784	4.38708691698140	14.02294079542258
C	2.13517113232371	5.13845220229995	13.20864923448175
C	3.68190813597476	7.08909254190201	12.81907089974411
H	3.73002889835214	7.85843568371249	13.61965519070544
H	3.90930517451081	7.61663580053104	11.87070448501363
H	4.47357804715385	6.34709853327615	12.99762220593399
C	1.56168676302554	2.72565524024466	15.75933026782641
H	0.50838887797297	2.96105258338454	15.98269342901412
H	1.69691867738661	2.47421424240721	14.69637224551659
C	2.12406755706153	1.70569203205614	16.66598982522334
H	3.10243881191790	1.29301229195857	16.37478669564023

C	1.54981180008564	1.25216384944604	17.80776583827139
H	0.57312151387577	1.61995132661634	18.14044163727644
H	2.03184766446553	0.49294921603035	18.43328535729630
O	5.18430323669571	8.07489691613290	16.27399872806832
C	4.16897405273368	7.20401240273876	16.53612310607947
C	5.63765506402316	5.87561512742446	15.44611132787920
C	6.12198580881004	7.34921929110531	15.40901185664477
H	6.05646889028973	7.79772328461891	14.40541732386723
H	7.12751374226160	7.50776609041097	15.82489038579178
C	6.57252906788248	4.88546856063099	16.20683250634361
H	5.46953454276023	5.47153069391122	14.43390159956049
C	6.79330679776818	5.33742749334559	17.66144891647668
H	7.43908492637443	4.61614620098473	18.19129066527876
H	5.83973538854229	5.39306499908653	18.20875371934156
H	7.28452495848283	6.32580411475250	17.72141790872620
C	5.94015340042220	3.48000914028165	16.18609940991821
H	6.60986514255466	2.75316434071735	16.68020182979696
H	5.75623902882559	3.14032425662421	15.15176173618515
H	4.96982050626691	3.47024623352199	16.71455318279116
C	7.91695862067817	4.83228536716555	15.45100095783906
H	8.44221098420646	5.80471755018506	15.45525378881277
H	7.77074147855986	4.52645407062440	14.39922157769738
H	8.58845255469136	4.09616154103594	15.92669858188004
C	4.00912564168013	3.43720445345264	19.38071206743395
C	5.00926341231532	3.15990026386110	20.32081491879773
C	5.50084957403852	4.18079953320074	21.15150970146781
H	5.35584185625061	6.27633352768863	21.69772295485782
H	6.29337998997596	3.96503669190363	21.87550209950927
H	3.61984101914469	2.64986603741024	18.72629228881470
H	5.41491084989021	2.14574068345018	20.39737944519561
C	-0.66909330337704	3.40993542781639	20.42553966313073

C	-1.80824636783166	3.47902708243847	19.60932170856123
C	-1.72174090536611	4.05446976474529	18.32969578804896
H	-0.41441744072163	4.97349084254483	16.85873591718935
H	-2.76361462501608	3.08139853491137	19.96683872145347
H	-2.60759641493188	4.10654997439369	17.68858327591385
H	1.44866870716327	3.85302017588019	20.60149379911894
H	-0.73354003418285	2.96015148980110	21.42173819672427
H	1.28357649597439	8.27852292329877	12.51442580801341
H	1.43157192333601	7.35328085342897	11.02169835444833
H	-0.47957444075954	6.83112337712831	13.37584534981031
H	-0.90023380378946	7.19208301187197	11.68369259020637

3_CF₃**TS14_CF₃****TS15_CF₃****(*Re*/chair/axial)-TS20_Ph_i**

Pd	3.73563277499944	10.11836741467525	20.65752971440068
P	5.09208303340328	10.05429590318874	22.43000238149444
O	3.06911535531621	11.17057047802440	18.73661263195849
N	5.66988580674513	10.40031999290604	19.57366721547773
C	6.22928825029883	11.50515608450292	22.37099591869635
C	6.51160916497078	12.22936126422437	23.54580486209936
H	6.05847483844504	11.90746213746853	24.48728970702220
C	7.36854060335858	13.33842066032568	23.53520410079784
H	7.57107415455986	13.87537264332835	24.46775421551656
C	7.97089833587017	13.74616944245022	22.33608867284715
H	8.64536823007154	14.60779154948677	22.31700337821624
C	7.70132555771386	13.04661803323373	21.15558596270321

H	8.15528263353815	13.35769351798418	20.21199077196601
C	6.83164259508117	11.93418783463004	21.14708782903764
C	4.45616374496971	10.06856697991072	24.15026396397082
C	5.00779828351401	9.29195561259845	25.18857601246095
C	3.33309180233309	10.88186609914820	24.41256946624459
C	6.26301953242973	8.63490400212967	22.42087605067024
C	8.49836495200485	7.66827932651991	22.51746201234580
C	7.65367375046437	8.78735782377870	22.58196258419064
H	8.07520282981068	9.78300626217779	22.74974068660404
C	0.79767242521571	11.04838129478040	18.04394474108249
C	-0.46857127497261	11.89090689104548	17.82929736219054
C	-0.72707382716787	12.97616693699836	18.88564178016093
C	0.52886431085928	13.82603453849460	19.10492758435734
H	0.81055729320186	14.31998837129182	18.15416745884707
H	0.34166191280637	14.63054659853366	19.83983599369842
C	1.67528855838192	12.92323866446625	19.57627279579810
H	2.63540540345558	13.46229330238863	19.65365702612227
H	1.45389261170623	12.54655805810880	20.59845559399256
C	1.91422653711526	11.70057925938742	18.69684829398734
C	1.08046137339695	10.04935291651776	16.95745936309331
C	1.88660190741416	9.58647498931853	21.49810262852402
H	2.16960045343658	8.82764746679907	22.24361564064357
H	1.42123521388576	10.46980931598711	21.96828169358055
C	1.25882013235491	9.11648874393044	20.30074519522929
H	1.52508491128998	8.11760312583196	19.93443852577239
C	0.25827790514996	9.84389100396194	19.59494829319683
H	-0.26473682806280	10.61117491332984	20.18044770592068
H	-0.40830471901128	9.25731967343838	18.95177225209227
O	7.37708939033263	11.68266470671941	18.81396969273712
C	6.57717691433783	11.28565767809698	19.85202798424892
C	5.82062346194288	9.99955337640764	18.15885736673199

C	6.81419655219848	11.05742778885402	17.61684317143199
H	6.31270397080921	11.84763788783715	17.03359672859094
H	7.65633638284700	10.64871448219216	17.03881267839152
C	6.29068591057023	8.51641104807809	18.04259964983867
H	4.83375399326624	10.10167298698708	17.67819129361008
C	7.63526804990779	8.30696616673786	18.76446390388299
H	7.96770862602519	7.25994541429960	18.65419573154705
H	7.53971463376174	8.51436278311814	19.84259985362254
H	8.43365141275879	8.95326652376460	18.35670228258515
C	5.22750047010045	7.60199206261072	18.68156292865422
H	5.56911603369509	6.55126150822308	18.67166686112706
H	4.27185683830397	7.65608301032073	18.13499885669665
H	5.03267781632474	7.89427424471858	19.72657911505089
C	6.41689554312550	8.16752179042160	16.54559710219055
H	7.21528891380878	8.74516391197700	16.04530177816622
H	5.46836846668933	8.36275254489472	16.01326856649286
H	6.66212829392089	7.09748323193157	16.42372735973882
C	5.72969234530875	7.34670447175009	22.20797727655019
C	6.57325899661768	6.22998548949790	22.15726505909926
C	7.96111838984319	6.38984585016135	22.30413080747740
H	9.57974432672158	7.79779924967499	22.63197292945597
H	8.62250938230349	5.51906873000067	22.24842345246774
H	4.64949051437074	7.23244130084865	22.06514765486703
H	6.14883596019572	5.23520269969409	21.98673333723352
C	4.44626901334379	9.33626117976076	26.47317590471080
C	3.33765274178850	10.15801329616229	26.73183126943655
C	2.78393407595947	10.93411437552171	25.70005956959940
H	2.89875880398841	11.46693200732173	23.59447113452629
H	2.90108344743225	10.18908975653341	27.73553959891184
H	1.91471072584834	11.57046258368561	25.89649549839640
H	5.87663800842644	8.65740508422926	24.98825883119594

H	4.87822324754138	8.72899546420692	27.27575323206753
H	-1.34600393692485	11.21964507081166	17.75655829773376
H	-0.39081296980086	12.39431834982965	16.84426234922694
H	-1.02709445471132	12.51778225266209	19.84752827662444
H	-1.57835832096215	13.60183569244708	18.56008044885124
C	2.12437970456768	9.09728679548472	17.07075343912664
C	0.27731688546279	9.98867282485706	15.79452524129317
C	0.52044100761259	9.04857390408204	14.78171916538982
C	1.56804952702974	8.12664534110048	14.90498451060759
C	2.36107362212511	8.15508482765673	16.06312959251828
H	2.73327310862392	9.10410013326618	17.97290946497617
H	3.16973786921045	7.42570610968212	16.18878088585308
H	1.75813870612830	7.39039722530689	14.11674256175424
H	-0.11968381259564	9.03968200458010	13.89247455218331
H	-0.55470912053681	10.68474565368990	15.66358468551812

(Re/chair/axial)-TS20_Ph_ii

Pd	3.79884310566052	10.48326238860468	20.71859568109034
P	5.16147312754165	10.15569755727529	22.45012112668862
O	3.03932137039093	11.43469686797301	18.89486851023080
N	5.71834100897182	10.70888284983228	19.60318204841075
C	6.47592525438939	11.44789639285569	22.48262910063016
C	6.86608825265225	12.02762395122223	23.70592303515040
H	6.38069377810964	11.69529751007473	24.62748094510340
C	7.86991955187800	13.00386939121136	23.76691308812312
H	8.15287893573987	13.43023632875423	24.73496010824838
C	8.51502771276524	13.41837364953370	22.59262239541887
H	9.30458449307686	14.17534104917272	22.62902997517061
C	8.14027098496407	12.86151761994370	21.36576399357893
H	8.62681183625202	13.18086839344039	20.44134905857824
C	7.12098869085164	11.88763876761822	21.28561917772739

C	4.53755495532021	10.12778695093951	24.17471750425345
C	4.99690734758463	9.22092206364053	25.15015006231768
C	3.52261235386168	11.05048231730003	24.50625331802761
C	6.13547697704612	8.59981629181903	22.32477412630927
C	8.21747488577177	7.33506763905006	22.37079076795095
C	7.52718183885319	8.54629188638826	22.53274391811095
H	8.07037976217181	9.45504931917681	22.80949062535054
C	0.90775262133261	10.92614695955209	18.03474025542802
C	-0.43145206518786	11.48315510470537	17.53615744620819
C	-0.96319019179559	12.67231068308987	18.35555156676435
C	0.14360874386611	13.70395034500758	18.61864129379337
H	0.51488940470668	14.09704104309024	17.65152495151262
H	-0.25400324748169	14.56840255228464	19.18166572481642
C	1.30988424070106	13.05425806590483	19.38222201751262
H	2.16446706878416	13.74341014804153	19.50014424819427
H	0.98270922239118	12.79049768309650	20.41156557315945
C	1.82154434796617	11.79485995824994	18.70289889614982
C	1.51286552955490	9.91232580055397	17.10009802891787
C	1.97678424941675	9.97287487290799	21.64392835029504
H	2.27608750214870	9.34201399582807	22.49407478112674
H	1.48979809268349	10.90284535809684	21.98698467027267
C	1.31234073714819	9.30206903187661	20.56158935523873
H	1.62642461915043	8.27887344462823	20.31711143666090
C	0.30181675190915	9.89858217438251	19.78557974009943
H	-0.20663556737571	10.76422395757981	20.22580021705008
H	-0.37293560996840	9.24840903050780	19.21922481409922
O	7.64427922834409	11.70418527407526	18.94314458526665
C	6.76770811905349	11.38938848108703	19.94736492752833
C	5.82042259016383	10.37446193668885	18.16552659096553
C	7.00561807962797	11.25974171970108	17.70441875137801
H	6.67874582752173	12.16055689341423	17.15743893649790

H	7.77264999384521	10.73235370994062	17.11838451166975
C	6.00789827516654	8.83814366997460	17.95642348074080
H	4.87202299662010	10.67533794090761	17.69031220919798
C	7.22908429059011	8.32100411705979	18.73844640681120
H	7.35771421953196	7.23751145239394	18.57025797360831
H	7.10426885493742	8.47763601899646	19.82081030586813
H	8.16461972285839	8.81906948381975	18.42276998538501
C	4.72954844223781	8.12283882185051	18.43462522210011
H	4.83149706526664	7.02973256370911	18.30722299915483
H	3.84759432343949	8.46036534697530	17.86669664996101
H	4.53632611366441	8.33372434812106	19.50171556925008
C	6.19276076973770	8.56730404943714	16.44968398487940
H	7.12999087949802	8.99998731610024	16.05434724256636
H	5.34576493228481	8.97087175609569	15.87011136172704
H	6.23376729454283	7.47862494563380	16.26780308430680
C	5.44309196382231	7.42457098598123	21.96583987129183
C	6.13231738899451	6.21469564955431	21.81845473477136
C	7.52284798858770	6.16954881116283	22.01325355957576
H	9.30177714633176	7.30405712902122	22.52119263768526
H	8.06476091306389	5.22742835885767	21.88052515304240
H	4.36451905470980	7.47583096163619	21.78230598213492
H	5.58687969487306	5.30929052388381	21.53301822184052
C	4.45533367594490	9.24692392018047	26.44382775149206
C	3.45695827626876	10.17764338072580	26.77283458600414
C	2.99309391717389	11.08151303228250	25.80272420718692
H	3.15471846453249	11.73505423631207	23.73380086729792
H	3.03493662468895	10.19397630837974	27.78312649352208
H	2.20785100683284	11.80230963198357	26.05346719964395
H	5.77952356943986	8.49991967141171	24.89432593809591
H	4.81583378820692	8.53917652531973	27.19788432446667
H	-1.18357842890449	10.67070958043173	17.50376856271085

H	-0.29693385596391	11.80074048450624	16.48103997114879
H	-1.36382367434794	12.31711586498828	19.32401130632088
H	-1.81137259632110	13.13655587610875	17.81935235196702
C	2.41272417065604	10.37510726450916	16.11221248125457
C	1.15389885248315	8.55104256444675	17.06700989767974
C	1.67487638161601	7.68325329692358	16.09355012977672
C	2.55989641722039	8.16073258194197	15.11833702279598
C	2.92440719309687	9.51719544675304	15.13075805876494
H	2.70050482011524	11.43112987535399	16.12168241397409
H	3.60693576068314	9.90945974906864	14.36855917793904
H	2.96388831549780	7.48557750146323	14.35685841560089
H	1.38342158955905	6.62734269555985	16.10111242581988
H	0.46453688840187	8.15072885005880	17.81407954356154

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Pd	3.83031608689796	10.58445826114228	20.71314443077207
P	5.19568097029458	10.25361978085612	22.45038151968413
O	3.10622845581470	11.16636025390674	18.69998916477042
N	5.85376607416624	10.68368812749591	19.60737129541250
C	6.55707514245615	11.49988391666147	22.46825500259304
C	6.94804422174755	12.09561355796627	23.68443515979349
H	6.43757230157989	11.80193357967961	24.60522405235602
C	7.98281977446895	13.03840209136687	23.74249576786578
H	8.26312965629023	13.47554076322295	24.70653930917901
C	8.66264745249711	13.40522191588271	22.57158521771025
H	9.47660671164575	14.13601712726459	22.60563205944603
C	8.29269570238570	12.83026922008360	21.35232081846603
H	8.80831286340948	13.10878439015273	20.43045620834373
C	7.24360518729946	11.88757281479329	21.27520780383997
C	4.59146550530633	10.26583859001953	24.18260229033745
C	4.94050387542658	9.28843453122344	25.13512898116744

C	3.68459951697051	11.28849902748505	24.54025700305856
C	6.11863277564709	8.66519522580349	22.33079384001095
C	8.16286691543802	7.33792960931402	22.34567052489847
C	7.51343351000354	8.57225879595020	22.50149382751357
H	8.09132228084512	9.46821109249165	22.74743671955561
C	0.79770832663521	11.23537644822521	18.15103021604730
C	-0.33944122436288	12.19144564825194	17.73541635210700
C	-0.41960019867825	13.46180491905768	18.59070601773393
C	0.93623932964692	14.18024049373206	18.60567241726389
H	0.88758882807028	15.10423351126361	19.21046472176795
H	1.20011502892764	14.48765209682120	17.57470955640538
C	2.01463289777237	13.23982635405932	19.16098090469614
H	3.03141035506030	13.66670087131192	19.10805715925347
H	1.81955731621886	13.04904988390492	20.24466336298351
C	2.04703078374176	11.86166995266351	18.54653370396226
C	0.88427651588540	10.04719278041841	17.21968099160714
C	1.95474159153147	10.13387852364347	21.65434788126515
H	2.00640869816852	9.06380851644017	21.37293718175112
H	2.11969403450802	10.30058519798885	22.72751893102208
C	0.87804541183953	10.85378693570837	21.07405876695584
H	0.55105912640243	11.77942577019384	21.56872925925657
C	0.24485432273843	10.48295305121346	19.84289709857352
H	-0.81215834111375	10.77667145363800	19.76482136255955
H	0.41301460147350	9.43009936530465	19.58015436667230
O	7.79273824867841	11.65924851102918	18.94102966265982
C	6.90298029723472	11.36621582936794	19.94328359855079
C	5.94423789518586	10.35355259730354	18.17169348254088
C	7.19014405244612	11.15651010725703	17.70873635217041
H	6.93415301143158	12.02839468231494	17.08366280229183
H	7.95513913717711	10.55349162033381	17.19539352686916
C	6.00857410887977	8.81247472062118	17.94262129266594

H	5.02379320618378	10.72839162377290	17.69528485920148
C	7.21994853688574	8.20098869902256	18.67006338317593
H	7.25080758074135	7.10911905032136	18.51019379170177
H	7.15576321474026	8.37850210216104	19.75538265484348
H	8.17908963012168	8.61532126109276	18.30796766701008
C	4.70859315466798	8.17678094459485	18.47419842470038
H	4.72965563604357	7.08220710834783	18.32239685739540
H	3.82214030080981	8.58594006127675	17.96208917054365
H	4.58821862618080	8.37670596429237	19.55355146628009
C	6.10051875373454	8.55540235913611	16.42478958564487
H	7.03000098052107	8.95921349316597	15.98292944672652
H	5.24258532690488	9.00919614612589	15.89600479939145
H	6.08418192256006	7.47016450709542	16.22132030175910
C	5.38323429308161	7.50335108732225	22.01558224741834
C	6.03159377299086	6.26998856950799	21.87508712745770
C	7.42493796073980	6.18631544584557	22.03221713789977
H	9.24948892357577	7.27762457226776	22.46817272940331
H	7.93471186963744	5.22561739842932	21.90551075981346
H	4.30119723414314	7.58108122277308	21.86455663204227
H	5.45104339110774	5.37600695492298	21.62498256686020
C	4.39817895394456	9.33985248591907	26.42787769068596
C	3.50979148030053	10.36753884088541	26.78214455217691
C	3.15697592382626	11.34494452435875	25.83668287959559
H	3.40244695681183	12.03661044021444	23.79013851349549
H	3.08786181530369	10.40400569212986	27.79189231077214
H	2.45899678129986	12.14448214722536	26.10631211518224
H	5.64053155449052	8.49261786489024	24.86298550424569
H	4.67476083558725	8.57636264350321	27.16283439834940
H	-1.30069468441297	11.64534724120024	17.76230045620738
H	-0.18541384950212	12.47364055053766	16.67445629243919
H	-0.70360666698261	13.19681416362632	19.62799358589545

H	-1.21386605068916	14.12482396574736	18.20147620137074
C	1.99855630799946	9.83361938219742	16.38017573308792
C	-0.20748299429073	9.16008249393883	17.09724225132682
C	2.02990964450112	8.76168950187354	15.47727037997032
C	0.94450681890964	7.87780063318413	15.38283386257675
C	-0.17917669315595	8.08696687612347	16.19576831090194
H	-1.09509351531417	9.30689207136144	17.72171042470082
H	-1.04023584358582	7.41298834430741	16.12941945978761
H	0.97125635823772	7.03940064432650	14.67886956500278
H	2.91059193688616	8.61893594455925	14.84123999354841
H	2.84886147837271	10.51511246158459	16.44276194300364

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Pd	3.83042577294365	11.03734755246992	20.74827770477079
P	5.02462424908963	10.11833136179891	22.39476020665699
O	3.23938364214926	11.39942632234920	18.49736147257600
N	5.94841987812926	11.17131702599808	19.77757791372607
C	6.56616506577823	11.05616359633180	22.78787358746006
C	7.01479080344914	11.12353563010459	24.12223446801601
H	6.45375828971528	10.59263182280620	24.89545999093313
C	8.16019292455574	11.84773165553853	24.47830476861963
H	8.48150982510683	11.87384776965732	25.52468527043332
C	8.88974858826254	12.52723989556906	23.49275706247691
H	9.78465634689226	13.09914500847477	23.75704541820949
C	8.47086216091220	12.46691522968520	22.16043809005961
H	9.03441653838691	12.98370549491449	21.38095891326310
C	7.31878905344301	11.73937559657485	21.78567619211661
C	4.26755658500103	9.86867446327795	24.04592357696118
C	4.10377376726586	8.60277038417065	24.64129128302850
C	3.74604281761643	11.00940683531616	24.69897291947299
C	5.64025956042800	8.45648198891771	21.91912982063588

C	7.41413431987521	6.85836774820268	21.43542958834872
C	7.00601297266917	8.11761194944723	21.90281041166572
H	7.75017975328926	8.84094808799277	22.24969316711207
C	0.91238763153748	11.12489819168531	18.02505914843258
C	-0.22041779921962	11.69313638956920	17.15122886853987
C	-0.24257680155409	13.22235707763478	17.01678657724262
C	1.12885040050921	13.74545611330589	16.58045838337376
H	1.11649309506467	14.84406674878411	16.45793149583125
H	1.39082956298104	13.31607471883133	15.59354752070216
C	2.17865507498262	13.33195275329450	17.61733670743436
H	3.20540029491852	13.58930099963745	17.30408940077442
H	2.00476285172366	13.88255392836328	18.56995970534435
C	2.17193325286846	11.85618934193886	17.99029172947888
C	0.96006189313215	9.61778498269433	18.06546793914666
C	1.96924024221219	11.14965987974467	21.73606547793662
H	1.58724560283043	10.11838866482566	21.81509303230936
H	2.25068097220753	11.56746059798995	22.71348664369022
C	1.28362204855921	12.01344314251169	20.83973281837092
H	1.50447085545932	13.08805297452802	20.90534033907986
C	0.32415930998811	11.59410136993141	19.86601207747025
H	-0.39936694327789	12.36540308435640	19.57423356081740
H	-0.14559617809367	10.62140673737831	20.06034737300505
O	7.91485491487732	12.28184914657457	19.52526921328191
C	6.98467099086421	11.70418439699188	20.35206834970159
C	6.17120025196694	11.22722594630464	18.31237678303870
C	7.31955396957721	12.25105238280633	18.19043665110344
H	6.96186188455453	13.27072592190491	17.96235644323488
H	8.11673973331080	11.97426500581746	17.48497789534446
C	6.48604718660328	9.80884037444821	17.73907632814810
H	5.23929179412252	11.58830163204299	17.85177117731584
C	7.77802692877068	9.23164193846871	18.34840101442373

H	7.97616922819786	8.22864096933692	17.93087264376428
H	7.67850195724959	9.11810195364579	19.44074750421853
H	8.66307380934904	9.85979982595418	18.14025045469370
C	5.30901730665146	8.86743132398956	18.05385598481080
H	5.48881463450310	7.86981882017301	17.61428864072768
H	4.36254683422850	9.26406319371015	17.65476768905705
H	5.18356849461684	8.74466753753583	19.14094697674842
C	6.62787735157144	9.93850435176800	16.20858006406220
H	7.47467154537711	10.58603333354969	15.91517052653899
H	5.70686364350065	10.35417175207499	15.76141240368212
H	6.80305923616376	8.94540741219462	15.75844934467297
C	4.68820637063591	7.51314277514281	21.47301512360234
C	5.09722086451769	6.24828291727372	21.03437566292867
C	6.46387576362990	5.92176848615596	21.00332367905412
H	8.48034845379686	6.60967140586113	21.41175788753857
H	6.78548117687985	4.94068467783646	20.63920192131345
H	3.62789917045961	7.78847539878138	21.45673101072560
H	4.35036491499810	5.52240779732335	20.69590791572741
C	3.43300020352771	8.48061316912879	25.86741603054072
C	2.92587641893380	9.61796261175829	26.51452650212188
C	3.08980737840781	10.88464298648408	25.92952959831918
H	3.87658501759348	11.99740916027761	24.24274928651742
H	2.40296322590850	9.51878189575658	27.47129521831221
H	2.69659545067102	11.77649179943573	26.42855002419224
H	4.50654847799638	7.71398534713958	24.14675821027369
H	3.31333322862174	7.49138984361715	26.32189945969203
H	-1.19272471168051	11.34082398209225	17.54567687349816
H	-0.13120215936575	11.26385113637872	16.13301145532036
H	-0.51714105209260	13.69184240876214	17.98151770540436
H	-1.02733666948170	13.51114452880853	16.29385438315659
C	1.91134782429748	8.90239291540799	18.83604212557045

C	0.00775576917182	8.84795534477664	17.35475622776795
C	1.92869402407831	7.50305456671878	18.85705739508137
C	0.98832885563615	6.75935037378013	18.12897853636362
C	0.02087499900403	7.44569605416139	17.38343697570440
H	-0.76346374176846	9.34047069149605	16.75840141851776
H	-0.73186765552029	6.89087990503488	16.81234070323926
H	1.00676200877699	5.66428243214007	18.14527809854998
H	2.70163132748393	6.99292647447077	19.44145307623641
H	2.65520508703722	9.45054857810335	19.41874078063694

(Si/chair/axial)-TS20_Ph_i

Pd	2.65792751378017	4.84018302582293	16.08464869336874
P	2.32715686937040	5.55858980205105	18.16319496518921
O	3.25291005652154	4.59275587356556	14.01754770272920
N	4.50723761051538	6.24815721446481	16.36551808865874
C	2.47328415907075	7.38297968631378	18.31588487766362
C	1.55306273296469	8.09736219585785	19.11094206598004
H	0.76936843573199	7.54610627058383	19.63656968778411
C	1.62572456068907	9.48758772472130	19.25162376341480
H	0.89918325547766	10.00700462149709	19.88503437231257
C	2.64120732306993	10.20550466761447	18.59610448997738
H	2.71481629413632	11.29196366623093	18.70670479682720
C	3.56199642289672	9.52305540241938	17.80005970909380
H	4.35020024044330	10.06818148692962	17.27577081840631
C	3.49177413821363	8.11987660744986	17.63321753384155
C	0.73542686039760	5.17681591068248	18.98045631936460
C	0.62974808909199	4.44934371840018	20.18051642574439
C	-0.43732693299311	5.55550083369674	18.28756010852342
C	3.61914297554146	4.93613419851505	19.31380777013706
C	5.31387965850903	5.24964238354917	21.03584488630367
C	4.28309577183527	5.76686563639777	20.23627264087584

H	4.00012688303682	6.82070872351711	20.31748929602716
C	1.16390135902630	5.24413792537130	13.03045453750048
C	0.48018858282539	5.47279185129756	11.66945799815930
C	0.69571797052434	4.33011359440371	10.66686897124568
C	2.19072305306402	4.00871048783092	10.53566405056461
H	2.36061477523329	3.20955353571906	9.79125546905915
H	2.72454399388895	4.90670433024219	10.16704747402915
C	2.77071373691338	3.59618466385990	11.89830248908380
H	3.86828406579186	3.48374561847996	11.86347073085758
H	2.37185664179025	2.59624522922006	12.18187648693254
C	2.44123309774303	4.56652844538115	13.02014990270959
C	1.03551589218160	6.43881003209752	13.94133225974380
C	1.19080440499042	3.27690151618108	16.02539412281071
H	1.81891436446758	2.50545076542150	15.54467754783462
H	0.97745716174773	3.06981960427018	17.08291643991835
C	0.11048846935341	3.78484100308563	15.26059960495094
H	-0.64807307343159	4.36252143994293	15.80070464006454
C	0.06838838842806	3.78170252765909	13.83925777232576
H	-0.89464201216000	4.03888374285508	13.37676976430915
H	0.54113812776400	2.92303997806538	13.34453324795953
O	5.37398035136835	8.34084683941040	16.14919594747538
C	4.44824319348364	7.49705372472307	16.71791576021776
C	5.63517968396190	6.07346979754805	15.43214974507463
C	6.19898857444049	7.51387790210705	15.27597942721843
H	6.10392588543615	7.91083374833868	14.25256063720149
H	7.24387026995003	7.62425992285549	15.61032304243413
C	6.63174753214139	5.00286563067735	15.96813532421402
H	5.22351622073900	5.69977045697171	14.47786853239934
C	7.10562682888068	5.36184929423526	17.38866762299417
H	7.80596057678297	4.59501235348717	17.76372468792734
H	6.25124521906312	5.41155627355231	18.08336281264697

H	7.63287136926977	6.33359709551564	17.41891991133287
C	5.90199089491772	3.64457586869953	15.99538315294702
H	6.57674162132105	2.85064498000101	16.36414609773055
H	5.54289925395758	3.36769563385957	14.98897755708731
H	5.01949576025477	3.69028149099388	16.65756939809024
C	7.82834030773249	4.91350497370112	15.00043009905303
H	8.41241954898980	5.85152214013198	14.96803909607434
H	7.49186292243852	4.68363821466382	13.97270778907022
H	8.51667583513876	4.10994093357890	15.31698736210046
C	3.99238793043761	3.57944844256200	19.21158742008234
C	5.00911855165998	3.06117889222976	20.02370282945160
C	5.67784786978656	3.89829859980481	20.93218579126882
H	5.83494498066107	5.90600964771856	21.74090969146728
H	6.48570578061606	3.49857300278117	21.55397933654257
H	3.49224218704852	2.94456761610370	18.47185287477583
H	5.29385510369006	2.00773651772810	19.93345739333806
C	-0.63494317766597	4.10948287163313	20.68610006632919
C	-1.79751208391578	4.49947241351088	20.00372685020661
C	-1.69571055414460	5.22852393924223	18.80597472604002
H	-0.34660808411022	6.11080679228597	17.34659211475007
H	-2.78229955099940	4.23287334384339	20.40139493105861
H	-2.60070346745376	5.53180246664818	18.26870404516905
H	1.53645117759947	4.15239460960083	20.71676960547263
H	-0.71102660228204	3.54216052675273	21.61987320408372
H	-0.59983540840301	5.65151332130973	11.82878348917463
H	0.87835639779972	6.41417962554837	11.23858806387222
H	0.15211893549631	3.42570728574117	11.00112586060555
H	0.26929273371646	4.61156348248257	9.68659366364064
C	-0.19507220910074	6.79376236172351	14.52976912054884
C	2.12815875712795	7.31594168024718	14.12018792356881
C	-0.31243058304827	7.94582711992333	15.32378759625524

C	2.00438866050979	8.48619406680093	14.87969447079837
C	0.78958752361020	8.79235633947235	15.51119033466439
H	0.70635680793498	9.68264776379946	16.14207400363782
H	2.86608567332362	9.15064102611737	14.99227954457303
H	-1.27546559367587	8.18880535682024	15.78694000871369
H	-1.07190756696961	6.15939942877494	14.37082175313690
H	3.08516204204006	7.06847824207619	13.65351676120081

(Si/chair/axial)-TS20_Ph_ii

Pd	2.68142206815327	4.83145155512418	16.11763817934807
P	2.31686360988224	5.55183726838711	18.19002004694855
O	3.32094263845195	4.57343355429298	14.06709975649432
N	4.55776470957566	6.20275775883284	16.45943029719865
C	2.49233891931236	7.37255042157932	18.35289110329815
C	1.56662063409266	8.10120620025662	19.12841584553664
H	0.76131568362896	7.56264699005559	19.63418768020662
C	1.66040720307994	9.48957868771168	19.27449152387770
H	0.92877420890510	10.02025197147241	19.89252459271239
C	2.70321414923006	10.19105011418656	18.64439467452879
H	2.79328365097162	11.27578507675053	18.75970654293215
C	3.63016313273965	9.49441111800862	17.86813177364255
H	4.44011762974586	10.02674180832433	17.36419857169383
C	3.53937108375465	8.09297195105525	17.69609744132833
C	0.70084004608520	5.19529900784085	18.97086430803354
C	0.55674233403664	4.46445258463441	20.16490250652250
C	-0.45018116134556	5.59673983847531	18.25474603142456
C	3.57084869820255	4.90172640742829	19.36726934255827
C	5.22749660641806	5.17789121396236	21.13215539056652
C	4.22500044236349	5.71626243598312	20.31086115406893
H	3.95692216838119	6.77404109631341	20.39158560676932
C	1.26615341965706	5.26378926648877	13.03540951708243

C	0.61873823795806	5.50894708627036	11.65957526338421
C	0.83698043605276	4.36558555897067	10.65836420167244
C	2.32877461763479	4.01849342257097	10.56010813758497
H	2.50171099109147	3.21870511891589	9.81709515366984
H	2.88649986884688	4.90808499580622	10.20685725414682
C	2.86995583728523	3.59160782566374	11.93424492515479
H	3.96583259538967	3.45955908896330	11.92439650144350
H	2.44676224636977	2.59817751365031	12.20505010598889
C	2.53185478939933	4.56409599019129	13.05164166221323
C	1.13833966882020	6.45837100581684	13.94670229683965
C	1.19049066128693	3.29045967940751	16.02411416627365
H	1.81662363309786	2.50985361072363	15.55599269384329
H	0.95138321199112	3.08681523090176	17.07670097775788
C	0.13746530935349	3.81935074729517	15.23673987784407
H	-0.62242008016075	4.40973998460214	15.76099193320328
C	0.12764968558081	3.82000849476018	13.81435510893058
H	-0.82015249209272	4.09488366625351	13.33103159970996
H	0.59565401394516	2.95357975456955	13.32869217698482
O	5.45180406541196	8.28509347710760	16.24704987373260
C	4.50594674386382	7.45472115095171	16.80280733728812
C	5.69917128026803	6.01137751305605	15.54554843423525
C	6.29230079275480	7.44165193500876	15.40515181677299
H	6.24021857157069	7.83737380061092	14.37831909449961
H	7.32680287265415	7.53447288134261	15.77572669975820
C	6.66621660011719	4.92044855742132	16.09380578138316
H	5.29798890030271	5.64922075938560	14.58224871851514
C	7.11612042767306	5.26106886191735	17.52660928743980
H	7.79537519779267	4.47971108583698	17.91040068180648
H	6.24799768925481	5.32055536878593	18.20325495487357
H	7.65897979310354	6.22342858881632	17.57533839487600
C	5.91286806398819	3.57483397371087	16.09595593170764

H	6.56532319502392	2.76705158425389	16.47463126333470
H	5.57180744265175	3.31027882248104	15.08001206920541
H	5.01667770892131	3.63208953505076	16.73843752539825
C	7.88109450806599	4.81767599354542	15.15053144224167
H	8.48154377413381	5.74578869649649	15.13790791142922
H	7.56241395375038	4.60150825137950	14.11418639069967
H	8.54888779301323	3.99998620513110	15.47485275861374
C	3.92486465864933	3.53991805198514	19.26564967670728
C	4.91305742296825	3.00061657065943	20.09905144776680
C	5.57243340882778	3.82152351861495	21.02888889817864
H	5.74147379325580	5.82164368457252	21.85386159688369
H	6.35841672467639	3.40527773569951	21.66764725287831
H	3.43300708912960	2.91762818863102	18.50983409423687
H	5.18326705271424	1.94333267209724	20.00905951460738
C	-0.72413838967166	4.14382499051199	20.64146793195711
C	-1.86492893360285	4.55636595836320	19.93603545216752
C	-1.72485877717982	5.28883646898294	18.74426777839119
H	-0.33004570788369	6.15462566141677	17.31867655449609
H	-2.86246120329164	4.30472375513817	20.31104159747133
H	-2.61274247906770	5.60981402298911	18.18902402941584
H	1.44641146445827	4.14978597172662	20.71925014767046
H	-0.82992474244253	3.57377527678178	21.57067783469431
H	-0.46123694015703	5.70705416326115	11.79423108560174
H	1.04420659617345	6.44414293759551	11.24153605638954
H	0.27032291446851	3.46985378395124	10.97733093683393
H	0.43786276486200	4.65727788483596	9.66963307427156
C	2.24205037723971	7.31560386003222	14.15280343362456
C	-0.09911624657020	6.83427070076746	14.50698187751115
C	2.12128302886420	8.48683341781680	14.91128997867431
C	-0.21438533622948	7.98685952376141	15.30053630793405
C	0.89772943388240	8.81347487060684	15.51501917518071

H	0.81562671686870	9.70411599009426	16.14554469879804
H	-1.18344382272584	8.24608999916000	15.74179822405301
H	2.99181241855312	9.13553519418522	15.04503491333080
H	3.20523287870892	7.05217471760115	13.70804938961247
H	-0.98320064696689	6.21598828337252	14.32624474943090

(Si/boat/axial)-TS20_Ph_i

Pd	2.40182689026886	4.85546287353063	16.21424101849329
P	2.10804664837011	5.50014743237204	18.31674252250079
O	3.16410749409551	5.18095172123209	13.96352942714848
N	4.30077421629942	6.14158089563353	16.43157245244756
C	2.32883354990743	7.31940997531252	18.47248289598529
C	1.38944277907984	8.08797755992678	19.18814642317804
H	0.56041233967905	7.57885236599235	19.68609227029491
C	1.49589310461889	9.48153130634465	19.27633098943806
H	0.74908671197354	10.04734388425132	19.84301148787207
C	2.56475210894858	10.14357178398004	18.65194452408565
H	2.66106217038852	11.23167137880069	18.71836370864879
C	3.51002425194653	9.40273500391512	17.93590121617456
H	4.34071867748261	9.90378678710269	17.43371733672065
C	3.40319711806002	7.99874148650797	17.81889567731514
C	0.52900773383013	5.17557374592608	19.18697153789382
C	0.45719447453397	4.66738927259736	20.49852913196916
C	-0.66080750324015	5.42045072045542	18.46713054541672
C	3.38620161473938	4.82742604953953	19.45393475430645
C	5.09950085284097	5.06048195301706	21.17124478476795
C	4.09661753341704	5.62733147525151	20.36952030787446
H	3.87048615310459	6.69519552588300	20.44606184591530
C	1.01198418960271	5.36657754887720	12.97388222736493
C	0.23089144544447	5.46663211439619	11.65565193253031
C	0.84736206495765	4.69215030145564	10.47940309721753

C	2.35242435170076	4.96554847576956	10.37233025554059
H	2.78827510317298	4.44421129973837	9.50040883295026
H	2.51919257709093	6.04920199676184	10.21323017297517
C	3.05139292949692	4.52456042117142	11.66563806090272
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C	2.43264084584917	5.12059023695974	12.92465371595784
C	0.46888884060923	6.25800156801467	14.05535031784858
C	0.88736547367453	3.41329943106475	16.09973243486854
H	1.13524577083784	2.72684871166688	16.92484639079382
H	-0.09481364684214	3.89126665605726	16.23153360389643
C	1.22769480598271	2.99842956196348	14.77698901062336
H	2.08925052707625	2.33179735522554	14.64585419673026
C	0.53833184473636	3.45125325274981	13.62184424961164
H	-0.51300962648078	3.73012745411779	13.75907700537684
H	0.72592247390451	2.91429474283098	12.68456113177204
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C	4.38801064145417	7.32144223909105	16.96195851894788
C	5.51414628377103	5.89442772504788	15.62581213016378
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H	6.22723172543434	7.79939832733071	14.71637291216021
H	7.29186676075897	7.20379195710459	16.03613394407963
C	6.31862048784187	4.67103180427011	16.15981824884074
H	5.17270367324707	5.65662355073654	14.60472750019850
C	6.72432959670684	4.87785317628429	17.63007226575794
H	7.27312154328906	3.99653240373185	18.00540711474321
H	5.83648020309376	5.01645369811850	18.26643612031682
H	7.38278184933286	5.75655469810307	17.75971837206630
C	5.43609970972753	3.41331008844303	16.03180821293812
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H	5.12464081056742	3.25555631151741	14.98440078739270

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C	7.56923122074900	4.49259696039867	15.27487312329912
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H	8.12985057530885	3.59291553025486	15.58479218431622
C	3.68411253069210	3.45132820605716	19.36245697073819
C	4.67231580564833	2.88462416692085	20.17663703196046
C	5.38826492151110	3.69051473025939	21.07763595070029
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H	4.89784423086477	1.81627022475265	20.09498525690267
C	-0.79184658048470	4.41139422360779	21.08425413826072
C	-1.97319551322070	4.66954340206966	20.37098057260818
C	-1.90468127548917	5.18017376059451	19.06378590192118
H	-0.60114524209334	5.81088012031188	17.44576834207791
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H	1.37782415591782	4.47636317154290	21.05856625213778
H	-0.84187944392063	4.01333789281258	22.10341104277317
H	-0.81210972213054	5.13010753588551	11.81244489123345
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C	1.27813543156282	7.20813377113424	14.72659967057432
C	-0.90841402035942	6.24258784992647	14.37358935738772
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C	-1.45235258149341	7.11327610033701	15.32848529123658
H	-1.57554292089161	5.53875328832997	13.86524017974820
C	-0.63251995364658	8.04759482523894	15.98090868366653
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H	2.34163388393454	7.25917904330842	14.48867271500027
H	-1.05055722357832	8.72941583079450	16.72864282630395
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(Si/boat/axial)-TS20_Ph_ii

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N	4.32783374114625	6.14819606314982	16.41909131649314
C	2.36040774364490	7.34916989544770	18.45014902377565
C	1.42635299036456	8.12782805168207	19.16192384864026
H	0.59132053165552	7.62738931594784	19.65864067255490
C	1.54548986591902	9.52049282780540	19.24776726014765
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C	2.62200585212650	10.17140967948662	18.62483675893019
H	2.72812251543642	11.25871718070841	18.68936230432994
C	3.56227705212042	9.42045377015639	17.91276719951351
H	4.39891796683759	9.91281713911447	17.41186302441914
C	3.44281239863328	8.01726010147157	17.79823769737570
C	0.53724712906442	5.22429334379359	19.16198164489087
C	0.45568694915452	4.71726504816874	20.47340353810677
C	-0.64749524228057	5.48104031805561	18.43790858258280
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C	5.10079055899652	5.06779990157281	21.16123537897758
C	4.10587348947201	5.64301804397495	20.35555913136297
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C	1.04222169573958	5.40037820070812	12.94937878181468
C	0.26746035236663	5.50555469556729	11.62782008890045
C	0.88063801428485	4.72213673454660	10.45578400002983
C	2.38878950748253	4.98006739007190	10.35397768175833
H	2.82273138863886	4.45230585359878	9.48497564050744

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H	3.01786715856363	3.42894423122611	11.74650858626401
C	2.46058602683970	5.14013741716494	12.90629706871401
C	0.50400226852657	6.29964387724532	14.02682815247374
C	0.88815000181795	3.45324006806292	16.08005144796322
H	1.12721315929060	2.76537993560309	16.90658834457137
H	-0.08941232828146	3.94138828037931	16.20887913473328
C	1.22775357860940	3.03362900741860	14.75863703093738
H	2.08260920613584	2.35781274964091	14.63063823187572
C	0.54662373662249	3.49265508104892	13.60098873402728
H	-0.50211795536041	3.78260994492242	13.73501437417664
H	0.73103127965047	2.95252063160702	12.66491478427888
O	5.54736415873661	8.05168100834187	16.63349431147067
C	4.42380119805958	7.32903322128383	16.94572237322061
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C	6.29187833010645	7.24652423298951	15.66873294241433
H	6.27786320181710	7.78319953622404	14.70536116026046
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C	6.33179820368941	4.65775789442698	16.15461554209508
H	5.19950920254677	5.65214150539947	14.59520439371393
C	6.73557809748340	4.86261769381094	17.62568589053818
H	7.27451059066041	3.97637165275612	18.00370598933386
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H	7.40249310100136	5.73482804447900	17.75594363832771
C	5.43722973784255	3.40862373667335	16.02607859743043
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H	4.51505997802003	3.51970157381686	16.62644897972253
C	7.58292385498868	4.46578577974738	15.27324956001030

H	8.28321490713196	5.31793036343824	15.34669206774716
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H	8.13417797650039	3.56141018845632	15.58628686124739
C	3.67463832872644	3.46927926114461	19.35149116838130
C	4.65483455785676	2.89436967299212	20.16958763354923
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H	5.66222127647303	5.69572291638658	21.86115272408281
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H	4.86996955244149	1.82367274035162	20.09061744392936
C	-0.79793990850440	4.47413286978850	21.05481174163397
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C	-1.89582434297039	5.25358929009226	19.03025210833710
H	-0.58022991003591	5.87063527303356	17.41669319395577
H	-2.95067533916080	4.55313544928808	20.79466076602457
H	-2.80962889073622	5.46339667106185	18.46420535658698
H	1.37237152756839	4.51705243012431	21.03669997934417
H	-0.85558473885924	4.07691245035223	22.07389265097929
H	-0.77952978108374	5.18004914330775	11.78124299787302
H	0.20429436815426	6.57808729571056	11.35194673951592
H	0.70896940255544	3.63688295949729	10.59136140927647
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C	-0.87466455314433	6.29923022846141	14.33951242205669
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H	2.38531797717151	7.28201607697030	14.46577366690036
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CO₂

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