

Supporting Information

Evidence for a kinetic FLP reaction pathway in the activation of benzyl chlorides by alkali metal-phosphine pairs

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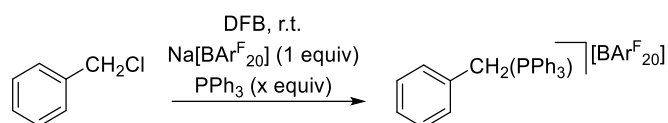
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Experimental

General information

Experiments were performed under inert conditions using standard Schlenk techniques or a glove box (Vacuum Atmospheres Company) as appropriate. Subsequent manipulation of air-stable products was carried out under ambient conditions. Dichloromethane (DCM), acetonitrile, diethylether and *n*-hexane were purified using a solvent purification system, deoxygenated and stored over 4 Å molecular sieves prior to use. Chloroform-*d* (CDCl₃), 1,2-dichlorobenzene (DCB), *tert*-butylmethylether (TBME), dimethylformamide (DMF) and 1,2-difluorobenzene (DFB) solvents were stirred over CaH₂ at room temperature under nitrogen atmosphere overnight prior to distillation under reduced pressure. Tetrahydrofuran (THF) was distilled under nitrogen from sodium and benzophenone and stored over 4 Å molecular sieves. Glassware for reactions were oven-dried overnight prior to use in experiments. Column chromatography using silica (230-400 mesh) was carried out using analytical grade eluent mixtures of *n*-hexane and ethyl acetate. ¹H, ¹³C, ¹⁹F and ³¹P NMR spectra were all carried out at 298 K and recorded using Bruker AV-400 and AV-500 spectrometers. The chemical shifts (δ) for ¹H and ³¹P{¹H} spectra were referenced to solvent, bis(triphenylphosphine)iminium tetrakis(pentafluorophenyl)borate {[PPN][BAR^F₂₀]} or hexamethylphosphoramide (HMPA). The starting materials Na[B(C₆F₅)₄]¹ and K[B(C₆F₅)₄]² were prepared using reported methods. All other reagents were obtained commercially and used as received.

Order in PPh₃



$\text{Na}[\text{BAr}^{\text{F}}_{20}]$ (35.0 mg, 1.0 equiv, 0.05 mmol) and PPh_3 (0.25, 0.5, 1.0 equiv) were dissolved in DFB (0.5 mL). The solution was added to a J. Young's NMR tube containing BnCl (6.2 mg, 1.0 equiv, 0.05 mmol) and $[\text{PPN}][\text{BAr}^{\text{F}}_{20}]$ (30.3 mg, 0.025 mmol) as an internal standard. The reaction was monitored at 298 K by ^{31}P NMR spectroscopy to determine the concentration of the product $[\text{BnPPH}_3][\text{BAr}^{\text{F}}_{20}]$ and the remaining starting material.

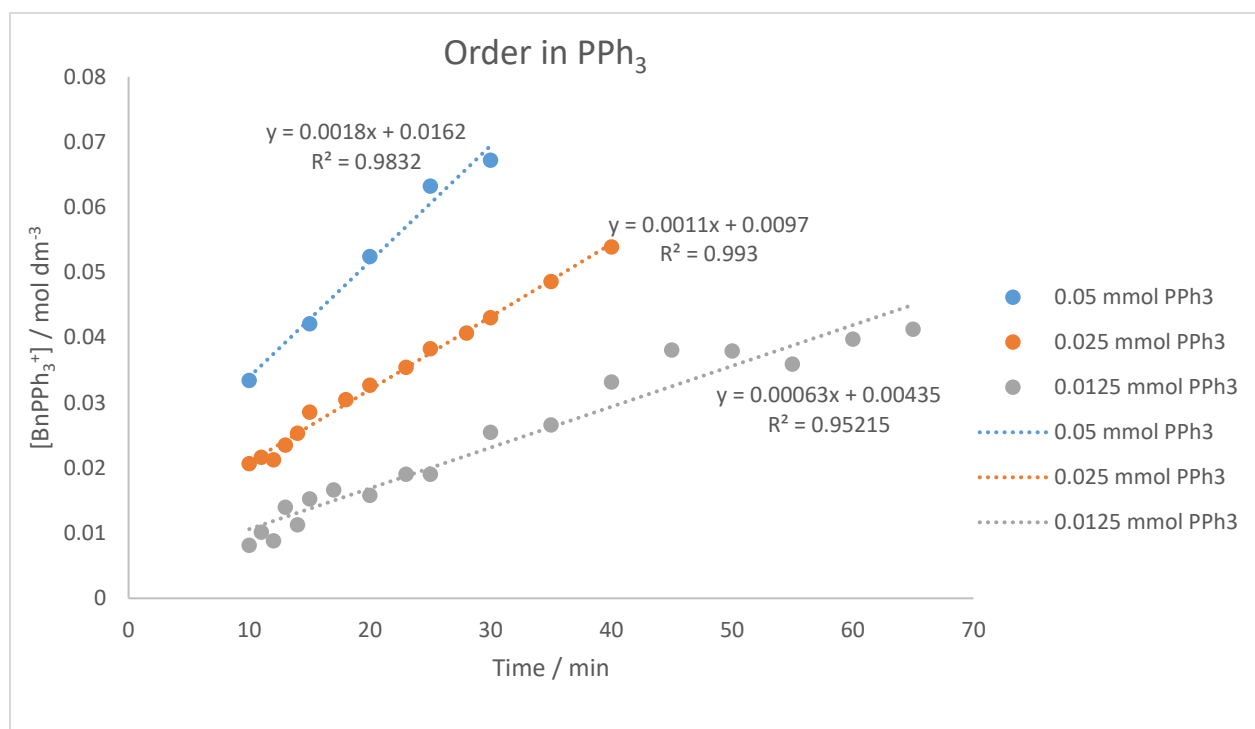
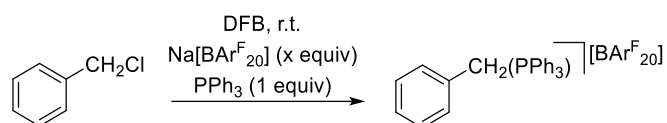


Figure S1. Initial rates plot of time versus concentration of PPh_3 for determination of order in PPh_3

PPh_3 eq.	k_{obs}
0.25	6.3×10^{-4}
0.5	1.1×10^{-3}
1.0	1.8×10^{-3}

Order in Na[BAr^F₂₀]



PPh₃ (13.0 mg, 1.0 equiv, 0.05 mmol) and Na[BAr^F₂₀] (0.25, 0.5, 1.0 equiv) were dissolved in DFB (0.5 mL). The solution was added to a J. Young's NMR tube containing BnCl (6.2 mg, 1.0 equiv, 0.05 mmol) and [PPN][BAr^F₂₀] (30.3 mg, 0.025 mmol) as an internal standard. The reaction was monitored at 298 K by ³¹P NMR spectroscopy to determine the concentration of the product [BnPPH₃][BAr^F₂₀] and the remaining starting material.

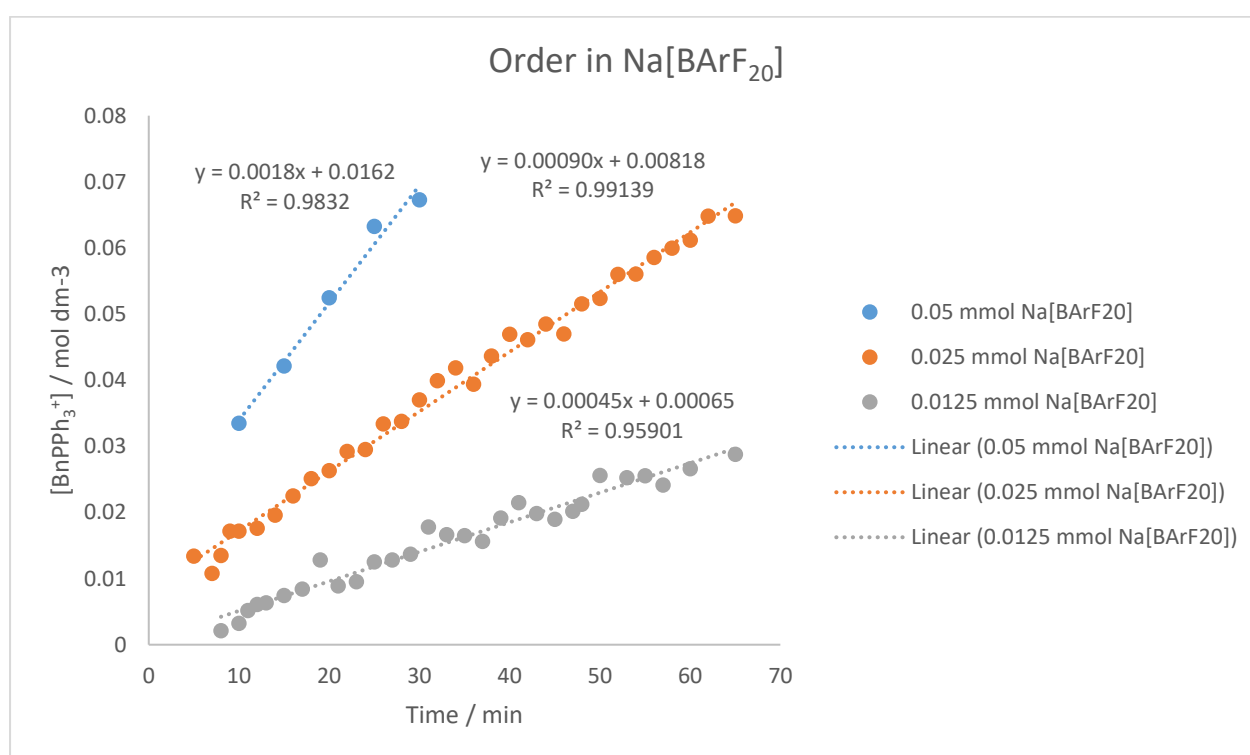
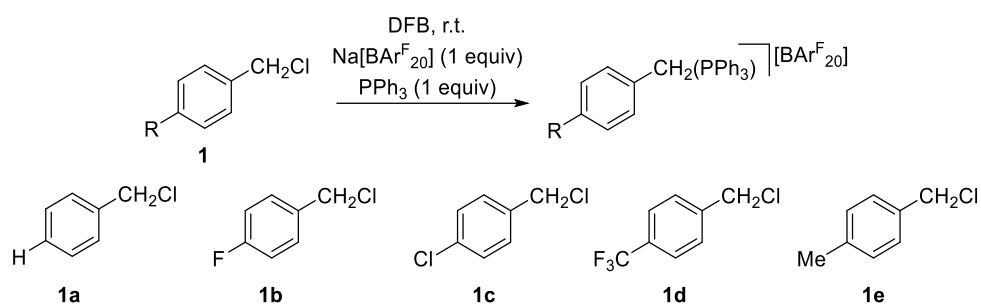


Figure S2. Initial rates plot of time versus concentration of Na[BAr^F₂₀] for determination of order in Na[BAr^F₂₀]

Eq. Na[BAr ^F ₂₀]	k _{obs}
0.25	4.5x10 ⁻⁴
0.5	9.0x10 ⁻⁴
1.0	1.8x10 ⁻³

Hammett plot analysis



PPh₃ (13.0 mg, 1.0 equiv, 0.05 mmol) and Na[BAr^F₂₀] (35.0 mg, 1.0 equiv, 0.05 mmol) were dissolved in DFB (0.5 mL). The solution was added to a J. Young's NMR tube containing a combinations of compounds **1a**, **1b**, **1c**, **1d** and **1e** such that the combined concentration of compounds **1** was equal to 1.0 equiv. The reaction was monitored at 298 K by ¹H and ³¹P NMR spectroscopies to determine the ratio of the products (and thus their relative rate values).

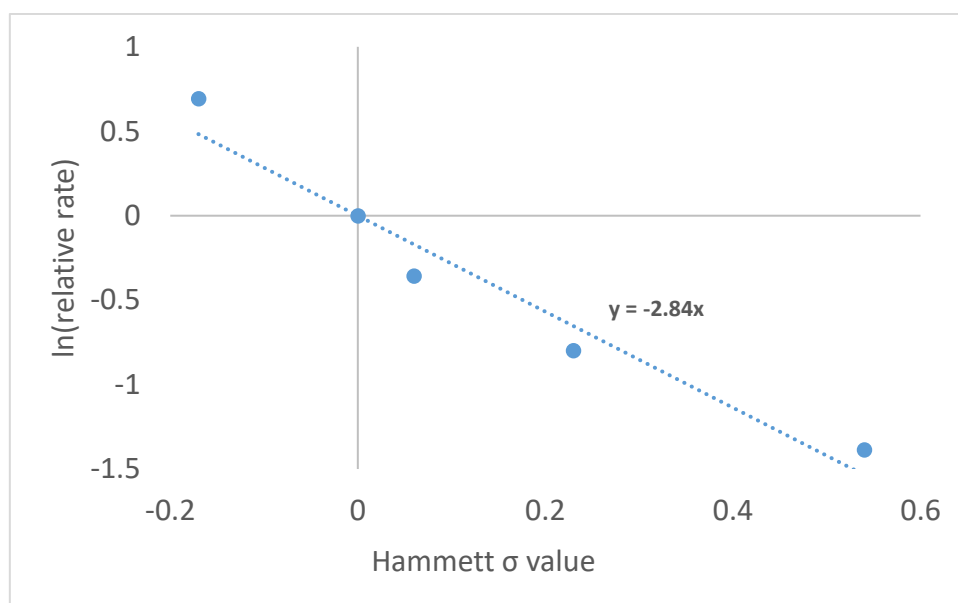
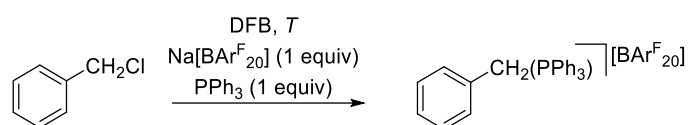


Figure S3. Plot of natural logarithmic of rate versus Hammett σ -values (i.e. Hammett plot analysis) for reaction of PPh₃ and Na[BAr^F₂₀] with various benzyl chlorides. $\rho = -2.84 \pm 0.37$.

Activation barrier for reaction between PPh₃ and BnCl with Na[BAr^F₂₀] additive



PPh₃ (13.0 mg, 1.0 equiv, 0.05 mmol) and Na[BAr^F₂₀] (35.0 mg, 1.0 equiv, 0.05 mmol) were dissolved in DFB (0.5 mL). The solution was added to a J. Young's NMR tube containing BnCl (6.2 mg, 1.0 equiv, 0.05 mmol). A sealed capillary containing neat hexamethylphosphoramide was added for an internal standard. The reaction was monitored at 298 K, 303 K, 308 K, 313 K or 318 K by ³¹P NMR spectroscopy to determine the concentration of the product and the remaining starting material (PPh₃).

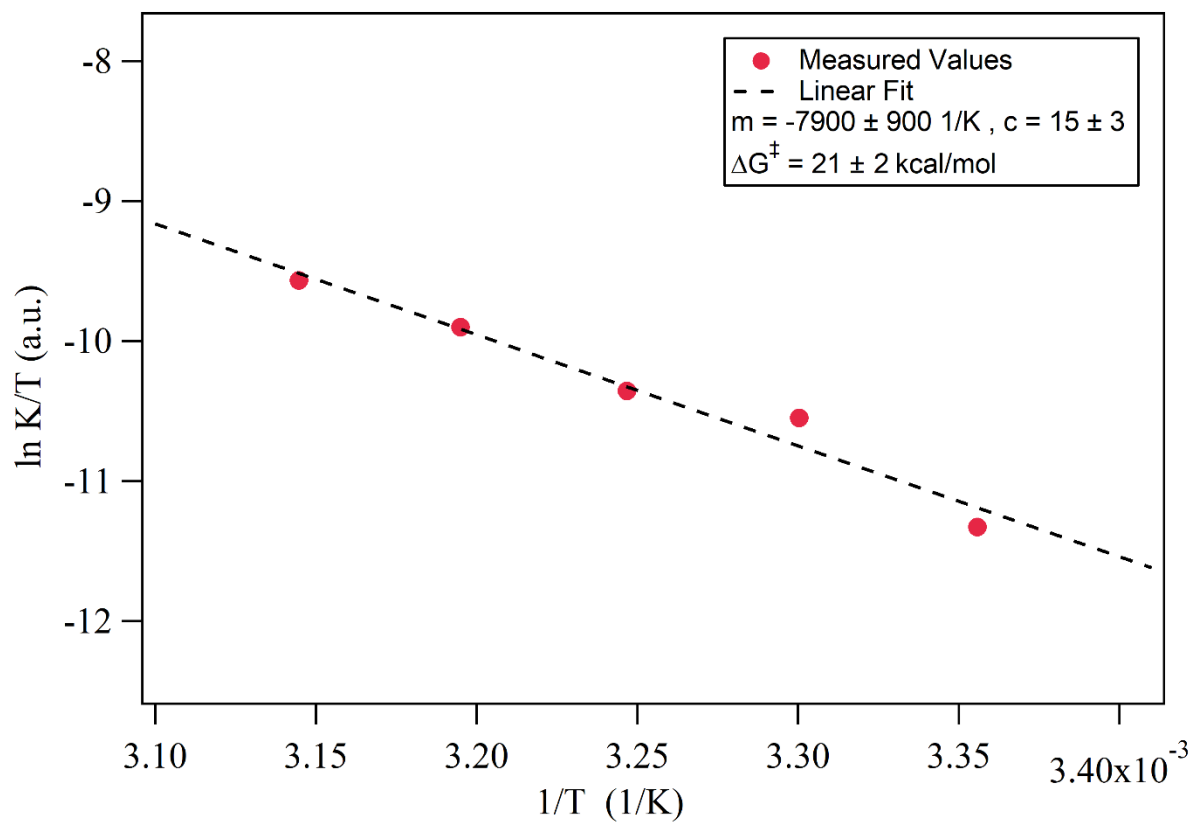
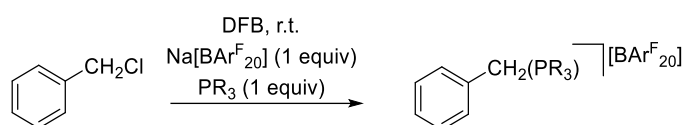


Figure S4. Eyring plot for reaction between PPh_3 , $\text{Na}[\text{BAr}^{\text{F}}_{20}]$ and BnCl at 298 K, 303 K, 308 K, 313 K and 318 K.

Activation parameters: $\Delta H^\ddagger = 15.6 \text{ kcal mol}^{-1}$, $\Delta S^\ddagger = -0.017 \text{ kcal mol}^{-1} \text{ K}^{-1}$, $\Delta G^\ddagger = 20.7 \pm 2.0 \text{ kcal mol}^{-1}$

Rates of reaction with different phosphines



PR₃ attempted:

PPh₃ PPh₂Me P(4-CF₃-C₆H₄)₃ PPh₂(All) PCy₃ P(1-Np)₃

PPh₂Cy PPhCy₂ P(4-Anis)₃ PPh₂(2-BrC₆H₄) P(4-Tol)₃

PR₃ (1.0 equiv, 0.05 mmol) and Na[BAR^F₂₀] (35.0 mg, 1.0 equiv, 0.05 mmol) were dissolved in DFB (0.5 mL). The solution was added to a J. Young's NMR tube containing BnCl (6.2 mg, 1.0 equiv, 0.05 mmol) and [PPN][BAR^F₂₀] (30.3 mg, 0.025 mmol) as an internal standard. The reaction was monitored via ³¹P NMR spectroscopy for the first 60 minutes of reaction (or thereabouts). The reaction with phosphine P(4-CF₃-C₆H₄)₃ was monitored for 10 days, after which a yield of 17% was observed, giving a rate 590 times less than PPh₃.

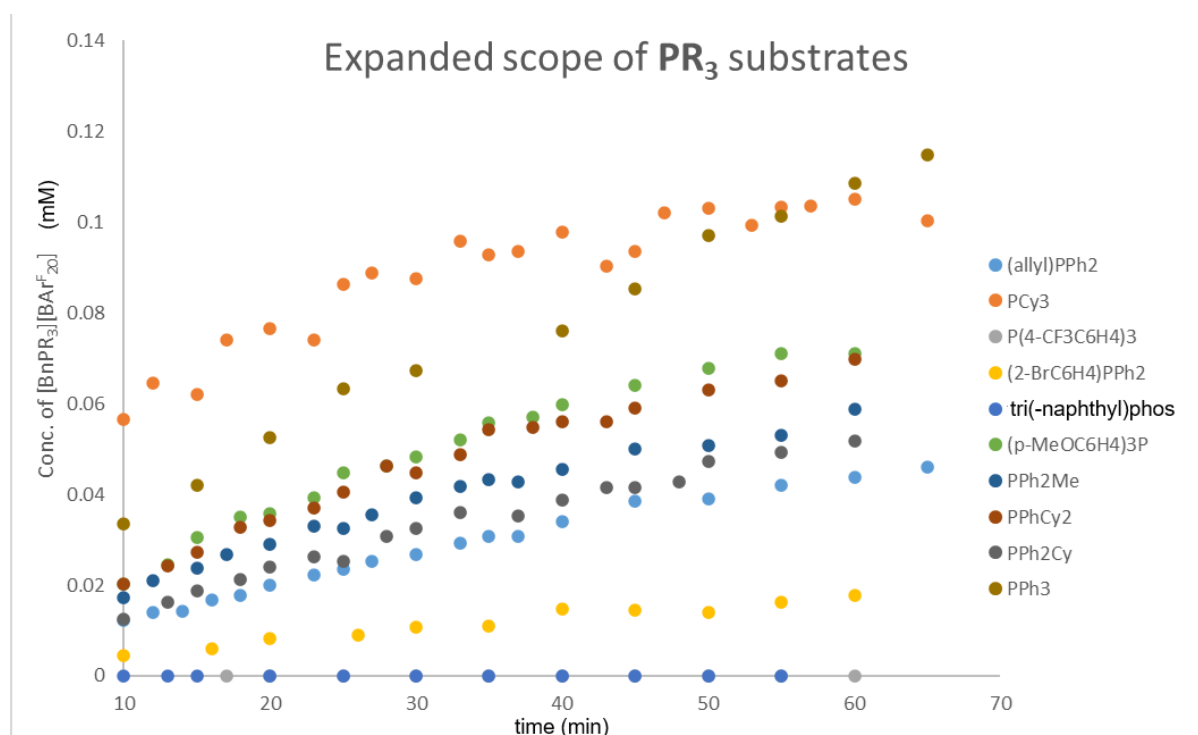


Figure S5. Plot of product concentration versus time for the reaction of various phosphines (PR₃) with BnCl and Na[BAR^F₂₀] at room temperature.

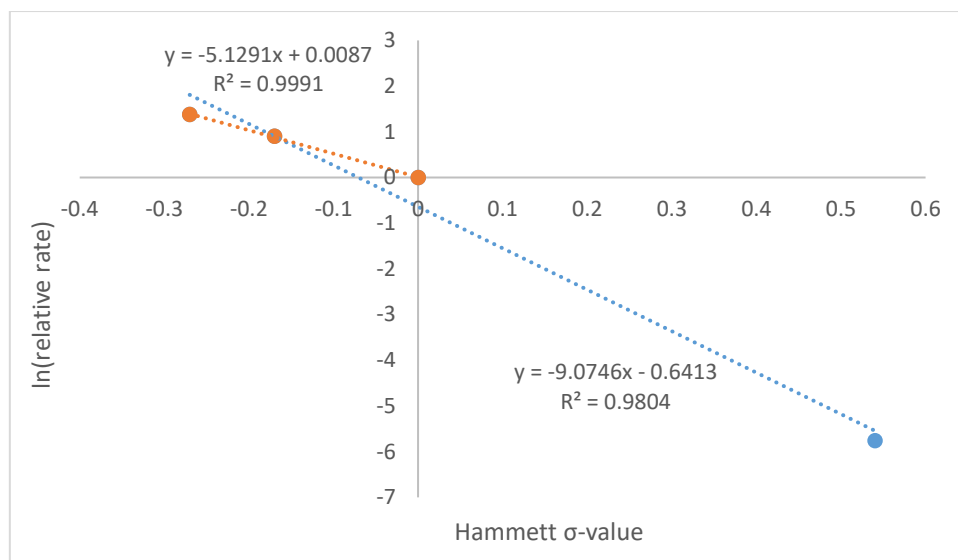


Figure S6. Plot of natural logarithm of relative reaction rates vs Hammett σ -values for aryl substituents of homoleptic triarylphosphines (PAr_3).

Addition of Na[BAr^F₂₀] to PPh₃

³¹P NMR signal evidence for LP ground state

A sample of PPh₃ (13.1 mg, 0.05 mmol) was dissolved in 1 mL DFB. [PPN][BAr^F₂₀] (7.2 mg, 0.006 mmol) was added as an internal reference and the sample analysed by ³¹P NMR spectroscopy. Na[BAr^F₂₀] (35.8 mg, 0.05 mmol) was added and the sample analysed again with ³¹P NMR spectroscopy.

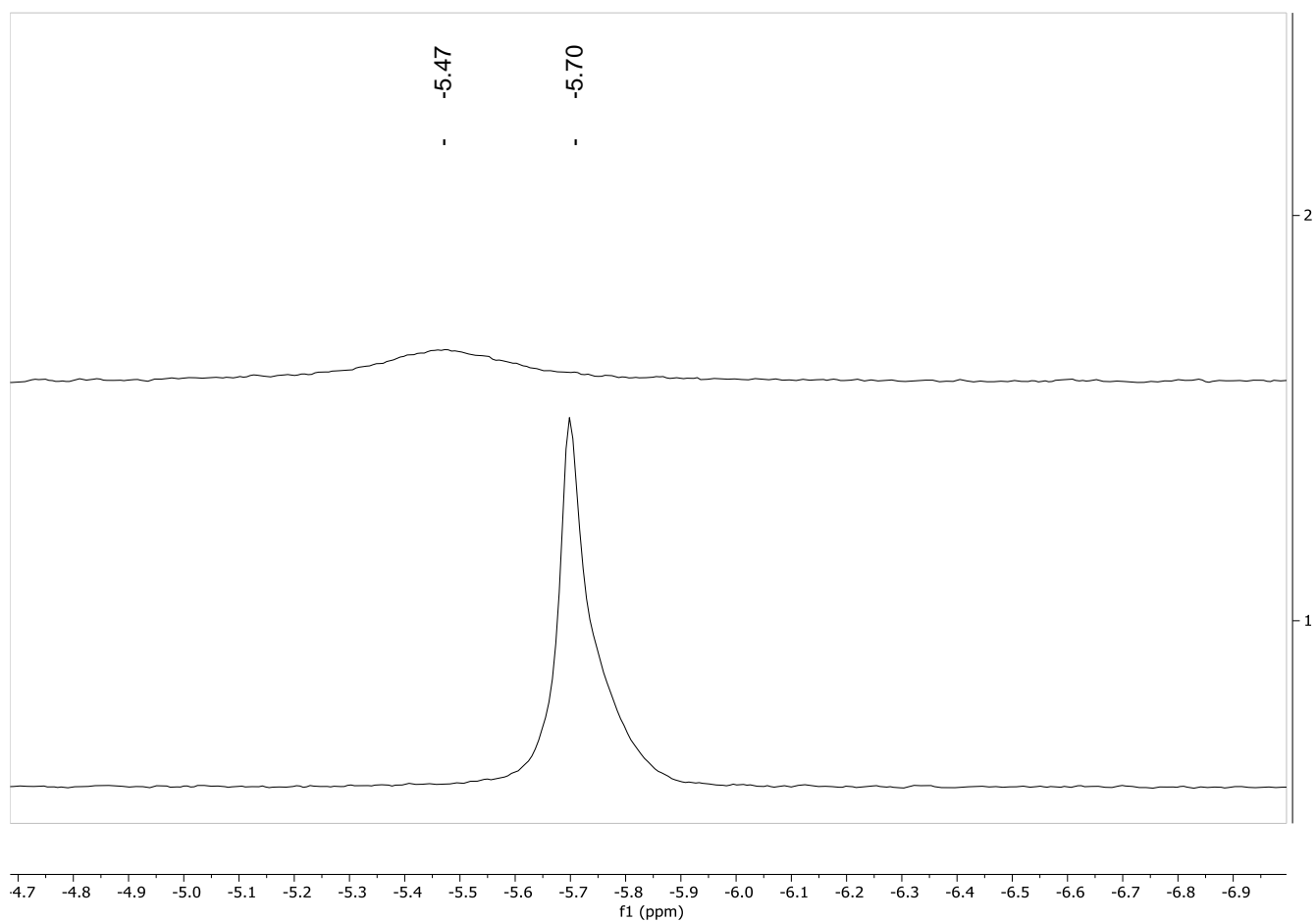


Figure S7. ³¹P NMR spectra of samples of PPh₃ (bottom) and Na[BAr^F₂₀] + PPh₃ in DFB relative to [PPN][BAr^F₂₀] internal standard.

DOSY evidence for LP ground state

A sample of PPh₃ (13.0 mg, 1.0 equiv, 0.05 mmol) was dissolved in 0.65 mL DFB and 0.1 mL toluene-*d*₈. The sample was analysed by ¹H DOSY NMR. Na[BAR^F₂₀] (35.0 mg, 1.0 equiv, 0.05 mmol) was then added and the sample reanalysed by ¹H DOSY NMR.

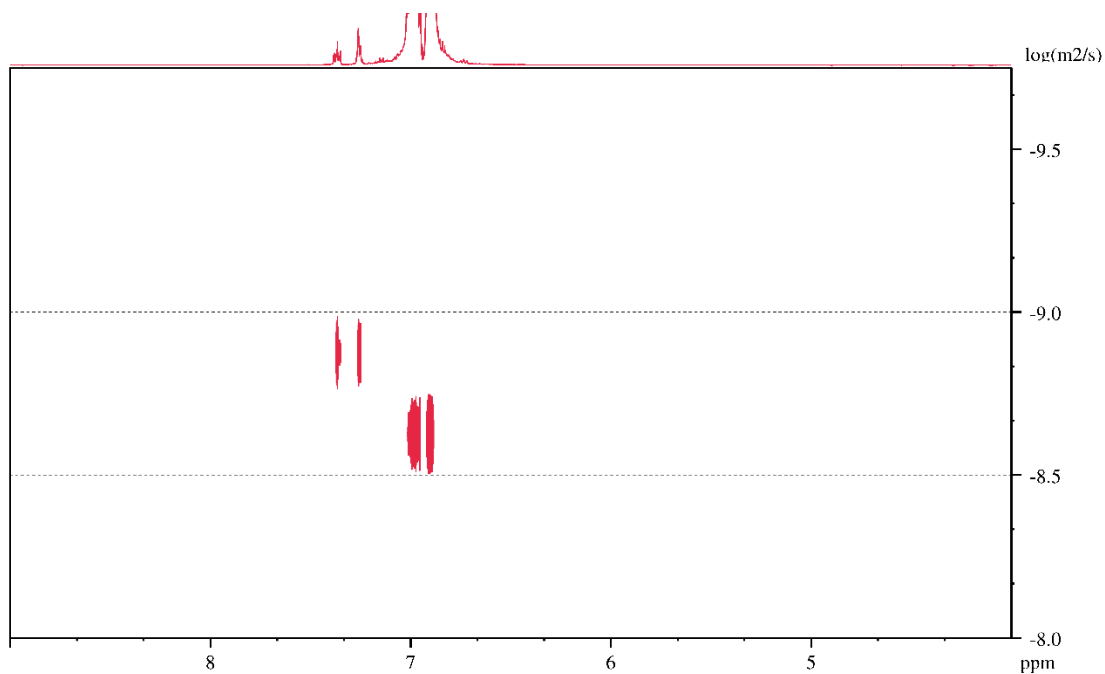


Figure S8. ¹H DOSY NMR spectrum of PPh₃. Diffusion rate = $9.18 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$.

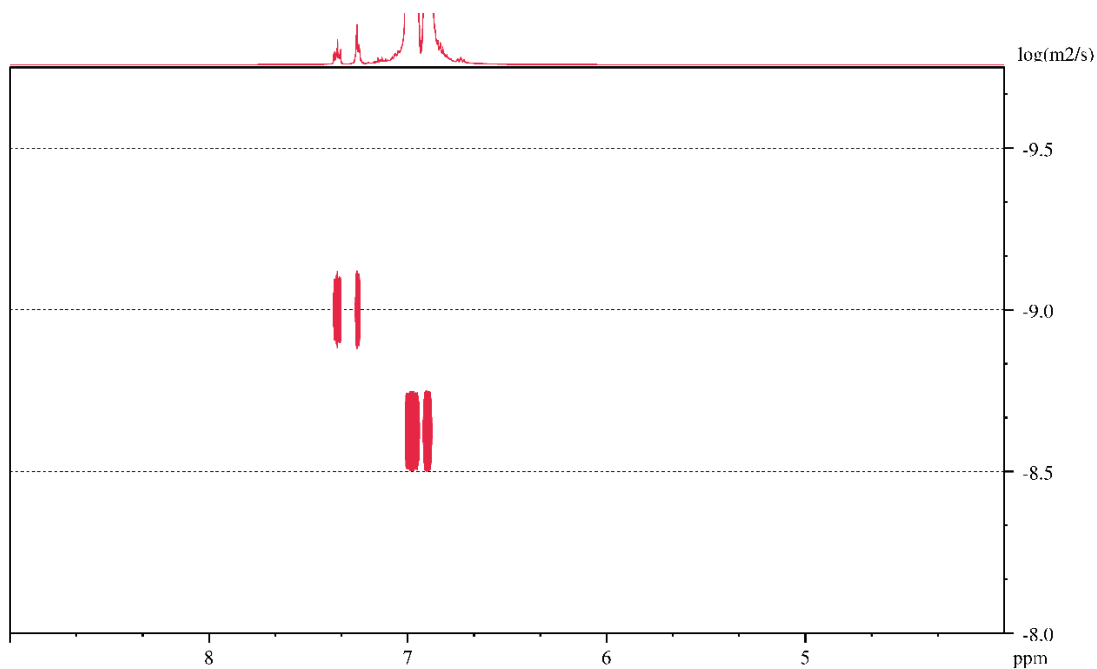


Figure S9. ¹H DOSY NMR spectrum of PPh₃/Na[BAR^F₂₀]. Diffusion rate = $8.43 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$.

Computational Studies

Computational methodology

To gain insight into the mechanism of formation of the heterocyclic compounds, we performed DFT calculations with the Gaussian 16 suite of programs (Revision A.03).³

The calculations were performed using the range-separated hybrid dispersion-corrected ω B97X-D exchange-correlation functional.⁴ The solvation effects were taken into account by computing the solvation free energies employing the SMD implicit solvation model (solvent: Dichloromethane $\rightarrow \epsilon = 8.93$).⁵ Geometry optimisations and transition state locations were performed in solution phase utilizing the SMD model. All the converged geometries were analysed by vibrational frequency calculations to identify the nature of the obtained structures. The vibrational analysis revealed that all located transition states possess only one negative Hessian eigenvalue, while no imaginary frequencies were obtained for the reported minima.

The formula used to calculate the free energy: $G = E_0' + (G_0(\text{DCM}) - E_0(\text{DCM})) + \Delta G_{\text{conc}}$. The reported Gibbs free energies were obtained by combining ω B97X-D/Def2TZVPP electronic energies (E_0') with the thermal and entropic contributions computed at the ω B97X-D/Def2SVP level at $T = 298.15$ K ($G_0 - E_0$).⁶ The $G_{\text{sol}}(\text{DCM})$ is the solution-phase Gibbs free energy, which was derived from a single point energy calculation at the ω B97X-D/Def2SVP level for the geometry optimized in solution phase by employing the SMD model. The value of ΔG_{conc} (0.0030119 Hartree at 298.15 K ≈ 1.89 kcal/mol) corresponds to concentration correction to the Gibbs free energy when shifting from ideal gas standard state ($p = 1$ atm) to the standard concentration in solution phase ($c = 1$ mol/dm³). The conformational analysis was carried out in the MacroModel software (Release 2017-1).⁷

Computational results

Cl anion removal

The thermodynamics of the pathway involving the formation of benzylic carbocation was also considered (Figure S10). The free energy change associated with the C-Cl bond cleavage in the benzyl chloride was computed to be 183.1 kcal/mol, hence, the spontaneous Cl⁻ anion dissociation is highly unlikely under the applied conditions.

The DFT computations estimated that the reaction, resulting in NaCl and the complex wherein the benzylic carbocation is positioned in close proximity of the [BAr^F₂₀]⁻ anion, was thermodynamically still rather unfavorable ($\Delta G = 30.6$ kcal/mol). The respective transition state is expected to lie higher than the product side. Therefore, the Na[BAr^F₂₀]-assisted C-Cl bond cleavage can be excluded as well.

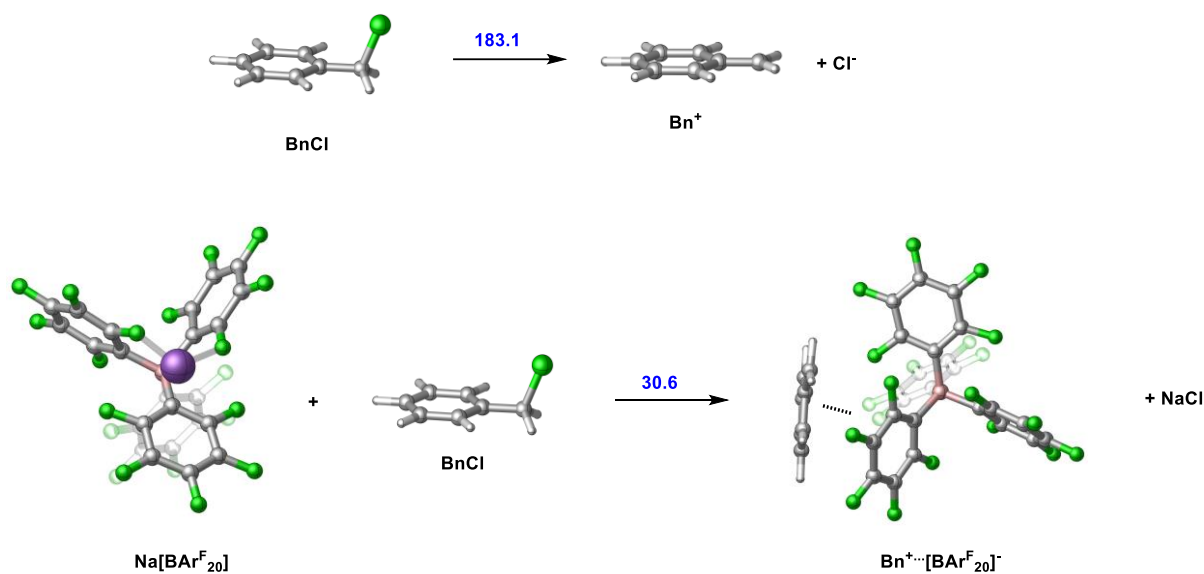


Figure S10. Gibbs energy changes associated with the removal of Cl anion.

Transition states of C-Cl cleavage

Guided by the computational results above, we assessed a pathway in which PPh₃ is involved in the C-Cl bond-breaking step as a nucleophile. At the outset, we chose the monomeric state of the Na[BAR^F₂₀], as a possible reference state in our calculations. The barrier for C-Cl cleavage was calculated by computing the free energy difference between the respective TS and the Na[BAR^F₂₀] reference state. Considering the large conformational space, an extensive conformational search was performed for the transition states, and some representative examples are shown in Figure S11. These TSs correspond to the formation of the loosely bound complex [Bn-PPh₃]⁺⋯NaCl⋯[BAR^F₂₀]⁻. The lowest barrier related to C-Cl activation is estimated to be 21.9 kcal/mol with respect to the separate state Na[BAR^F₂₀]⁻ + PPh₃ + BnCl, which points to a kinetically feasible C-Cl activation.

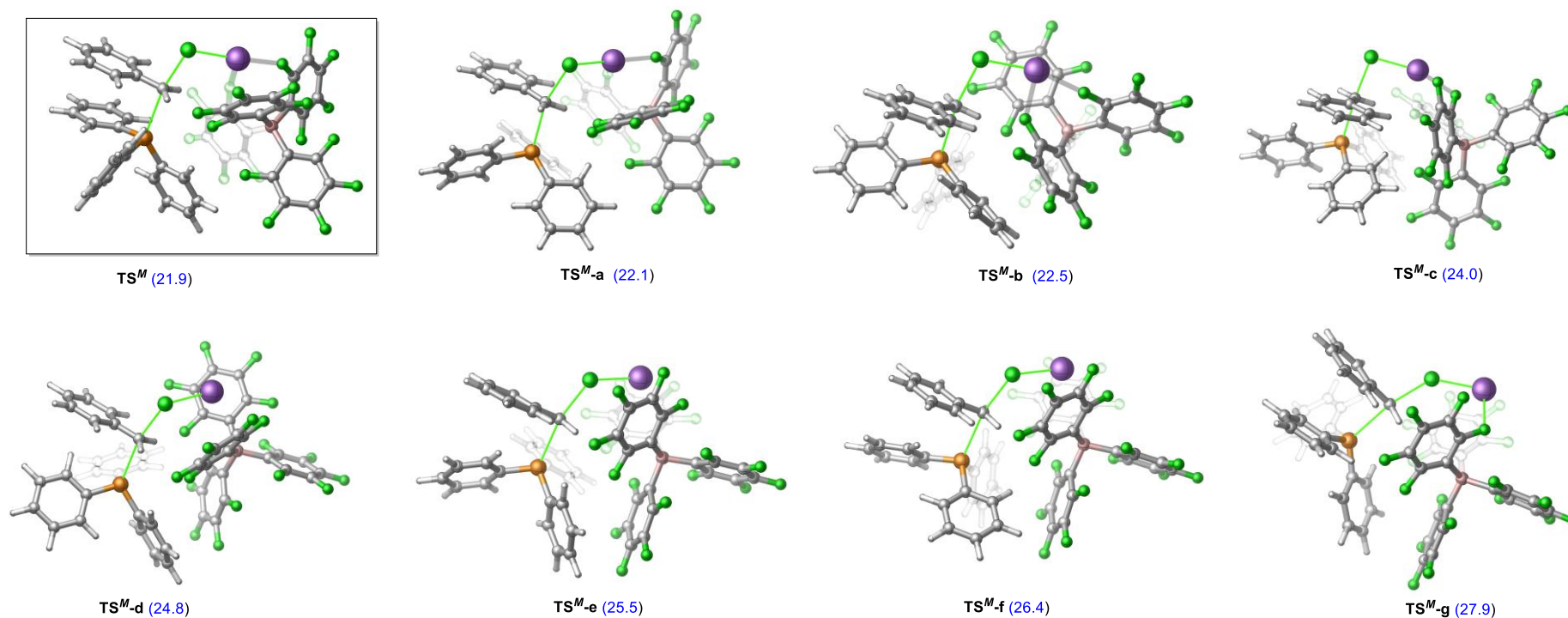


Figure S11. DFT-optimized conformers of **TS^M** transition state. Relative stabilities are given in parenthesis (in kcal/mol) with respect to separate state **Na[BAR^F₂₀]⁻ + PPh₃ + BnCl**.

Dimerization of Na[BAR^F₂₀]

Based on our previous experience, we examined the possibility of a dimeric form of the Na[BAR^F₂₀] species. In the dimer Na[BAR^F₂₀]···Na[BAR^F₂₀], one of the Na⁺ ions connects the two BAR^F₂₀-fragments, which may be retained in the solution to some extent. Various conformers were identified, shown in Figure S12 along with free energy change associated with the dimerization. The computed data suggest that the dimerization is slightly exergonic (-2.4 kcal/mol), and the existence of the dimeric form cannot be excluded.

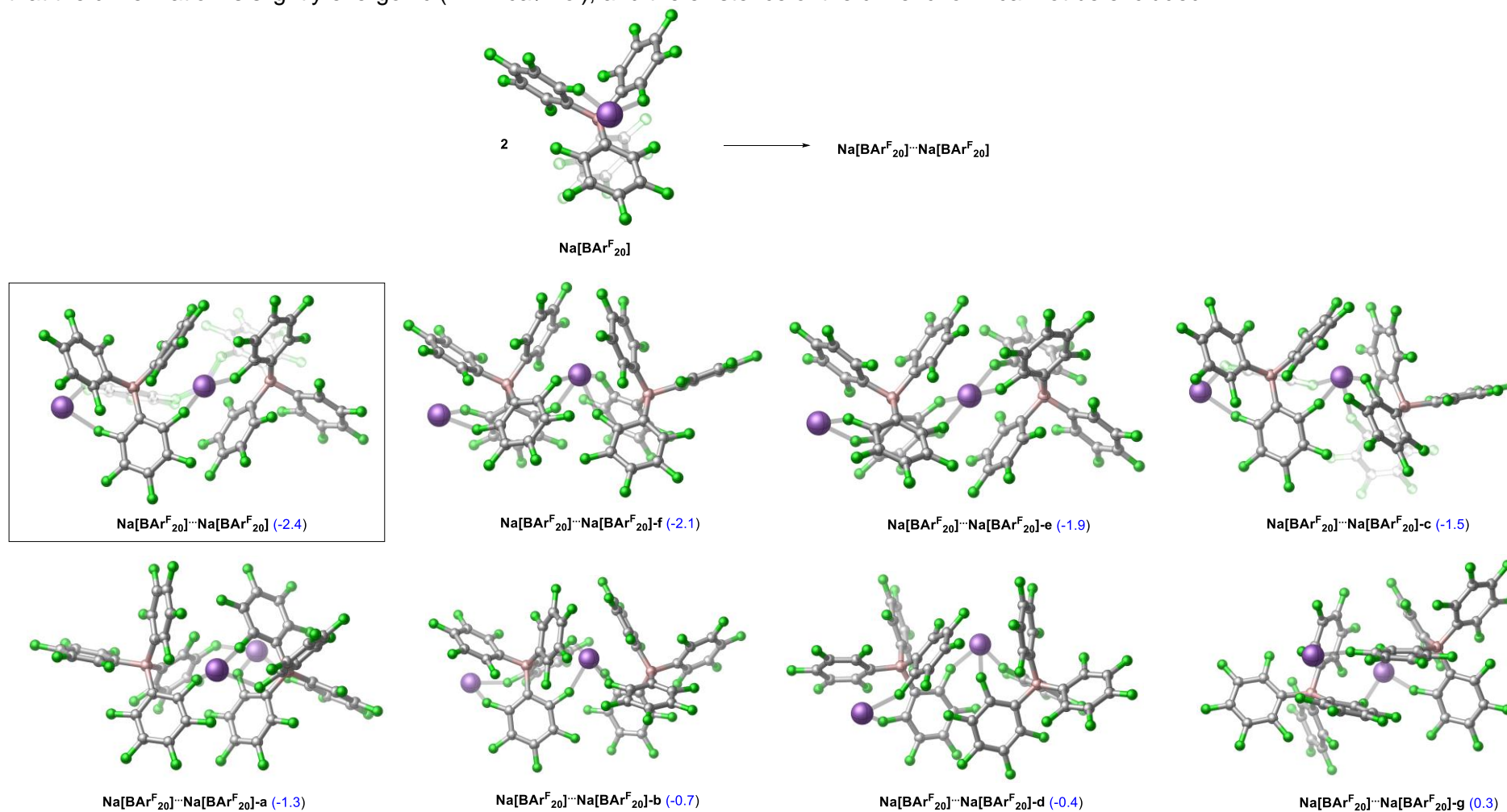


Figure 12. Gibbs energy changes associated with the dimerization of Na[BAR^F₂₀] species are given in parenthesis (in kcal/mol).

PPh₃ coordination to Na[BAr^F₂₀]

Next, DFT calculations were carried out to estimate the relative stability of the complex PPh₃⋯Na[BAr^F₂₀] in the solution phase. The coordination was predicted to be favored by 1.8 kcal/mol (Figure S13), thus, for the monomeric pathway, the PPh₃⋯Na[BAr^F₂₀] complex was used as the reference state (see Figure 4B in the main text).

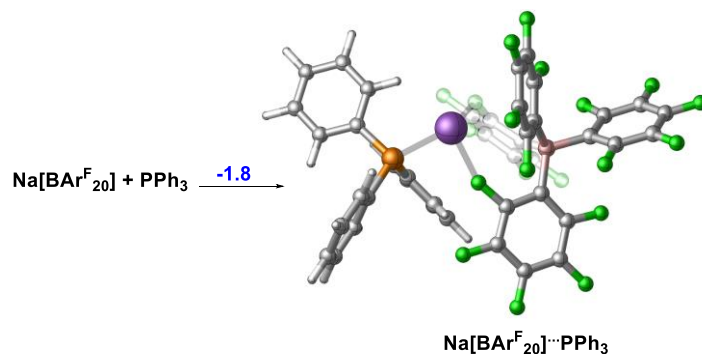


Figure S13. Gibbs energy change associated with the PPh₃ coordination to Na[BAr^F₂₀].

Similarly to the monomeric state, the thermodynamics of the PPh₃⋯Na[BAr^F₂₀]⋯Na[BAr^F₂₀] formation was computed (Figure S14). The formation of the adduct is only slightly exergonic (-0.8 kcal/mol), yet, this state was used as a reference state to estimate the overall reaction barrier on the dimeric pathway (see Figure 4C in the main text).

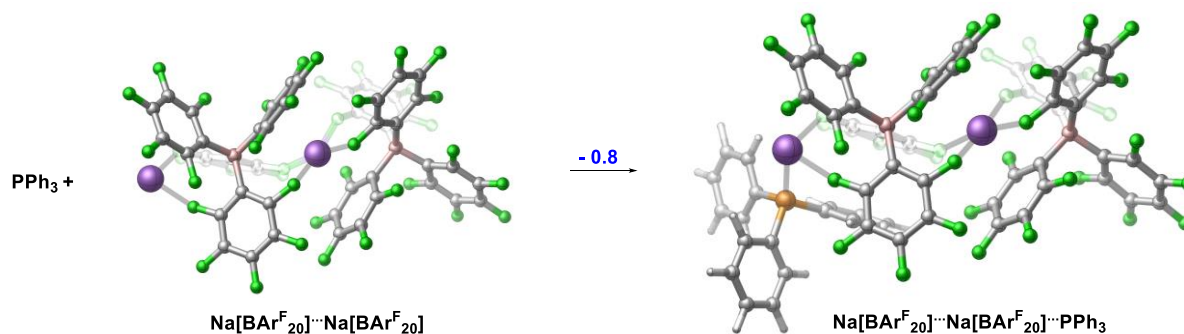


Figure 14. Gibbs energy change associated with the PPh₃ coordination to Na[BAr^F₂₀]⋯Na[BAr^F₂₀].

C-Cl activation without Na⁺ assistance

For Na⁺-free reaction path, the activation barrier corresponding to the nucleophilic substitution of the chloride by the PPh₃ is computed to be 29.2 kcal/mol with respect to the reference state PPh₃⋯Na[BAr^F₂₀] + BnCl (Figure S15). From a kinetic standpoint, this pathway is not competitive as the overall barrier height is about 6 kcal/mol higher than that of the Na[BAr^F₂₀]-assisted reaction.

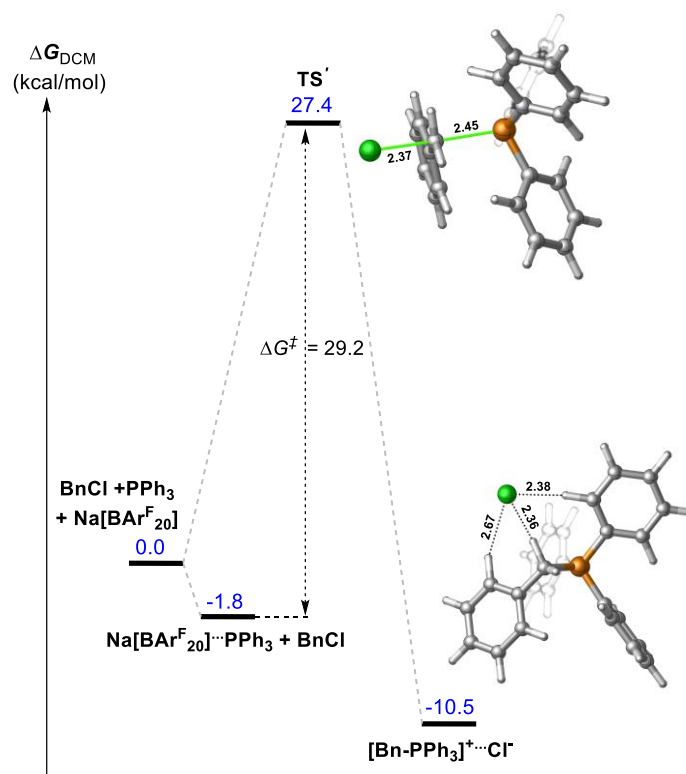


Figure 15. Gibbs energy change associated with the reaction between **BnCl** and **PPh₃** relative to a ground state with a monomeric Na[BAr^F₂₀]⁻⋯PPh₃ adduct.

Computed energy components of the reported structures.

Table S1. Summary of energy data (given in Hartree) computed for optimized structures at the ω B97X-D/Def2SVP level of theory. Note that **G** contains concentration correction. For the definition of various energy components, see Computational details section (above).

Structure	E_0'	$G_0(\text{DCM})$	$E_0(\text{DCM})$	G
BnCl	-731.1916	-730.6549	-730.7430	-731.1005
Bn ⁺	-270.7385	-270.3598	-270.4487	-270.6466
Cl ⁻	-460.1494	-460.0069	-459.9912	-460.1620
Na[BAr ^F ₂₀]	-3098.8349	-3095.2176	-3095.3528	-3098.6968
Bn ⁺ ...[BAr ^F ₂₀] ⁻	-3207.3799	-3203.4194	-3203.6667	-3207.1296
NaCl	-622.6001	-622.3980	-622.3762	-622.6189
PPh ₃	-1036.3385	-1035.2582	-1035.4881	-1036.1056
Na[BAr ^F ₂₀] ⁻ ...PPh ₃	-4135.1998	-4130.4845	-4130.8761	-4134.8052
Na[BAr ^F ₂₀] ⁻ ...Na[BAr ^F ₂₀] ⁻ ...PPh ₃	-7234.0649	-7225.7232	-7226.2808	-7233.5042
Na[BAr ^F ₂₀] ⁻ ...Na[BAr ^F ₂₀]	-6197.6985	-6190.4567	-6190.7548	-6197.3974
Na[BAr ^F ₂₀] ⁻ ...Na[BAr ^F ₂₀]-a	-6197.6977	-6190.4579	-6190.7569	-6197.3956
Na[BAr ^F ₂₀] ⁻ ...Na[BAr ^F ₂₀]-b	-6197.6979	-6190.4535	-6190.7537	-6197.3947
Na[BAr ^F ₂₀] ⁻ ...Na[BAr ^F ₂₀]-c	-6197.6987	-6190.4541	-6190.7538	-6197.3959
Na[BAr ^F ₂₀] ⁻ ...Na[BAr ^F ₂₀]-d	-6197.6951	-6190.4535	-6190.7514	-6197.3942
Na[BAr ^F ₂₀] ⁻ ...Na[BAr ^F ₂₀]-e	-6197.6958	-6190.4543	-6190.7504	-6197.3966
Na[BAr ^F ₂₀] ⁻ ...Na[BAr ^F ₂₀]-f	-6197.6996	-6190.4554	-6190.7550	-6197.3970
Na[BAr ^F ₂₀] ⁻ ...Na[BAr ^F ₂₀]-g	-6197.6945	-6190.4550	-6190.7535	-6197.3930
TS ^I	-1767.5057	-1765.8608	-1766.2010	-1767.1624
[Bn-PPh ₃] ⁺ ...Cl ⁻	-1767.5704	-1765.9200	-1766.2646	-1767.2227
Na[BAr ^F ₂₀] ⁻ ...BnCl...PPh ₃	-4866.3939	-4861.1288	-4861.6313	-4865.8884
TS ^M	-4866.3761	-4861.1101	-4861.6153	-4865.8679
TS ^M -a	-4866.3729	-4861.1081	-4861.6104	-4865.8676
TS ^M -b	-4866.3732	-4861.1085	-4861.6117	-4865.8670
TS ^M -c	-4866.3720	-4861.1058	-4861.6101	-4865.8646
TS ^M -d	-4866.3687	-4861.1012	-4861.6035	-4865.8633
TS ^M -e	-4866.3685	-4861.1013	-4861.6046	-4865.8623
TS ^M -f	-4866.3671	-4861.0985	-4861.6018	-4865.8607
TS ^M -g	-4866.3677	-4861.1004	-4861.6066	-4865.8585
[Bn-PPh ₃] ⁺ ...NaCl...[BAr ^F ₂₀] ⁻	-4866.4497	-4861.1744	-4861.6794	-4865.9417
Na[BAr ^F ₂₀] ⁻ ...Na[BAr ^F ₂₀] ⁻ ...BnCl...PPh ₃	-7965.2608	-7956.3684	-7957.0400	-7964.5861
TS ^P	-7965.2411	-7956.3481	-7957.0183	-7964.5679

[BAr^F₂₀]⁻Na[BAr^F₂₀]	-6035.4912	-6028.2971	-6028.5984	-6035.1870
[Bn-PPh₃]⁺	-1307.1846	-1305.6968	-1306.0456	-1306.8328

Cartesian coordinates of the reported structures

Cartesian coordinates of the optimized geometries are given below in standard XYZ format (units are in Å). The first line is the molecule name (as defined above in Table S1), the second line indicates total number of atoms.

BnCl

15

C	-1.689123	0.484596	-0.467371
C	-0.299046	0.447282	-0.567534
C	0.471289	1.547393	-0.172380
C	-0.173191	2.684399	0.329734
C	-1.562917	2.722783	0.430982
C	-2.323622	1.622466	0.032720
H	-2.280227	-0.378626	-0.782312
H	0.196846	-0.445686	-0.957974
H	0.421555	3.546768	0.643311
H	-2.055085	3.616721	0.821346
H	-3.413029	1.652676	0.110639
C	1.967281	1.499061	-0.260297
H	2.308462	0.826221	-1.056203
H	2.399530	2.494401	-0.418257
Cl	2.704204	0.870950	1.279478

Bn⁺

14

C	-1.617776	0.395521	-0.214380
C	-0.246405	0.394488	-0.319851
C	0.480011	1.628167	-0.192792
C	-0.235495	2.851683	0.044014
C	-1.607134	2.832434	0.144826
C	-2.288394	1.609525	0.015603
H	-2.185587	-0.530799	-0.307657
H	0.307517	-0.529607	-0.499701
H	0.326651	3.783206	0.139144
H	-2.166754	3.751155	0.324022
H	-3.378256	1.602086	0.097170
C	1.845390	1.638863	-0.298330
H	2.403221	0.715146	-0.481093
H	2.410072	2.571378	-0.202502

Cl⁻

1

Cl	-2.565130	0.891478	-0.023344
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Na[BAr^F₂₀]

46

B	-1.307678	-0.766735	0.039487
C	0.208840	-0.825117	-0.615395
C	1.397785	-1.061923	0.071088
C	0.343373	-0.778229	-2.004327
C	2.633410	-1.203588	-0.561130
C	1.551248	-0.912284	-2.676813
C	2.712960	-1.129721	-1.944175
C	-1.313656	-0.623738	1.690317
C	-0.649238	0.459839	2.271980
C	-2.029738	-1.389194	2.599726
C	-0.657803	0.740365	3.632817

C	-2.081003	-1.153371	3.971020
C	-1.385414	-0.074128	4.495202
C	-1.941330	-2.201002	-0.518868
C	-2.869960	-2.356194	-1.550059
C	-1.371645	-3.400546	-0.075636
C	-3.232079	-3.596085	-2.086701
C	-1.698930	-4.654230	-0.579460
C	-2.641046	-4.753943	-1.599451
C	-2.180830	0.567313	-0.414431
C	-3.527501	0.656764	-0.077376
C	-1.676250	1.725176	-1.006646
C	-4.350077	1.745362	-0.323586
C	-2.454967	2.851701	-1.276319
C	-3.800430	2.866006	-0.935383
F	1.423623	-1.182045	1.400783
F	3.732363	-1.422019	0.153086
F	3.879295	-1.264982	-2.559612
F	1.605189	-0.843649	-4.002481
F	-0.738251	-0.585338	-2.767998
F	-0.454547	-3.376655	0.890264
F	-1.126597	-5.748343	-0.101041
F	-2.973495	-5.935052	-2.090739
F	-4.133431	-3.669182	-3.055597
F	-3.492023	-1.304203	-2.089683
F	-2.775316	-2.450086	2.189908
F	-2.798940	-1.938006	4.764937
F	-1.414686	0.179453	5.794432
F	0.009538	1.779882	4.114876
F	0.055349	1.292249	1.503084
F	-4.133678	-0.393230	0.539731
F	-5.631643	1.726907	0.019828
F	-4.548713	3.929212	-1.186104
F	-1.912279	3.917545	-1.849733
F	-0.393286	1.829923	-1.350064
Na	-4.543669	-2.580403	0.780548

Bn⁺[BAr^F₂₀]⁻

59

B	-1.756656	-0.816813	0.194461
C	-0.427803	-0.866274	-0.795815
C	0.899331	-1.051785	-0.414276
C	-0.625602	-0.857523	-2.175672
C	1.951401	-1.168973	-1.324695
C	0.385215	-0.966461	-3.120037
C	1.696957	-1.125040	-2.688202
C	-1.376696	-0.644031	1.794520
C	-0.618611	0.461013	2.185924
C	-1.845618	-1.422860	2.849562
C	-0.304217	0.765778	3.504236
C	-1.556510	-1.156088	4.188364
C	-0.781984	-0.054180	4.520483
C	-2.496616	-2.253049	-0.172692
C	-3.671280	-2.416440	-0.902136
C	-1.834785	-3.446891	0.121170
C	-4.169739	-3.656959	-1.297937
C	-2.295504	-4.706169	-0.244143
C	-3.478020	-4.813176	-0.968508
C	-2.728693	0.502056	-0.066182

C	-3.952199	0.570345	0.604805
C	-2.419363	1.641549	-0.803507
C	-4.830248	1.644568	0.529274
C	-3.260439	2.750311	-0.893571
C	-4.479997	2.750947	-0.235005
F	1.251879	-1.139286	0.869684
F	3.197300	-1.334050	-0.892864
F	2.686487	-1.234404	-3.564320
F	0.108033	-0.920115	-4.422463
F	-1.867058	-0.719454	-2.662338
F	-0.682013	-3.415971	0.797559
F	-1.615832	-5.801392	0.079391
F	-3.936246	-6.002245	-1.337192
F	-5.296928	-3.734632	-2.002616
F	-4.403891	-1.366497	-1.290803
F	-2.624510	-2.487421	2.639378
F	-2.029690	-1.944170	5.149225
F	-0.501266	0.214590	5.789098
F	0.436196	1.829295	3.801437
F	-0.137753	1.297199	1.257833
F	-4.351276	-0.457301	1.359617
F	-5.996914	1.619609	1.164809
F	-5.310787	3.777856	-0.360317
F	-2.922449	3.793000	-1.652216
F	-1.279875	1.745024	-1.496944
C	-2.669887	1.639535	-4.369364
H	-2.503567	2.672156	-4.049335
C	-3.871004	1.019963	-4.151937
C	-4.056671	-0.352221	-4.534895
C	-4.925352	1.712274	-3.464807
C	-5.228762	-0.996552	-4.220520
H	-3.246481	-0.869638	-5.051756
C	-6.085497	1.046425	-3.144698
H	-4.783613	2.761387	-3.198127
C	-6.227612	-0.301061	-3.517680
H	-5.379276	-2.043396	-4.484536
H	-6.886029	1.550858	-2.602343
H	-7.145202	-0.829519	-3.247477
H	-1.841124	1.111844	-4.849305

NaCl

2

Na	0.662396	0.830671	0.000000
Cl	-1.774441	0.830671	0.000000

PPh₃

34

P	-4.087650	0.040965	0.015500
C	-3.191164	-1.568555	0.073897
C	-3.738344	-2.627830	-0.665762
C	-2.018227	-1.791452	0.806082
C	-3.116568	-3.875049	-0.689916
H	-4.661497	-2.473862	-1.232820
C	-1.402529	-3.043922	0.791764
H	-1.575465	-0.982578	1.391962
C	-1.946898	-4.086234	0.041849
H	-3.552480	-4.688065	-1.275438
H	-0.488502	-3.203598	1.368904

H	-1.462386	-5.065489	0.030835
C	-3.259949	0.991331	1.360559
C	-2.177899	1.858218	1.162078
C	-3.762624	0.823254	2.659571
C	-1.605868	2.534258	2.240764
H	-1.771892	2.007480	0.158809
C	-3.183480	1.489143	3.738500
H	-4.616009	0.159762	2.829917
C	-2.103684	2.348673	3.530335
H	-0.762766	3.208230	2.070602
H	-3.582923	1.343168	4.744978
H	-1.653008	2.877361	4.373664
C	-3.381334	0.821825	-1.497160
C	-4.023365	1.974586	-1.974022
C	-2.263462	0.336989	-2.187715
C	-3.547087	2.639544	-3.102516
H	-4.905694	2.359145	-1.453332
C	-1.794133	0.995911	-3.325134
H	-1.748945	-0.560772	-1.837078
C	-2.431083	2.149254	-3.782519
H	-4.054934	3.539466	-3.457616
H	-0.921546	0.605313	-3.854357
H	-2.060762	2.664365	-4.672111

Na[BAr^F₂₀]⁻PPh₃

80

B	-2.076441	-1.460407	1.157666
C	-0.530028	-1.273473	0.601023
C	0.602737	-0.997261	1.363077
C	-0.270230	-1.534256	-0.745934
C	1.891766	-0.946357	0.831352
C	0.994145	-1.493998	-1.319361
C	2.091218	-1.196730	-0.518399
C	-2.271170	-0.942470	2.724846
C	-1.984216	0.392840	3.024075
C	-2.745103	-1.661256	3.815343
C	-2.092101	0.950964	4.291405
C	-2.862758	-1.157860	5.108358
C	-2.526480	0.163905	5.351584
C	-2.294949	-3.100620	0.965403
C	-3.080652	-3.737168	0.001659
C	-1.497744	-3.972664	1.716334
C	-3.124582	-5.124079	-0.169808
C	-1.508043	-5.356183	1.581880
C	-2.334632	-5.940924	0.627373
C	-3.177167	-0.542880	0.325489
C	-4.535851	-0.746946	0.532150
C	-2.898258	0.544411	-0.502753
C	-5.560250	-0.000497	-0.029421
C	-3.886589	1.332830	-1.094188
C	-5.228053	1.067397	-0.853908
F	0.522887	-0.771294	2.677082
F	2.931031	-0.672636	1.613074
F	3.310352	-1.155236	-1.038034
F	1.164733	-1.742012	-2.613488
F	-1.281524	-1.835412	-1.568955
F	-0.671618	-3.482873	2.640509
F	-0.744470	-6.118217	2.351276

F	-2.368179	-7.254983	0.483679
F	-3.914001	-5.660423	-1.090459
F	-3.865258	-3.046043	-0.828266
F	-3.130741	-2.957382	3.689516
F	-3.301827	-1.927764	6.096392
F	-2.614918	0.670848	6.570898
F	-1.791728	2.226240	4.499974
F	-1.531396	1.203538	2.064476
F	-4.940073	-1.755713	1.343133
F	-6.831130	-0.281914	0.234715
F	-6.173293	1.812525	-1.405598
F	-3.549880	2.350539	-1.876352
F	-1.646399	0.908366	-0.777951
Na	-4.836213	-3.735100	2.392113
P	-6.690802	-2.422303	4.196694
C	-6.991017	-3.330315	5.760471
C	-5.908138	-4.030372	6.311329
C	-8.225664	-3.350491	6.420949
C	-6.052594	-4.725601	7.511158
H	-4.938538	-4.020430	5.805157
C	-8.371033	-4.055377	7.615441
H	-9.081238	-2.814017	6.003816
C	-7.285789	-4.740433	8.163418
H	-5.199963	-5.261304	7.934645
H	-9.338614	-4.067103	8.122527
H	-7.402683	-5.289923	9.100437
C	-8.363462	-2.183794	3.482213
C	-9.172351	-1.074429	3.760006
C	-8.841293	-3.175758	2.614474
C	-10.436341	-0.963143	3.181288
H	-8.815726	-0.289375	4.430921
C	-10.108358	-3.067716	2.043396
H	-8.217862	-4.044524	2.380105
C	-10.906775	-1.958700	2.324598
H	-11.057467	-0.092195	3.402938
H	-10.469467	-3.847940	1.369483
H	-11.896581	-1.867532	1.871256
C	-6.221268	-0.735380	4.750217
C	-5.952080	0.220215	3.759165
C	-6.078301	-0.377611	6.094611
C	-5.547598	1.506502	4.103825
H	-6.076973	-0.039816	2.707719
C	-5.673872	0.913480	6.438589
H	-6.276668	-1.106295	6.883314
C	-5.404199	1.855564	5.447863
H	-5.337462	2.236404	3.318598
H	-5.559209	1.178749	7.491771
H	-5.072018	2.859543	5.721193

Na[BAr^F₂₀]⁻Na[BAr^F₂₀]⁻PPh₃

126

B	-7.522467	-5.208268	-0.336430
C	-7.422208	-3.547717	-0.289774
C	-7.503645	-2.672494	-1.376409
C	-7.429156	-2.914187	0.958384
C	-7.551202	-1.281809	-1.245435
C	-7.478530	-1.536354	1.137259
C	-7.539477	-0.709480	0.019290

C	-9.052136	-5.455122	0.261637
C	-10.140068	-4.957904	-0.464536
C	-9.392285	-5.984228	1.507667
C	-11.460613	-5.022392	-0.037836
C	-10.705141	-6.071066	1.977656
C	-11.747928	-5.585766	1.201492
C	-6.339798	-5.971037	0.547564
C	-6.427985	-7.343413	0.756167
C	-5.167032	-5.429070	1.061796
C	-5.493834	-8.122771	1.421828
C	-4.192622	-6.148876	1.748319
C	-4.346664	-7.516930	1.921187
C	-7.312555	-5.818264	-1.868513
C	-8.176314	-6.634705	-2.589325
C	-6.136777	-5.539446	-2.559589
C	-7.948591	-7.074850	-3.889824
C	-5.852175	-5.929228	-3.858964
C	-6.780768	-6.707409	-4.539909
F	-7.527621	-3.125108	-2.631391
F	-7.617188	-0.508327	-2.316886
F	-7.595436	0.603159	0.154162
F	-7.476189	-1.013488	2.351502
F	-7.389035	-3.651391	2.068592
F	-4.882359	-4.114001	0.920490
F	-3.122208	-5.535718	2.224994
F	-3.430997	-8.224855	2.556758
F	-5.679037	-9.427392	1.559473
F	-7.507952	-8.013897	0.293437
F	-8.463245	-6.448722	2.346509
F	-10.956140	-6.607248	3.164630
F	-12.996667	-5.660021	1.630998
F	-12.441694	-4.552195	-0.795084
F	-9.936719	-4.398202	-1.658807
F	-9.346627	-7.061904	-2.055180
F	-8.830139	-7.852510	-4.500323
F	-6.551714	-7.093601	-5.781821
F	-4.721090	-5.582015	-4.446536
F	-5.186055	-4.782667	-1.959140
Na	-9.534202	-8.643470	-0.445572
B	-2.091901	-0.731633	-2.125159
C	-2.838701	-0.567987	-3.597378
C	-4.164992	-0.959750	-3.743189
C	-2.310156	0.039148	-4.736275
C	-4.921589	-0.842049	-4.898942
C	-3.024289	0.193185	-5.925234
C	-4.336995	-0.249236	-6.011963
C	-2.936526	0.339890	-1.177339
C	-3.780163	0.068936	-0.108630
C	-2.898812	1.694978	-1.521459
C	-4.501308	1.024564	0.601478
C	-3.606400	2.690800	-0.859206
C	-4.423219	2.353452	0.215565
C	-0.469155	-0.414904	-2.169256
C	0.232878	0.433355	-1.315790
C	0.335348	-1.148249	-3.043964
C	1.620522	0.576136	-1.346665
C	1.718149	-1.038081	-3.111862
C	2.370144	-0.163896	-2.249199

C	-2.090017	-2.302897	-1.564637
C	-1.598823	-2.557719	-0.278272
C	-2.349141	-3.454025	-2.313492
C	-1.405935	-3.829226	0.250412
C	-2.177185	-4.750661	-1.821765
C	-1.709415	-4.941077	-0.529848
F	-4.805541	-1.536519	-2.692529
F	-6.170859	-1.281641	-4.951107
F	-5.022439	-0.109920	-7.136503
F	-2.456503	0.773043	-6.975015
F	-1.069146	0.524119	-4.756589
F	-0.228410	-2.015254	-3.892920
F	2.418075	-1.759402	-3.980832
F	3.689710	-0.041135	-2.288580
F	2.229126	1.407764	-0.507740
F	-0.391352	1.167208	-0.390888
F	-2.125794	2.098926	-2.531617
F	-3.509894	3.957028	-1.241460
F	-5.105197	3.285509	0.861845
F	-5.258662	0.666201	1.629293
F	-3.977333	-1.202344	0.327480
F	-1.277263	-1.538047	0.517206
F	-0.937460	-3.984799	1.477743
F	-1.552928	-6.165719	-0.053456
F	-2.460428	-5.800318	-2.579681
F	-2.798041	-3.379981	-3.567127
Na	-4.748927	-2.856589	-0.933426
P	-8.005688	-10.554684	-2.034256
C	-6.494684	-9.949023	-2.883403
C	-5.554051	-9.257087	-2.106362
C	-6.260486	-10.099789	-4.253505
C	-4.400943	-8.731446	-2.679681
H	-5.718074	-9.149371	-1.034536
C	-5.100500	-9.574817	-4.828521
H	-6.981951	-10.624894	-4.883063
C	-4.172209	-8.888261	-4.048442
H	-3.684089	-8.189352	-2.058973
H	-4.929831	-9.696490	-5.900265
H	-3.274394	-8.466320	-4.504975
C	-8.901500	-11.501777	-3.320476
C	-8.504808	-12.777541	-3.744200
C	-10.024355	-10.903700	-3.906176
C	-9.216623	-13.437418	-4.743729
H	-7.634127	-13.259303	-3.292439
C	-10.732616	-11.562935	-4.911405
H	-10.346957	-9.911891	-3.577070
C	-10.328896	-12.830003	-5.330279
H	-8.900925	-14.431765	-5.067851
H	-11.604512	-11.085919	-5.364666
H	-10.884343	-13.349309	-6.114778
C	-7.365822	-11.854741	-0.903625
C	-8.223043	-12.290511	0.117341
C	-6.088302	-12.419408	-1.004942
C	-7.815437	-13.276078	1.014452
H	-9.225904	-11.861113	0.213856
C	-5.678062	-13.399319	-0.100696
H	-5.403639	-12.094228	-1.791468
C	-6.538940	-13.829571	0.908606

H	-8.494393	-13.607301	1.803507
H	-4.677696	-13.829493	-0.188197
H	-6.213588	-14.595603	1.616216

Na[BAr^F₂₀]⁻Na[BAr^F₂₀]

92

B	-7.027525	-5.335344	-0.674093
C	-7.128554	-3.676371	-0.602181
C	-7.213324	-2.801714	-1.689330
C	-7.341055	-3.068764	0.641284
C	-7.447223	-1.430371	-1.558911
C	-7.585255	-1.711669	0.818307
C	-7.635737	-0.881548	-0.297864
C	-8.565202	-5.747410	-0.196824
C	-9.643200	-5.356396	-1.000097
C	-8.935104	-6.277624	1.040876
C	-10.977653	-5.486945	-0.633830
C	-10.262648	-6.424104	1.453710
C	-11.291751	-6.028064	0.609869
C	-5.847692	-5.994758	0.292431
C	-5.757868	-7.380593	0.398609
C	-4.832044	-5.337972	0.978104
C	-4.803528	-8.073939	1.127686
C	-3.853837	-5.968985	1.742164
C	-3.829466	-7.354311	1.812289
C	-6.617833	-5.899408	-2.178169
C	-7.281711	-6.860858	-2.929625
C	-5.428841	-5.476183	-2.765601
C	-6.850357	-7.334162	-4.165907
C	-4.946564	-5.892414	-3.997392
C	-5.671144	-6.843648	-4.709420
F	-7.060496	-3.235654	-2.940657
F	-7.498136	-0.653216	-2.627975
F	-7.866656	0.411704	-0.165062
F	-7.775042	-1.213298	2.027634
F	-7.320842	-3.812954	1.747552
F	-4.717417	-3.990544	0.938219
F	-2.949167	-5.254028	2.388827
F	-2.904796	-7.977827	2.519294
F	-4.815878	-9.396609	1.176705
F	-6.678852	-8.155370	-0.228464
F	-8.018408	-6.687202	1.921732
F	-10.540910	-6.946265	2.638671
F	-12.551901	-6.168675	0.978960
F	-11.945290	-5.105162	-1.451729
F	-9.410072	-4.816792	-2.195895
F	-8.424444	-7.435260	-2.478867
F	-7.548743	-8.255386	-4.811661
F	-5.241522	-7.274580	-5.882184
F	-3.823678	-5.403547	-4.492639
F	-4.666336	-4.562975	-2.119555
Na	-8.829265	-8.694348	-0.608493
B	-2.038315	-0.239428	-1.804299
C	-2.642521	-0.157212	-3.346667
C	-3.893709	-0.697872	-3.623034
C	-2.074489	0.513707	-4.429266
C	-4.538938	-0.658858	-4.849483
C	-2.678561	0.593780	-5.684605

C	-3.916985	0.005462	-5.900286
C	-3.103963	0.710940	-0.955078
C	-4.016348	0.325911	0.018110
C	-3.198818	2.063667	-1.297100
C	-4.918753	1.178545	0.647480
C	-4.089524	2.957721	-0.715364
C	-4.965933	2.510876	0.268655
C	-0.471186	0.273450	-1.679734
C	0.028006	1.198462	-0.765466
C	0.504775	-0.355495	-2.455730
C	1.383260	1.510229	-0.651536
C	1.863411	-0.078524	-2.376946
C	2.309114	0.867129	-1.459941
C	-1.904382	-1.801552	-1.235819
C	-1.525701	-2.000987	0.097516
C	-1.950590	-2.972668	-1.997036
C	-1.247779	-3.243726	0.655741
C	-1.690754	-4.243744	-1.476691
C	-1.335683	-4.380563	-0.142435
F	-4.565611	-1.350035	-2.638077
F	-5.717759	-1.237694	-5.026972
F	-4.497945	0.074270	-7.088450
F	-2.078271	1.241240	-6.675021
F	-0.902324	1.139193	-4.325580
F	0.143309	-1.282173	-3.350530
F	2.734484	-0.708984	-3.157338
F	3.600776	1.148861	-1.360318
F	1.793602	2.408481	0.237645
F	-0.775276	1.845831	0.082609
F	-2.380323	2.570554	-2.221455
F	-4.112180	4.229793	-1.089562
F	-5.821783	3.344643	0.837709
F	-5.730981	0.718362	1.589286
F	-4.101449	-0.965119	0.431734
F	-1.411429	-0.953071	0.912771
F	-0.899644	-3.350708	1.927478
F	-1.081747	-5.577800	0.358902
F	-1.779399	-5.318072	-2.246506
F	-2.271842	-2.946440	-3.291256
Na	-4.503474	-2.706137	-0.895555

Na[BAr^F₂₀]⁻Na[BAr^F₂₀]-f

92

B	-1.796573	-0.469942	-1.621973
C	-0.304712	0.205669	-1.420201
C	0.767324	-0.304688	-2.154341
C	0.044528	1.177479	-0.485790
C	2.080491	0.127007	-2.019687
C	1.349032	1.641963	-0.315057
C	2.375123	1.113885	-1.085279
C	-1.548492	-2.014040	-1.053317
C	-1.251304	-2.192657	0.302758
C	-1.470794	-3.182193	-1.816038
C	-0.961962	-3.422652	0.884639
C	-1.190481	-4.440362	-1.274517
C	-0.933722	-4.561923	0.084697
C	-2.334063	-0.434471	-3.192471
C	-3.507667	-1.101889	-3.528490

C	-1.805314	0.323141	-4.236918
C	-4.125535	-1.071465	-4.769053
C	-2.376474	0.381424	-5.509244
C	-3.543283	-0.319226	-5.782108
C	-3.010528	0.349651	-0.833475
C	-3.948399	-0.153832	0.058425
C	-3.248607	1.680339	-1.191977
C	-5.034043	0.555581	0.563133
C	-4.308510	2.441461	-0.714055
C	-5.220827	1.870573	0.167949
F	0.549806	-1.261352	-3.064096
F	3.050071	-0.394172	-2.763599
F	3.620469	1.542665	-0.932684
F	1.616592	2.577644	0.589881
F	-0.865473	1.725071	0.323687
F	-0.709172	1.063635	-4.075968
F	-1.815495	1.117352	-6.460498
F	-4.098645	-0.264266	-6.983038
F	-5.254792	-1.735666	-4.989503
F	-4.130939	-1.858236	-2.594260
F	-1.691163	-3.171603	-3.130461
F	-1.174755	-5.515502	-2.048192
F	-0.663343	-5.743463	0.609257
F	-0.721508	-3.519445	2.182141
F	-1.256945	-1.142930	1.122046
F	-3.882657	-1.437970	0.497353
F	-5.892446	-0.025906	1.390462
F	-6.250510	2.570235	0.618247
F	-4.465880	3.700485	-1.100829
F	-2.421191	2.294213	-2.040849
Na	-4.065396	-3.223061	-0.790477
B	-7.250330	-5.113251	-0.810907
C	-8.132933	-3.721769	-0.615623
C	-9.499331	-3.616093	-0.388194
C	-7.520421	-2.489735	-0.832466
C	-10.204445	-2.415933	-0.346833
C	-8.162146	-1.260491	-0.812362
C	-9.529369	-1.221794	-0.558580
C	-6.894896	-5.070813	-2.435225
C	-5.653759	-4.873624	-3.030516
C	-7.936507	-5.083605	-3.359718
C	-5.442825	-4.701298	-4.395541
C	-7.798361	-4.930781	-4.731111
C	-6.527519	-4.727314	-5.259599
C	-8.053635	-6.485296	-0.336908
C	-8.179120	-7.669501	-1.064833
C	-8.492596	-6.573441	0.989182
C	-8.706884	-8.850254	-0.533794
C	-9.025832	-7.723338	1.559100
C	-9.133519	-8.877292	0.787670
C	-5.906820	-5.185562	0.162591
C	-5.020875	-6.256386	-0.003085
C	-5.619883	-4.364907	1.256329
C	-3.916896	-6.490328	0.808377
C	-4.513865	-4.552877	2.090362
C	-3.659917	-5.625581	1.868709
F	-10.267265	-4.721553	-0.220123
F	-11.511065	-2.412623	-0.129712

F	-10.176014	-0.070056	-0.535211
F	-7.496906	-0.140502	-1.046890
F	-6.197568	-2.450014	-1.091588
F	-8.404688	-5.505820	1.781783
F	-9.431276	-7.730786	2.818711
F	-9.640823	-9.981486	1.304954
F	-8.803252	-9.937776	-1.283595
F	-7.794685	-7.740487	-2.342802
F	-9.209477	-5.263386	-2.923900
F	-8.854765	-4.967765	-5.528054
F	-6.358938	-4.558649	-6.558358
F	-4.223139	-4.494274	-4.862105
F	-4.524604	-4.805693	-2.287102
F	-5.213331	-7.120009	-0.999510
F	-3.115399	-7.517094	0.581032
F	-2.619655	-5.822314	2.655628
F	-4.276686	-3.716038	3.087570
F	-6.392227	-3.323199	1.563853
Na	-10.713990	-6.402870	-1.705536

Na[BAr^F₂₀]⁻Na[BAr^F₂₀]-e

92

B	-7.054773	-5.425396	-0.579739
C	-7.250454	-3.822430	-0.967724
C	-7.133885	-2.728031	-0.109281
C	-7.738735	-3.504440	-2.240679
C	-7.438701	-1.416927	-0.487793
C	-8.048592	-2.217855	-2.661743
C	-7.881264	-1.157290	-1.777710
C	-8.640380	-5.928430	-0.614689
C	-9.526892	-5.379901	0.320023
C	-9.256313	-6.699283	-1.603094
C	-10.900960	-5.586288	0.309161
C	-10.634381	-6.931314	-1.656617
C	-11.463116	-6.371190	-0.693718
C	-6.303440	-5.693575	0.875247
C	-5.019205	-5.201657	1.089869
C	-6.752078	-6.493586	1.920074
C	-4.252096	-5.412681	2.225095
C	-6.034062	-6.755295	3.084077
C	-4.768907	-6.206474	3.243573
C	-6.082463	-6.236204	-1.650334
C	-5.262769	-5.684753	-2.630017
C	-5.982228	-7.621511	-1.571894
C	-4.491407	-6.427179	-3.520673
C	-5.216072	-8.419250	-2.407967
C	-4.458329	-7.810192	-3.402813
F	-6.691513	-2.878153	1.143229
F	-7.295819	-0.418803	0.368967
F	-8.143987	0.079219	-2.157297
F	-8.489845	-1.996327	-3.888238
F	-7.924112	-4.474885	-3.136076
F	-7.952016	-7.121499	1.853586
F	-6.543697	-7.536209	4.023865
F	-4.066845	-6.439119	4.337723
F	-3.048071	-4.877864	2.338246
F	-4.430854	-4.445198	0.132836
F	-8.547659	-7.279115	-2.575959

F	-11.148591	-7.684264	-2.617213
F	-12.765725	-6.586290	-0.723422
F	-11.674285	-5.047561	1.238077
F	-9.054935	-4.606274	1.296866
F	-5.162530	-4.344581	-2.781616
F	-3.788199	-5.826707	-4.464398
F	-3.723140	-8.537812	-4.225084
F	-5.205876	-9.736053	-2.269711
F	-6.706007	-8.287674	-0.635531
Na	-8.660067	-8.734071	0.383087
B	-2.025748	-0.139645	-1.880862
C	-2.772067	0.091442	-3.344541
C	-4.088631	-0.320407	-3.519613
C	-2.269056	0.803121	-4.434559
C	-4.857867	-0.125603	-4.655821
C	-2.994067	1.031050	-5.605278
C	-4.295810	0.563290	-5.723651
C	-1.897029	-1.733049	-1.410432
C	-2.039118	-2.863500	-2.216250
C	-1.415490	-2.004537	-0.123767
C	-1.748866	-4.161120	-1.783457
C	-1.122004	-3.276275	0.351096
C	-1.303430	-4.370943	-0.486503
C	-2.958784	0.765931	-0.855390
C	-3.817703	0.304224	0.134454
C	-2.978846	2.152651	-1.018283
C	-4.568665	1.124714	0.972094
C	-3.726265	3.017971	-0.228983
C	-4.529660	2.498423	0.780607
C	-0.427490	0.295535	-1.879269
C	0.430900	-0.324340	-2.790444
C	0.213481	1.124053	-0.960453
C	1.804335	-0.123805	-2.833473
C	1.589651	1.355762	-0.964874
C	2.392778	0.728194	-1.905468
F	-4.721049	-0.975242	-2.510222
F	-6.102600	-0.578642	-4.722608
F	-4.991625	0.775417	-6.829700
F	-2.447223	1.707252	-6.607037
F	-1.047478	1.334874	-4.417740
F	-2.220289	2.717975	-1.960948
F	-3.680373	4.328901	-0.427716
F	-5.241649	3.304668	1.553657
F	-5.316245	0.608970	1.937347
F	-3.983371	-1.025554	0.352721
F	-1.209164	-1.002318	0.729654
F	-0.683176	-3.453107	1.587069
F	-1.057606	-5.595856	-0.054105
F	-1.908521	-5.197844	-2.593925
F	-2.494732	-2.762488	-3.470234
F	-0.068369	-1.165798	-3.703261
F	2.555330	-0.739639	-3.740126
F	3.702271	0.935448	-1.919663
F	2.136676	2.164250	-0.063079
F	-0.460179	1.750311	0.007628
Na	-4.576607	-2.701740	-1.195161

Na[BAr^F₂₀]⁺Na[BAr^F₂₀]^{-c}

B	-1.637176	-0.707666	-1.136763
C	-0.556387	0.448321	-1.600005
C	-0.573794	1.789691	-1.226365
C	0.411198	0.122844	-2.551879
C	0.321220	2.735575	-1.727120
C	1.323167	1.029177	-3.077049
C	1.275952	2.354845	-2.659220
C	-2.602982	-0.242367	0.135776
C	-1.982643	0.043328	1.356776
C	-3.989101	-0.243559	0.212705
C	-2.663502	0.288903	2.542404
C	-4.725566	-0.018586	1.372693
C	-4.054304	0.246540	2.555725
C	-0.925323	-2.076182	-0.521973
C	-1.714953	-3.183704	-0.232135
C	0.400442	-2.216104	-0.113212
C	-1.277455	-4.352544	0.369991
C	0.897712	-3.368303	0.498094
C	0.056522	-4.444101	0.748186
C	-2.465024	-0.988012	-2.554290
C	-2.371231	-2.122178	-3.365824
C	-3.239007	0.043769	-3.099707
C	-3.039827	-2.255841	-4.586250
C	-3.923565	-0.045968	-4.307614
C	-3.814971	-1.208639	-5.066268
F	-1.473097	2.258768	-0.357802
F	0.257155	4.000698	-1.325676
F	2.131948	3.242402	-3.146579
F	2.227500	0.646568	-3.972018
F	0.501918	-1.134825	-2.999383
F	1.286366	-1.233554	-0.272131
F	2.173113	-3.435683	0.858520
F	0.517630	-5.540535	1.330309
F	-2.111748	-5.364136	0.585286
F	-3.027241	-3.167050	-0.564501
F	-4.753474	-0.508076	-0.879150
F	-6.050214	-0.073859	1.350866
F	-4.723295	0.462003	3.677731
F	-2.001491	0.552433	3.660919
F	-0.650508	0.096296	1.424946
F	-1.647284	-3.181894	-3.004229
F	-2.932369	-3.374105	-5.288300
F	-4.437772	-1.315688	-6.224639
F	-4.664504	0.960410	-4.742635
F	-3.369577	1.190436	-2.435278
Na	-4.699873	-2.478467	-1.913488
B	-7.441880	-4.847396	-1.314221
C	-6.727664	-5.935857	-2.346543
C	-7.263281	-7.132522	-2.807401
C	-5.400494	-5.757107	-2.728914
C	-6.581599	-8.053663	-3.598439
C	-4.664907	-6.625038	-3.521486
C	-5.266854	-7.798808	-3.963586
C	-6.551348	-5.057561	0.073778
C	-5.675677	-4.151483	0.660945
C	-6.523829	-6.307990	0.685890
C	-4.837678	-4.436688	1.735056

C	-5.725744	-6.656576	1.765335
C	-4.858972	-5.705427	2.295076
C	-9.066620	-5.096307	-1.103631
C	-9.747323	-5.167332	0.112829
C	-9.896753	-5.059343	-2.229089
C	-11.140753	-5.218514	0.215338
C	-11.284368	-5.111469	-2.176045
C	-11.914982	-5.193314	-0.937505
C	-7.425793	-3.288467	-1.891919
C	-7.121734	-2.877834	-3.192406
C	-7.872369	-2.258747	-1.055009
C	-7.191813	-1.547894	-3.617747
C	-7.954343	-0.923728	-1.433439
C	-7.592997	-0.560686	-2.727259
F	-8.523379	-7.507921	-2.474960
F	-7.173606	-9.173839	-3.983341
F	-4.597560	-8.657379	-4.712014
F	-3.412169	-6.351650	-3.844140
F	-4.736820	-4.649316	-2.324812
F	-9.353039	-4.974605	-3.442744
F	-12.006417	-5.089655	-3.284662
F	-13.232041	-5.249941	-0.860664
F	-11.722072	-5.296958	1.402692
F	-9.088607	-5.199445	1.274999
F	-7.334110	-7.293530	0.221375
F	-5.777406	-7.874258	2.282669
F	-4.067879	-6.008520	3.308255
F	-4.013350	-3.513301	2.204635
F	-5.553795	-2.898611	0.178340
F	-6.713707	-3.747627	-4.119685
F	-6.873945	-1.225527	-4.861947
F	-7.638816	0.702032	-3.106489
F	-8.354308	-0.000035	-0.577297
F	-8.224782	-2.538200	0.198620
Na	-9.391603	-7.980343	-0.405478

Na[BAr^F₂₀]⁻Na[BAr^F₂₀]-a

92

B	-1.922698	-0.378594	-1.223146
C	-2.439168	0.800587	-0.184014
C	-3.152624	0.617916	0.992194
C	-2.317454	2.139590	-0.564645
C	-3.689704	1.647892	1.759180
C	-2.819006	3.207826	0.169341
C	-3.520241	2.960994	1.345875
C	-0.342942	-0.200862	-1.684542
C	0.178595	-0.996804	-2.699223
C	0.614324	0.590129	-1.048557
C	1.500690	-1.008111	-3.116034
C	1.958520	0.618809	-1.422499
C	2.408596	-0.182384	-2.462873
C	-3.027181	-0.186413	-2.455241
C	-4.376371	-0.432585	-2.196797
C	-2.795660	0.381829	-3.709182
C	-5.421076	-0.169365	-3.069179
C	-3.809616	0.665435	-4.630135
C	-5.132709	0.388566	-4.310951
C	-1.911078	-1.904280	-0.579271

C	-2.410889	-3.053568	-1.174668
C	-1.184538	-2.147173	0.589998
C	-2.249011	-4.341766	-0.673500
C	-0.989666	-3.409632	1.135952
C	-1.531796	-4.521967	0.498984
F	-3.426859	-0.626264	1.459386
F	-4.396233	1.369332	2.849453
F	-4.022961	3.960868	2.051276
F	-2.652670	4.454081	-0.249577
F	-1.687049	2.447339	-1.700537
F	-1.560602	0.688600	-4.113699
F	-3.511524	1.191317	-5.807274
F	-6.099634	0.644732	-5.171659
F	-6.670931	-0.442578	-2.733375
F	-4.734036	-0.959239	-1.006826
F	0.296277	1.374179	-0.019146
F	2.813240	1.402707	-0.780162
F	3.680932	-0.164252	-2.825862
F	1.897550	-1.791723	-4.109567
F	-0.643269	-1.848025	-3.368254
F	-3.100957	-2.985919	-2.339796
F	-2.785078	-5.381998	-1.299373
F	-1.388637	-5.729455	1.020506
F	-0.309265	-3.563256	2.262335
F	-0.629426	-1.124779	1.243064
Na	-2.487425	-2.399091	-4.486313
B	-7.238420	-5.376455	-1.199321
C	-8.534849	-6.395900	-1.294967
C	-9.475204	-6.368390	-0.263893
C	-8.870342	-7.226460	-2.361024
C	-10.641465	-7.122773	-0.250591
C	-10.028849	-8.002893	-2.391901
C	-10.922153	-7.951345	-1.331389
C	-6.096937	-5.616077	-2.373608
C	-5.549570	-4.649029	-3.211470
C	-5.510474	-6.878332	-2.495181
C	-4.549010	-4.933794	-4.134530
C	-4.496572	-7.193920	-3.392470
C	-3.998811	-6.199541	-4.225650
C	-6.370663	-5.602764	0.193770
C	-6.420828	-6.703248	1.050755
C	-5.416787	-4.664749	0.559091
C	-5.634075	-6.822573	2.199141
C	-4.665364	-4.700872	1.722338
C	-4.752956	-5.808760	2.552788
C	-7.964478	-3.882235	-1.315208
C	-8.642550	-3.582119	-2.501619
C	-8.089834	-2.891581	-0.348724
C	-9.348888	-2.407687	-2.731186
C	-8.771565	-1.690697	-0.531406
C	-9.416346	-1.443245	-1.731929
F	-9.263865	-5.587541	0.803605
F	-11.486310	-7.056253	0.772877
F	-12.028953	-8.681439	-1.347639
F	-10.288984	-8.782098	-3.436621
F	-8.091848	-7.322413	-3.441952
F	-5.228365	-3.565228	-0.211207
F	-3.911148	-3.646641	2.058885

F	-4.032177	-5.886747	3.657772
F	-5.737192	-7.897365	2.968111
F	-7.245495	-7.722729	0.824670
F	-5.933478	-7.877723	-1.719907
F	-3.993249	-8.419833	-3.448300
F	-3.017151	-6.448179	-5.078759
F	-4.062319	-3.950038	-4.921289
F	-5.943098	-3.372070	-3.177098
F	-8.606477	-4.446125	-3.519173
F	-9.944737	-2.193341	-3.896437
F	-10.061175	-0.305047	-1.932771
F	-8.766597	-0.773569	0.433990
F	-7.506581	-3.001809	0.872287
Na	-5.479050	-1.618416	1.087876

Na[BAr^F₂₀]⁻Na[BAr^F₂₀]-b

92

B	-7.196140	-4.991783	-0.310357
C	-6.235878	-5.308202	-1.629005
C	-6.357508	-4.745717	-2.903082
C	-5.277687	-6.324855	-1.538728
C	-5.546060	-5.103047	-3.983465
C	-4.445955	-6.710112	-2.585317
C	-4.588099	-6.096923	-3.827697
C	-8.070004	-6.394433	-0.197205
C	-8.910952	-6.742935	-1.259861
C	-7.932640	-7.383825	0.776514
C	-9.574425	-7.959681	-1.362386
C	-8.580142	-8.621485	0.716507
C	-9.406569	-8.912123	-0.360998
C	-8.135734	-3.636740	-0.500607
C	-9.500774	-3.523137	-0.268919
C	-7.528884	-2.417054	-0.787636
C	-10.217632	-2.331172	-0.336794
C	-8.181720	-1.197540	-0.879480
C	-9.551849	-1.152045	-0.643535
C	-6.344430	-4.611070	1.070015
C	-7.047482	-4.354137	2.245290
C	-4.985643	-4.343642	1.194460
C	-6.501054	-3.878410	3.427035
C	-4.372255	-3.847985	2.342517
C	-5.137267	-3.608670	3.474356
F	-7.252671	-3.793527	-3.162127
F	-5.692590	-4.504137	-5.154243
F	-3.828350	-6.454942	-4.843328
F	-3.534974	-7.652810	-2.412823
F	-5.107364	-6.965322	-0.382925
F	-6.199821	-2.380509	-1.015589
F	-7.517556	-0.092478	-1.179613
F	-10.208157	-0.007630	-0.714681
F	-11.519177	-2.316183	-0.090859
F	-10.241783	-4.603931	0.080284
F	-7.157826	-7.194588	1.849636
F	-8.412012	-9.513045	1.682021
F	-10.030998	-10.074019	-0.431736
F	-10.363795	-8.217044	-2.393072
F	-9.107929	-5.876185	-2.252871
F	-8.385672	-4.576814	2.281135

F	-7.260376	-3.675043	4.491955
F	-4.583097	-3.140238	4.577763
F	-3.075375	-3.593902	2.350703
F	-4.139636	-4.524175	0.153882
Na	-10.160063	-5.897981	1.985195
B	-1.856652	-0.626473	-2.160147
C	-0.320442	-0.056347	-1.962772
C	0.676125	-0.501973	-2.832883
C	0.136729	0.751214	-0.924668
C	2.017170	-0.157954	-2.723921
C	1.473129	1.123007	-0.774862
C	2.421128	0.665328	-1.678384
C	-2.966122	0.094874	-1.154072
C	-3.835001	-0.524807	-0.266531
C	-3.186696	1.469864	-1.277252
C	-4.848780	0.116352	0.438687
C	-4.175436	2.165877	-0.591750
C	-5.025527	1.480383	0.271313
C	-1.652020	-2.256184	-1.871689
C	-1.723634	-3.292264	-2.805765
C	-1.239184	-2.665778	-0.597558
C	-1.470787	-4.632673	-2.497507
C	-0.973622	-3.984586	-0.246969
C	-1.108214	-4.984531	-1.205028
C	-2.491430	-0.301279	-3.661322
C	-3.725696	-0.830536	-4.024683
C	-1.970675	0.582746	-4.606796
C	-4.396512	-0.583998	-5.212449
C	-2.600073	0.872590	-5.818309
C	-3.820454	0.288385	-6.128106
F	0.350924	-1.299445	-3.857029
F	2.910866	-0.608115	-3.597963
F	3.695418	1.007497	-1.547742
F	1.845058	1.901952	0.235530
F	-0.691739	1.216250	0.013836
F	-1.103874	-1.763431	0.372100
F	-0.613069	-4.300269	0.986108
F	-0.887174	-6.248736	-0.891865
F	-1.579076	-5.566337	-3.432157
F	-2.072800	-3.064392	-4.075171
F	-2.413620	2.192976	-2.090188
F	-4.323508	3.473228	-0.760674
F	-5.988914	2.119747	0.916255
F	-5.652357	-0.573464	1.241450
F	-3.771506	-1.859576	-0.052070
F	-4.363778	-1.681924	-3.179844
F	-5.564186	-1.158232	-5.469220
F	-4.426882	0.558875	-7.273648
F	-2.041906	1.718879	-6.674306
F	-0.823252	1.228575	-4.400988
Na	-4.253045	-3.321666	-1.736524

Na[BAr^F₂₀]⁻Na[BAr^F₂₀]-d

92

B	-7.633124	-4.864101	-1.164920
C	-7.146481	-6.184928	-2.033118
C	-6.342406	-7.227224	-1.574688
C	-7.684374	-6.388541	-3.305747

C	-6.056804	-8.365107	-2.329535
C	-7.427900	-7.503355	-4.093547
C	-6.602750	-8.506578	-3.597357
C	-9.230260	-5.235907	-0.892724
C	-9.529238	-6.336693	-0.081227
C	-10.334653	-4.696847	-1.556728
C	-10.806790	-6.857896	0.088419
C	-11.634956	-5.193905	-1.425130
C	-11.873263	-6.282474	-0.596604
C	-7.430321	-3.430109	-1.975187
C	-7.971127	-2.256147	-1.462811
C	-6.665328	-3.214730	-3.116197
C	-7.823762	-0.990057	-2.009685
C	-6.492498	-1.973393	-3.724662
C	-7.065659	-0.841309	-3.165167
C	-6.750981	-4.617057	0.216731
C	-7.238787	-4.368437	1.492150
C	-5.363853	-4.514054	0.131147
C	-6.449203	-4.075332	2.601315
C	-4.518065	-4.256458	1.199695
C	-5.072128	-4.020318	2.453636
F	-5.790208	-7.198803	-0.359515
F	-5.275233	-9.318494	-1.836781
F	-6.343274	-9.582548	-4.324849
F	-7.965599	-7.621632	-5.301450
F	-8.495469	-5.465924	-3.836239
F	-5.952761	-4.212654	-3.686318
F	-5.711004	-1.872538	-4.796286
F	-6.883586	0.347712	-3.705415
F	-8.373952	0.064826	-1.432163
F	-8.707072	-2.307205	-0.327011
F	-10.210918	-3.646446	-2.372928
F	-12.637431	-4.628088	-2.080267
F	-13.096367	-6.760137	-0.452530
F	-11.015729	-7.893969	0.885217
F	-8.549885	-6.950035	0.581191
F	-8.571450	-4.377007	1.744857
F	-7.004808	-3.829577	3.776995
F	-4.293222	-3.721162	3.479188
F	-3.206491	-4.181024	1.040346
F	-4.766377	-4.684168	-1.069660
Na	-10.332028	-3.203361	0.938738
B	-1.437258	-0.833139	-1.243820
C	-0.651376	0.619799	-1.342401
C	0.455807	0.723756	-2.187055
C	-1.051130	1.823199	-0.766064
C	1.146914	1.904402	-2.426511
C	-0.388782	3.032819	-0.977546
C	0.717319	3.076275	-1.813392
C	-2.041477	-0.959977	-2.791653
C	-1.569065	-1.793503	-3.806582
C	-2.965344	-0.001256	-3.227600
C	-1.979307	-1.702787	-5.140440
C	-3.390431	0.136524	-4.542474
C	-2.893640	-0.728783	-5.512301
C	-2.604580	-0.859592	-0.065682
C	-2.230148	-0.600660	1.255696
C	-3.947528	-1.180900	-0.211359

C	-3.106773	-0.606154	2.334422
C	-4.875197	-1.164338	0.825837
C	-4.448915	-0.891509	2.115753
C	-0.440134	-2.077956	-0.794133
C	-0.902455	-3.386746	-0.856559
C	0.815170	-1.960174	-0.196460
C	-0.221935	-4.509051	-0.410635
C	1.548687	-3.052112	0.269474
C	1.030306	-4.336022	0.166552
F	0.914032	-0.365059	-2.815383
F	2.201078	1.925921	-3.234784
F	1.356234	4.218403	-2.025992
F	-0.818886	4.145521	-0.391877
F	-2.121043	1.895370	0.030763
F	-4.453362	-1.554398	-1.414153
F	-6.153152	-1.457113	0.608010
F	-5.311256	-0.921990	3.121020
F	-2.676641	-0.346439	3.560375
F	-0.963624	-0.288830	1.534479
F	-3.482179	0.863468	-2.352835
F	-4.267934	1.069016	-4.878868
F	-3.303536	-0.634390	-6.765574
F	-1.498885	-2.543271	-6.046718
F	-0.671173	-2.752392	-3.558455
F	-2.120267	-3.632279	-1.397783
F	-0.751397	-5.720044	-0.525708
F	1.716849	-5.377970	0.610006
F	2.740156	-2.868399	0.824224
F	1.395197	-0.773563	-0.018894
Na	-3.808361	-3.378088	-2.757499

Na[BAr^F₂₀]⁻Na[BAr^F₂₀]-g

92

B	-7.313834	-5.290490	-1.379895
C	-7.839892	-5.203598	-2.946051
C	-7.225355	-5.772969	-4.060293
C	-9.093041	-4.643928	-3.204422
C	-7.781324	-5.752353	-5.339461
C	-9.685230	-4.598345	-4.460391
C	-9.020427	-5.162556	-5.543363
C	-8.340121	-6.418730	-0.738550
C	-8.233785	-7.743979	-1.166035
C	-9.426804	-6.170614	0.098164
C	-9.096292	-8.761861	-0.778212
C	-10.319475	-7.159233	0.512589
C	-10.155862	-8.464490	0.071685
C	-7.363415	-3.834806	-0.581823
C	-7.196220	-3.784109	0.798351
C	-7.454023	-2.572593	-1.157265
C	-7.154412	-2.628060	1.563694
C	-7.430064	-1.375904	-0.443310
C	-7.265754	-1.394298	0.933626
C	-5.711994	-5.709572	-1.248549
C	-5.177897	-6.648162	-0.373737
C	-4.739135	-5.028522	-1.977666
C	-3.819500	-6.936887	-0.260369
C	-3.375382	-5.287244	-1.925837
C	-2.902725	-6.247529	-1.038220

F	-6.042318	-6.386746	-3.967559
F	-7.135311	-6.303270	-6.360740
F	-9.563005	-5.136622	-6.751909
F	-10.874720	-4.033830	-4.632188
F	-9.793308	-4.098536	-2.203667
F	-7.496280	-2.412677	-2.500186
F	-7.480672	-0.219479	-1.099387
F	-7.198585	-0.273662	1.625135
F	-6.964387	-2.694751	2.873497
F	-7.036703	-4.937259	1.489864
F	-9.684587	-4.944347	0.562313
F	-11.329325	-6.856034	1.320557
F	-10.996136	-9.414827	0.454760
F	-8.923903	-10.003764	-1.214998
F	-7.245418	-8.094044	-1.996172
F	-5.956181	-7.312596	0.508989
F	-3.405684	-7.806545	0.656742
F	-1.606693	-6.471192	-0.917902
F	-2.514691	-4.606715	-2.663913
F	-5.117385	-4.036534	-2.813339
Na	-5.201291	-5.961506	2.533830
B	-1.846134	-0.408800	-1.166000
C	-1.005110	0.786471	-0.388308
C	-0.647571	1.927420	-1.110064
C	-0.717217	0.853636	0.972976
C	-0.023827	3.037963	-0.556292
C	-0.092332	1.947028	1.573106
C	0.256098	3.048808	0.805720
C	-3.285711	0.381209	-1.458290
C	-3.714843	0.900962	-2.681129
C	-4.053971	0.800019	-0.363925
C	-4.810319	1.758580	-2.819810
C	-5.137416	1.664635	-0.450544
C	-5.522460	2.150415	-1.696191
C	-2.007296	-1.782019	-0.247167
C	-0.855707	-2.412418	0.234748
C	-3.186591	-2.433058	0.090017
C	-0.854938	-3.544312	1.044694
C	-3.236117	-3.540847	0.926753
C	-2.070483	-4.111678	1.403084
C	-1.079321	-0.960366	-2.524493
C	-1.760314	-1.784510	-3.411063
C	0.270597	-0.798458	-2.838032
C	-1.217613	-2.390500	-4.533314
C	0.873841	-1.384939	-3.951137
C	0.129965	-2.187800	-4.805791
F	-0.899992	1.987767	-2.422231
F	0.297970	4.084186	-1.308542
F	0.846346	4.097445	1.361526
F	0.159554	1.943437	2.877801
F	-1.037326	-0.142323	1.805113
F	-4.383859	-2.016523	-0.381750
F	-4.409958	-4.095416	1.272398
F	-2.137385	-5.182584	2.188215
F	0.278714	-4.070501	1.477395
F	0.340267	-1.896857	-0.040412
F	-3.738852	0.380269	0.863730
F	-5.806120	2.027028	0.632497

F	-6.564244	2.955928	-1.807435
F	-5.166536	2.198832	-4.018397
F	-3.084807	0.607744	-3.822895
F	-3.074679	-2.036529	-3.197815
F	-1.960096	-3.150815	-5.326731
F	0.694397	-2.750217	-5.863242
F	2.163101	-1.186823	-4.193791
F	1.080970	-0.067067	-2.073941
Na	-5.151328	-1.676152	-2.626933

TS'

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C	-14.195078	-6.022278	6.490335
C	-15.431259	-5.380948	6.506613
C	-15.538671	-4.063180	6.971810
C	-14.386795	-3.397798	7.411826
C	-13.150008	-4.036584	7.384361
C	-13.050788	-5.352441	6.929120
H	-14.123051	-7.050908	6.129382
H	-16.325366	-5.905062	6.159963
H	-14.466043	-2.370043	7.774364
H	-12.258386	-3.507003	7.727925
H	-12.081241	-5.855731	6.912759
C	-16.849916	-3.392043	7.026894
H	-17.735531	-3.865940	6.616388
H	-16.942123	-2.399145	7.454438
Cl	-16.711126	-2.285533	4.933788
P	-17.508561	-4.352621	9.183739
C	-17.975661	-6.101696	8.963432
C	-18.810331	-6.404828	7.876497
C	-17.541194	-7.134799	9.802280
C	-19.205003	-7.718698	7.636356
H	-19.161836	-5.609129	7.213769
C	-17.933350	-8.450498	9.554275
H	-16.897170	-6.918438	10.656969
C	-18.763192	-8.744805	8.473210
H	-19.856592	-7.942462	6.788800
H	-17.588871	-9.249377	10.214881
H	-19.067524	-9.776351	8.281651
C	-18.987562	-3.544325	9.878653
C	-19.967284	-4.250141	10.589857
C	-19.133248	-2.163195	9.688667
C	-21.073941	-3.579521	11.107160
H	-19.866341	-5.327484	10.741857
C	-20.238763	-1.494919	10.213522
H	-18.378076	-1.602885	9.131208
C	-21.210137	-2.202845	10.921053
H	-21.834407	-4.135743	11.659955
H	-20.343832	-0.418346	10.062141
H	-22.079490	-1.680468	11.327128
C	-16.247602	-4.307892	10.497509
C	-16.423574	-3.570455	11.675680
C	-15.027442	-4.968133	10.277255
C	-15.398209	-3.499315	12.618580
H	-17.364563	-3.049235	11.865129
C	-14.009624	-4.898663	11.225216
H	-14.871380	-5.546980	9.363376
C	-14.191528	-4.162042	12.396548

H	-15.547826	-2.923538	13.534764
H	-13.067083	-5.419654	11.042433
H	-13.390677	-4.104513	13.137397

[Bn-PPh₃]⁺·Cl⁻

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C	-4.683508	-5.708791	3.582854
C	-5.980791	-5.595325	4.081880
C	-6.426406	-4.386763	4.631976
C	-5.555890	-3.288807	4.664230
C	-4.260937	-3.403675	4.160761
C	-3.818865	-4.614024	3.625278
H	-4.347784	-6.657095	3.156326
H	-6.652723	-6.456246	4.043689
H	-5.919862	-2.345489	5.085785
H	-3.591758	-2.540340	4.189698
H	-2.802257	-4.703627	3.234660
C	-7.805438	-4.249342	5.227072
H	-8.570327	-4.815944	4.675081
H	-8.098857	-3.178535	5.262967
Cl	-8.028829	-0.892017	5.839207
P	-7.883638	-4.804153	6.960698
C	-7.648659	-6.595340	7.063269
C	-8.275092	-7.417493	6.115408
C	-6.940936	-7.169695	8.125973
C	-8.170958	-8.801538	6.220387
H	-8.851838	-6.986579	5.293985
C	-6.841642	-8.556559	8.224318
H	-6.468216	-6.541555	8.883225
C	-7.451541	-9.371330	7.271830
H	-8.656313	-9.437669	5.477506
H	-6.285449	-8.999980	9.052648
H	-7.370177	-10.457690	7.350842
C	-9.520162	-4.433512	7.636743
C	-10.189540	-5.396865	8.405038
C	-10.109383	-3.182762	7.398108
C	-11.447933	-5.110679	8.928702
H	-9.737989	-6.372565	8.595215
C	-11.369563	-2.911517	7.928788
H	-9.576649	-2.406322	6.827564
C	-12.039277	-3.870151	8.688814
H	-11.968165	-5.863303	9.524784
H	-11.828062	-1.937274	7.745266
H	-13.027644	-3.649484	9.098747
C	-6.587165	-3.972982	7.903096
C	-6.894974	-2.885144	8.726763
C	-5.251675	-4.368997	7.729637
C	-5.871389	-2.206674	9.385099
H	-7.927072	-2.557439	8.855370
C	-4.236379	-3.683835	8.389801
H	-4.997153	-5.209694	7.080422
C	-4.545961	-2.603540	9.217156
H	-6.114814	-1.357823	10.026992
H	-3.198595	-3.993835	8.252254
H	-3.746734	-2.066108	9.732606

Na[BAr^F₂₀]⁻·BnCl·PPh₃

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C	-15.114329	-7.192293	6.974864
C	-15.867508	-6.386410	6.119585
C	-15.270171	-5.309259	5.458086
C	-13.907984	-5.055102	5.655287
C	-13.151517	-5.868378	6.493292
C	-13.755592	-6.937965	7.158777
H	-15.594162	-8.022145	7.498504
H	-16.931916	-6.588193	5.976908
H	-13.438130	-4.205156	5.157327
H	-12.091524	-5.652624	6.643366
H	-13.165870	-7.570115	7.826703
C	-16.093278	-4.394573	4.608900
H	-17.155284	-4.660507	4.603499
H	-15.981529	-3.350835	4.914043
Cl	-15.583934	-4.448146	2.837450
P	-17.288241	-3.044250	7.809616
C	-17.934179	-4.425229	8.840572
C	-18.810575	-5.325909	8.220163
C	-17.604413	-4.622915	10.188612
C	-19.351544	-6.398289	8.929975
H	-19.072882	-5.186888	7.167119
C	-18.137468	-5.699212	10.896436
H	-16.924983	-3.930682	10.691774
C	-19.011642	-6.588674	10.269098
H	-20.034405	-7.091139	8.432549
H	-17.870229	-5.842836	11.946147
H	-19.427040	-7.432332	10.825494
C	-18.398558	-1.645251	8.260462
C	-19.408741	-1.720916	9.227045
C	-18.229450	-0.442667	7.557121
C	-20.221017	-0.616228	9.489587
H	-19.568217	-2.645926	9.785529
C	-19.024439	0.666790	7.834747
H	-17.448481	-0.365084	6.799862
C	-20.028009	0.580750	8.800719
H	-21.006395	-0.692479	10.245574
H	-18.854276	1.601149	7.296008
H	-20.658903	1.446399	9.016059
C	-15.722015	-2.615052	8.684498
C	-15.432087	-1.347959	9.203411
C	-14.742321	-3.617134	8.768161
C	-14.200417	-1.095928	9.810246
H	-16.165891	-0.542307	9.140482
C	-13.518595	-3.368087	9.384032
H	-14.944612	-4.611705	8.361217
C	-13.244883	-2.104963	9.911365
H	-13.986185	-0.097732	10.199041
H	-12.771167	-4.162865	9.443594
H	-12.280946	-1.902758	10.382683
B	-13.786898	1.132308	4.427850
C	-14.387622	2.556941	5.015448
C	-14.190225	3.822534	4.467359
C	-15.305104	2.521471	6.067510
C	-14.822336	4.972109	4.942972
C	-15.956936	3.637714	6.574157
C	-15.715138	4.881246	6.000851
C	-12.547169	1.325620	3.344494
C	-11.417676	2.049198	3.737165

C	-12.413313	0.715369	2.104727
C	-10.273179	2.189720	2.962070
C	-11.289391	0.813952	1.288626
C	-10.204786	1.561944	1.722148
C	-15.164960	0.479388	3.768998
C	-15.955997	-0.513139	4.348451
C	-15.749561	1.108663	2.664213
C	-17.223395	-0.867389	3.875306
C	-16.999562	0.781711	2.151050
C	-17.747608	-0.217622	2.765841
C	-13.050523	0.186672	5.575112
C	-12.615148	-1.092277	5.240462
C	-12.610847	0.613507	6.828525
C	-11.803048	-1.896431	6.025702
C	-11.805289	-0.159212	7.664827
C	-11.402080	-1.425574	7.269075
F	-13.374127	4.013438	3.428091
F	-14.584987	6.151385	4.378929
F	-16.328067	5.963189	6.459959
F	-16.815131	3.527047	7.583328
F	-15.593962	1.353825	6.654022
F	-15.103749	2.098672	2.049497
F	-17.483458	1.412108	1.091823
F	-18.939178	-0.546478	2.298785
F	-17.934216	-1.810603	4.476541
F	-15.535499	-1.176102	5.432605
F	-13.403008	-0.065433	1.596164
F	-11.247639	0.190626	0.117852
F	-9.120570	1.675162	0.970546
F	-9.244421	2.904918	3.396689
F	-11.403683	2.660929	4.923186
F	-12.955917	-1.621870	4.035121
F	-11.404491	-3.091196	5.603164
F	-10.640829	-2.171102	8.054824
F	-11.428509	0.310195	8.847142
F	-12.912849	1.822736	7.299927
Na	-14.365298	-1.991067	2.318950

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C	-17.196254	-6.751132	-3.159799
C	-17.775402	-5.675457	-3.823557
C	-17.001494	-4.550136	-4.150743
C	-15.640143	-4.521957	-3.806370
C	-15.063973	-5.600212	-3.145013
C	-15.841619	-6.714103	-2.820667
H	-17.801067	-7.623865	-2.904879
H	-18.832983	-5.699019	-4.095069
H	-15.040823	-3.645524	-4.061870
H	-14.006217	-5.572596	-2.875721
H	-15.388620	-7.559510	-2.297638
C	-17.599152	-3.420645	-4.838738
H	-18.654017	-3.407522	-5.091217
H	-17.020781	-2.519182	-5.019478
Cl	-17.232407	-4.104093	-7.112942
P	-18.372427	-2.265427	-2.528142
C	-19.939123	-3.051159	-1.986174
C	-20.726812	-3.734703	-2.918068

C	-20.393280	-2.929259	-0.663883
C	-21.943119	-4.303120	-2.533761
H	-20.403879	-3.818178	-3.957271
C	-21.603209	-3.500292	-0.280721
H	-19.795592	-2.382540	0.070454
C	-22.379164	-4.190569	-1.215748
H	-22.550433	-4.832003	-3.271671
H	-21.946801	-3.402228	0.751564
H	-23.330243	-4.635563	-0.913969
C	-18.685920	-0.513002	-2.074781
C	-19.589808	0.189519	-2.884084
C	-18.138106	0.123098	-0.953448
C	-19.954428	1.496809	-2.568740
H	-20.019245	-0.288703	-3.766355
C	-18.497291	1.435235	-0.647256
H	-17.435968	-0.403034	-0.304336
C	-19.409542	2.121311	-1.447759
H	-20.656124	2.029269	-3.213100
H	-18.060401	1.922295	0.227428
H	-19.685474	3.149989	-1.206159
C	-17.099196	-2.866001	-1.366808
C	-17.263106	-4.034745	-0.613520
C	-15.851336	-2.222798	-1.357541
C	-16.207383	-4.536691	0.147757
H	-18.215239	-4.568544	-0.621009
C	-14.803528	-2.718319	-0.586282
H	-15.691687	-1.325414	-1.958025
C	-14.978543	-3.879297	0.168084
H	-16.350208	-5.451725	0.727142
H	-13.842935	-2.198362	-0.583369
H	-14.154819	-4.273518	0.767626
B	-18.244712	1.527469	-7.446093
C	-19.496496	2.604531	-7.501006
C	-20.550580	2.451020	-6.600272
C	-19.684525	3.618196	-8.437748
C	-21.676566	3.262134	-6.565447
C	-20.803205	4.452246	-8.449708
C	-21.806669	4.276596	-7.507187
C	-17.526705	1.430159	-5.952171
C	-17.621889	2.369750	-4.925552
C	-16.605964	0.419008	-5.695958
C	-16.868444	2.308567	-3.752657
C	-15.859497	0.288485	-4.534801
C	-15.997394	1.250335	-3.541170
C	-16.956578	1.962551	-8.397972
C	-16.284051	1.178101	-9.325289
C	-16.355711	3.207086	-8.183173
C	-15.134297	1.564092	-10.009974
C	-15.215442	3.649444	-8.842317
C	-14.591952	2.816657	-9.766084
C	-19.007537	0.125290	-7.912015
C	-19.496641	0.019749	-9.218900
C	-19.410060	-0.911090	-7.068932
C	-20.278126	-1.036100	-9.675632
C	-20.209686	-1.979914	-7.475772
C	-20.638166	-2.051489	-8.793373
F	-20.497798	1.478951	-5.681862
F	-22.621752	3.073144	-5.650135

F	-22.873609	5.063322	-7.504792
F	-20.917418	5.409283	-9.364272
F	-18.788010	3.854235	-9.398703
F	-16.889375	4.057011	-7.303347
F	-14.712542	4.851067	-8.592632
F	-13.499285	3.213647	-10.399795
F	-14.555979	0.741019	-10.875364
F	-16.710759	-0.075317	-9.625266
F	-16.379697	-0.532489	-6.634717
F	-15.024956	-0.734045	-4.370732
F	-15.297195	1.163861	-2.419040
F	-16.978056	3.262792	-2.838794
F	-18.442064	3.416297	-5.012174
F	-19.219011	0.975187	-10.105895
F	-20.685149	-1.082722	-10.935731
F	-21.380456	-3.064446	-9.205632
F	-20.552883	-2.927963	-6.612999
F	-19.044762	-0.938355	-5.784538
Na	-16.941191	-1.914834	-8.364293

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95

C	-15.052557	-7.330460	6.642499
C	-15.935317	-6.361958	6.176610
C	-15.477137	-5.060709	5.915030
C	-14.120949	-4.755097	6.106991
C	-13.236181	-5.729034	6.554350
C	-13.703893	-7.015228	6.830819
H	-15.413776	-8.338756	6.855503
H	-16.987497	-6.606745	6.017758
H	-13.769002	-3.744287	5.899005
H	-12.183602	-5.480245	6.701491
H	-13.012557	-7.779761	7.192938
C	-16.382989	-4.022897	5.451297
H	-17.438282	-4.228724	5.288598
H	-16.049115	-2.995374	5.423127
Cl	-16.035720	-4.073641	3.106479
P	-17.125375	-3.214973	7.931502
C	-17.866134	-4.628457	8.820071
C	-18.728354	-5.456958	8.089553
C	-17.644441	-4.898226	10.177193
C	-19.360716	-6.537268	8.703606
H	-18.909251	-5.255073	7.030221
C	-18.271105	-5.983309	10.787515
H	-16.982595	-4.257128	10.763829
C	-19.128765	-6.803669	10.052743
H	-20.031543	-7.175340	8.123963
H	-18.091487	-6.186453	11.845729
H	-19.617942	-7.653454	10.534548
C	-18.274752	-1.822718	8.257848
C	-19.387582	-1.940412	9.100860
C	-18.039526	-0.598953	7.612873
C	-20.235858	-0.851046	9.301638
H	-19.598091	-2.883187	9.609970
C	-18.874698	0.493698	7.832370
H	-17.185145	-0.490575	6.945970
C	-19.979354	0.368293	8.675117
H	-21.100231	-0.956928	9.961323

H	-18.653411	1.445291	7.344482
H	-20.640831	1.221237	8.843584
C	-15.596999	-2.806810	8.854621
C	-15.239133	-1.491829	9.182236
C	-14.696568	-3.844838	9.144878
C	-14.018561	-1.224911	9.800155
H	-15.910110	-0.660012	8.963461
C	-13.478957	-3.573574	9.766093
H	-14.949245	-4.878335	8.895283
C	-13.136752	-2.262941	10.098382
H	-13.755692	-0.193912	10.045987
H	-12.793111	-4.394618	9.987227
H	-12.179865	-2.047602	10.577836
B	-13.777220	1.244803	4.386576
C	-14.344399	2.711212	4.899443
C	-14.116518	3.944649	4.293530
C	-15.274684	2.743974	5.940590
C	-14.731504	5.127424	4.706610
C	-15.914212	3.894005	6.382458
C	-15.640029	5.104307	5.754882
C	-12.547875	1.333055	3.281875
C	-11.395064	2.052165	3.606379
C	-12.449834	0.623107	2.091796
C	-10.259292	2.104840	2.807633
C	-11.336003	0.633308	1.256406
C	-10.227248	1.384849	1.617453
C	-15.174802	0.597563	3.769162
C	-15.981425	-0.343933	4.401803
C	-15.752932	1.179789	2.636214
C	-17.262842	-0.691773	3.967692
C	-17.013746	0.852168	2.151941
C	-17.779938	-0.093041	2.827497
C	-13.057452	0.349601	5.585096
C	-12.649111	-0.953695	5.316264
C	-12.611972	0.828855	6.817417
C	-11.856348	-1.734367	6.143849
C	-11.826809	0.080555	7.695589
C	-11.446048	-1.210795	7.362764
F	-13.288706	4.068670	3.253704
F	-14.463805	6.273633	4.090565
F	-16.238552	6.218139	6.152781
F	-16.791220	3.845133	7.380638
F	-15.594825	1.611188	6.579763
F	-15.088767	2.119234	1.963753
F	-17.493005	1.433498	1.062635
F	-18.982520	-0.419603	2.386813
F	-17.989311	-1.583053	4.626440
F	-15.547058	-0.972013	5.506766
F	-13.462104	-0.172753	1.663145
F	-11.324809	-0.078099	0.136067
F	-9.152399	1.412670	0.844143
F	-9.204887	2.821481	3.174008
F	-11.346279	2.742121	4.748289
F	-13.006788	-1.537209	4.145146
F	-11.493137	-2.960497	5.785066
F	-10.695620	-1.929079	8.183224
F	-11.448009	0.595945	8.858707
F	-12.890074	2.066581	7.226340

Na -14.502776 -2.072314 2.517195

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C -16.455953 -12.428685 12.347635
C -16.723991 -11.136950 11.910399
C -15.695987 -10.346412 11.370259
C -14.401919 -10.880321 11.253052
C -14.135594 -12.170509 11.697167
C -15.160352 -12.942621 12.248970
H -17.257388 -13.037584 12.771324
H -17.731009 -10.724239 11.987072
H -13.607603 -10.274243 10.813043
H -13.125718 -12.577555 11.614976
H -14.949180 -13.955851 12.598754
C -15.976940 -8.991320 10.937531
H -16.948820 -8.547568 11.127334
H -15.193523 -8.365502 10.519918
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P -15.409062 -7.852950 13.335864
C -16.868041 -8.135263 14.403678
C -17.664977 -7.056246 14.813060
C -17.270257 -9.438485 14.737165
C -18.818025 -7.274355 15.564384
H -17.390552 -6.034990 14.546134
C -18.421125 -9.651572 15.494304
H -16.674649 -10.296158 14.420239
C -19.192424 -8.569656 15.918092
H -19.427780 -6.421878 15.872002
H -18.717278 -10.671228 15.750289
H -20.095802 -8.736845 16.508020
C -14.955642 -6.114024 13.719154
C -14.490639 -5.758138 14.994281
C -15.125938 -5.119488 12.751335
C -14.220619 -4.426296 15.296047
H -14.348390 -6.525065 15.760080
C -14.860668 -3.783360 13.057973
H -15.473260 -5.384626 11.754531
C -14.411850 -3.435463 14.329831
H -13.863512 -4.158121 16.293026
H -15.007957 -3.013583 12.296911
H -14.207801 -2.389763 14.571563
C -14.022191 -8.798184 14.067456
C -12.846296 -8.836871 13.303159
C -14.053652 -9.460597 15.299847
C -11.725195 -9.525435 13.759402
H -12.806616 -8.319901 12.339853
C -12.933118 -10.159932 15.750175
H -14.949273 -9.430352 15.922896
C -11.769925 -10.196310 14.982347
H -10.816053 -9.544388 13.154117
H -12.970685 -10.674720 16.712998
H -10.895150 -10.745398 15.338445
B -20.358032 -5.614192 10.532672
C -19.869785 -4.146017 11.116263
C -19.834876 -3.041762 10.262727
C -19.271630 -3.932000 12.356374
C -19.269427 -1.816723 10.596168

C	-18.677504	-2.727282	12.729688
C	-18.676632	-1.659095	11.844607
C	-20.562949	-6.754723	11.719674
C	-20.077022	-8.053627	11.737376
C	-21.476821	-6.486588	12.743663
C	-20.457562	-9.029939	12.653715
C	-21.877821	-7.415635	13.695357
C	-21.370603	-8.708910	13.644248
C	-19.140642	-5.898927	9.432518
C	-19.234283	-5.742588	8.046771
C	-17.833010	-6.054073	9.899431
C	-18.128876	-5.746574	7.191267
C	-16.707019	-6.046694	9.088356
C	-16.853891	-5.896426	7.714854
C	-21.850028	-5.640068	9.824316
C	-22.250073	-6.783679	9.137838
C	-22.840999	-4.668366	9.938714
C	-23.499794	-6.974651	8.568970
C	-24.115717	-4.809499	9.387868
C	-24.450562	-5.967869	8.700155
F	-20.347569	-3.138747	9.031467
F	-19.274083	-0.806990	9.732957
F	-18.115332	-0.505895	12.180616
F	-18.101861	-2.604151	13.921470
F	-19.206936	-4.900648	13.273565
F	-17.626544	-6.208187	11.211292
F	-15.490919	-6.201093	9.599944
F	-15.797131	-5.919264	6.922736
F	-18.296078	-5.609986	5.883583
F	-20.409789	-5.566728	7.440316
F	-22.028480	-5.274731	12.837203
F	-22.734162	-7.081956	14.652382
F	-21.745224	-9.615441	14.533946
F	-19.959559	-10.260274	12.584861
F	-19.194425	-8.477615	10.801094
F	-21.373012	-7.807417	8.974298
F	-23.791743	-8.091338	7.913716
F	-25.657644	-6.113575	8.173851
F	-25.015611	-3.843849	9.524838
F	-22.624109	-3.530778	10.598570
Na	-19.210398	-8.674939	8.527995

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C	-13.979786	-6.414727	0.390270
C	-14.009840	-5.065433	0.052027
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C	-11.606059	-4.947372	0.307450
C	-11.577730	-6.295195	0.649477
C	-12.765080	-7.029515	0.695646
H	-14.906443	-6.989603	0.417941
H	-14.962358	-4.584307	-0.184391
H	-10.678720	-4.370825	0.264211
H	-10.625899	-6.778394	0.880243
H	-12.743275	-8.087312	0.966933
C	-12.856962	-2.892817	-0.316073
H	-13.799315	-2.360196	-0.391210
H	-11.941302	-2.306602	-0.326944

Cl	-12.782269	-3.018112	-2.651118
P	-13.101868	-2.005253	2.196605
C	-11.608079	-1.562086	3.151898
C	-10.469947	-2.365182	2.993865
C	-11.565272	-0.476620	4.036496
C	-9.309414	-2.092432	3.716373
H	-10.492688	-3.215114	2.306983
C	-10.400298	-0.201711	4.751483
H	-12.444726	0.157308	4.171457
C	-9.272758	-1.008562	4.594072
H	-8.429065	-2.726370	3.588832
H	-10.375587	0.647097	5.438752
H	-8.361742	-0.790446	5.156288
C	-13.987794	-3.207654	3.243484
C	-13.520272	-3.643206	4.489575
C	-15.173102	-3.751927	2.730746
C	-14.236860	-4.599410	5.209149
H	-12.596896	-3.234808	4.906247
C	-15.897534	-4.691867	3.458415
H	-15.545244	-3.420034	1.761350
C	-15.425465	-5.122232	4.698384
H	-13.865260	-4.932935	6.180793
H	-16.828812	-5.089982	3.051451
H	-15.986203	-5.866253	5.268801
C	-14.124476	-0.488953	2.203147
C	-15.335183	-0.370237	2.894163
C	-13.671031	0.588923	1.426598
C	-16.088321	0.800825	2.796694
H	-15.705630	-1.193767	3.505358
C	-14.412128	1.764716	1.351080
H	-12.730172	0.509608	0.874669
C	-15.629628	1.868491	2.027324
H	-17.035878	0.875154	3.334699
H	-14.048474	2.596067	0.744150
H	-16.221898	2.783274	1.949284
B	-19.179141	-2.184105	-0.355601
C	-19.715270	-1.754029	1.147520
C	-20.966879	-1.245283	1.484931
C	-18.795047	-1.756800	2.193963
C	-21.292326	-0.804109	2.768474
C	-19.070705	-1.332273	3.485942
C	-20.339054	-0.842738	3.776514
C	-18.115337	-0.957784	-0.708284
C	-18.610906	0.346499	-0.796310
C	-16.738100	-1.033247	-0.864418
C	-17.829630	1.466849	-1.055797
C	-15.914720	0.047852	-1.164034
C	-16.461631	1.317398	-1.253838
C	-20.383420	-2.330084	-1.478818
C	-20.410164	-1.754932	-2.746837
C	-21.433986	-3.213450	-1.222908
C	-21.419223	-1.997015	-3.679400
C	-22.461077	-3.483834	-2.118202
C	-22.452666	-2.867374	-3.364810
C	-18.488397	-3.695489	-0.402054
C	-17.852706	-4.118351	-1.565362
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C	-17.290681	-5.370120	-1.763113

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C	-17.390200	-6.321653	-0.757306
F	-21.942287	-1.133762	0.581308
F	-22.506874	-0.331138	3.028190
F	-20.632501	-0.419959	4.998411
F	-18.138876	-1.372221	4.434992
F	-17.555755	-2.203491	1.965262
F	-21.490004	-3.852444	-0.049619
F	-23.438196	-4.326473	-1.801717
F	-23.417443	-3.111487	-4.240936
F	-21.388083	-1.410685	-4.871909
F	-19.441696	-0.929790	-3.159982
F	-16.076535	-2.218473	-0.783471
F	-14.616462	-0.145912	-1.382489
F	-15.699295	2.365826	-1.521230
F	-18.377069	2.672754	-1.126357
F	-19.920462	0.565849	-0.664869
F	-17.693764	-3.257151	-2.601958
F	-16.620045	-5.628650	-2.888344
F	-16.869469	-7.528970	-0.910902
F	-18.126500	-6.854612	1.404193
F	-19.179936	-4.473780	1.738961
Na	-15.321366	-3.029618	-3.004555

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C	-11.484283	-5.499728	8.966604
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C	-12.260044	-3.460261	7.916271
C	-11.033953	-2.843397	8.215257
C	-10.050838	-3.546137	8.903357
C	-10.275059	-4.873290	9.278880
H	-11.655028	-6.537946	9.258810
H	-13.429404	-5.273950	8.055699
H	-10.863257	-1.810052	7.907146
H	-9.103344	-3.059729	9.144402
H	-9.499244	-5.424768	9.815135
C	-13.296197	-2.720032	7.214996
H	-14.295339	-3.134351	7.105903
H	-13.136534	-1.682482	6.935735
Cl	-12.827976	-3.378835	4.998856
P	-14.186590	-1.492464	9.498149
C	-15.602432	-0.335629	9.535654
C	-15.568241	0.880210	10.231734
C	-16.764421	-0.695778	8.841561
C	-16.683844	1.715406	10.238773
H	-14.666884	1.180243	10.771132
C	-17.882128	0.136773	8.858396
H	-16.794778	-1.629162	8.275735
C	-17.842942	1.342296	9.557627
H	-16.644838	2.665834	10.774894
H	-18.782620	-0.153116	8.312310
H	-18.714079	2.000860	9.561078
C	-12.745071	-0.441142	9.897720
C	-11.953003	-0.565766	11.043440
C	-12.385502	0.497786	8.919877
C	-10.810929	0.222887	11.195966
H	-12.218556	-1.277497	11.827070

C	-11.247664	1.284035	9.073016
H	-13.003794	0.617153	8.027636
C	-10.452042	1.142070	10.211546
H	-10.199254	0.115447	12.094758
H	-10.982660	2.004418	8.297667
H	-9.553990	1.752399	10.331622
C	-14.438346	-2.581838	10.945993
C	-15.635914	-2.592938	11.673954
C	-13.430974	-3.500926	11.283071
C	-15.818576	-3.500192	12.717541
H	-16.434405	-1.888740	11.430666
C	-13.614961	-4.401312	12.330158
H	-12.486960	-3.507762	10.734990
C	-14.810995	-4.405724	13.048565
H	-16.756523	-3.494541	13.277638
H	-12.817626	-5.104580	12.581561
H	-14.957091	-5.114342	13.867104
B	-13.947126	1.565459	4.103403
C	-14.170550	2.324052	5.560668
C	-13.191416	2.919456	6.352994
C	-15.476849	2.548144	6.003362
C	-13.470702	3.638656	7.515576
C	-15.803834	3.264436	7.147399
C	-14.785543	3.804904	7.923921
C	-12.364885	1.148241	3.807762
C	-11.646547	1.389558	2.634194
C	-11.657824	0.420418	4.769137
C	-10.320784	0.987377	2.448450
C	-10.335241	0.008653	4.636368
C	-9.658616	0.291836	3.452977
C	-14.526047	2.705821	3.051710
C	-15.743502	2.675038	2.374468
C	-13.824910	3.906104	2.917158
C	-16.215201	3.729543	1.592149
C	-14.252711	4.980794	2.148011
C	-15.467492	4.892186	1.477476
C	-14.744298	0.112705	3.997052
C	-14.880861	-0.513098	2.755977
C	-15.263703	-0.624992	5.060020
C	-15.534241	-1.724293	2.547459
C	-15.932139	-1.837284	4.901197
C	-16.065542	-2.398699	3.640659
F	-11.892459	2.832621	6.041049
F	-12.484697	4.170553	8.231106
F	-15.069572	4.485200	9.025996
F	-17.072064	3.452197	7.492060
F	-16.507171	2.063057	5.302333
F	-12.656202	4.064085	3.548992
F	-13.522149	6.086667	2.055925
F	-15.903317	5.903472	0.738922
F	-17.382596	3.630144	0.964921
F	-16.553692	1.614167	2.438393
F	-12.261269	0.087963	5.914008
F	-9.729168	-0.660692	5.605575
F	-8.407836	-0.099546	3.286250
F	-9.696151	1.249711	1.310752
F	-12.193568	2.027455	1.603191
F	-14.342533	0.057119	1.664509

F	-15.619787	-2.248911	1.332192
F	-16.662909	-3.566989	3.483695
F	-16.390387	-2.497922	5.959185
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Na	-12.421828	-1.722785	3.094389

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C	-14.940610	-7.533996	6.517066
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C	-15.357645	-5.218146	5.950825
C	-14.060959	-4.884943	6.370556
C	-13.215669	-5.869319	6.871843
C	-13.655909	-7.192252	6.948854
H	-15.278880	-8.570856	6.570891
H	-16.792117	-6.810103	5.671468
H	-13.725557	-3.846620	6.310649
H	-12.210468	-5.606028	7.207358
H	-12.991968	-7.964141	7.344951
C	-16.255240	-4.186107	5.457988
H	-17.303893	-4.405026	5.279509
H	-15.930468	-3.151508	5.396412
Cl	-15.860991	-4.367344	3.129863
P	-17.088684	-3.177647	7.844759
C	-18.817968	-3.316585	8.435694
C	-19.569806	-4.405134	7.984635
C	-19.393148	-2.414342	9.343770
C	-20.886030	-4.582783	8.414366
H	-19.134011	-5.115430	7.280154
C	-20.706794	-2.590708	9.768602
H	-18.816018	-1.563964	9.715059
C	-21.455841	-3.674678	9.302628
H	-21.469901	-5.425907	8.038642
H	-21.152826	-1.874871	10.462418
H	-22.491391	-3.802094	9.625075
C	-16.778137	-1.392292	7.618514
C	-17.803824	-0.523064	7.226970
C	-15.461773	-0.908611	7.662410
C	-17.525680	0.803572	6.903837
H	-18.832337	-0.878663	7.174721
C	-15.185862	0.419385	7.343344
H	-14.640744	-1.569961	7.951873
C	-16.216528	1.279282	6.962225
H	-18.343312	1.462114	6.603774
H	-14.156521	0.782541	7.388753
H	-15.998181	2.319426	6.709424
C	-16.116764	-3.658062	9.324394
C	-15.805148	-2.770224	10.363817
C	-15.722558	-4.998523	9.428767
C	-15.104358	-3.217441	11.482152
H	-16.109059	-1.722570	10.302124
C	-15.023973	-5.444397	10.550677
H	-15.960592	-5.703257	8.628220
C	-14.711251	-4.553934	11.576740
H	-14.866329	-2.517927	12.286853
H	-14.720038	-6.491510	10.617753
H	-14.160265	-4.900621	12.454211
B	-20.610666	-2.390849	3.024307

C	-21.299164	-2.078213	4.497693
C	-22.324325	-2.906769	4.957405
C	-21.031112	-0.990226	5.324886
C	-22.992140	-2.727544	6.162382
C	-21.673040	-0.769832	6.542846
C	-22.662194	-1.643309	6.966738
C	-20.020856	-3.938740	2.886715
C	-19.820478	-4.848196	3.921615
C	-19.523653	-4.383070	1.662891
C	-19.210369	-6.091477	3.759024
C	-18.902226	-5.607090	1.447868
C	-18.728105	-6.475454	2.518480
C	-19.244090	-1.481106	2.756573
C	-18.956883	-0.707959	1.630827
C	-18.210522	-1.537486	3.696516
C	-17.758552	-0.004449	1.466188
C	-17.001470	-0.861264	3.574497
C	-16.770149	-0.087044	2.440188
C	-21.839753	-2.062420	1.971789
C	-22.307485	-0.750344	1.874882
C	-22.577925	-2.991765	1.242848
C	-23.388268	-0.362394	1.093560
C	-23.671219	-2.649985	0.446129
C	-24.081167	-1.326914	0.369970
F	-22.693649	-3.967515	4.230834
F	-23.926747	-3.585136	6.559448
F	-23.283686	-1.449052	8.121559
F	-21.332598	0.266661	7.303660
F	-20.116433	-0.071630	4.995575
F	-18.373148	-2.271711	4.797577
F	-16.056798	-0.967771	4.496280
F	-15.624193	0.555023	2.291488
F	-17.550121	0.717622	0.374736
F	-19.818074	-0.599992	0.620731
F	-19.565746	-3.562131	0.588143
F	-18.400845	-5.902748	0.251913
F	-18.102383	-7.628567	2.360980
F	-19.039474	-6.886094	4.811449
F	-20.183409	-4.567627	5.170876
F	-21.690442	0.223521	2.553341
F	-23.767435	0.909759	1.036464
F	-25.118861	-0.985561	-0.381576
F	-24.327881	-3.585728	-0.231695
F	-22.279968	-4.294341	1.268424
Na	-17.079726	-3.082058	1.277158

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C	-15.554096	-6.490795	1.057272
C	-16.372286	-5.546666	0.447548
C	-15.932806	-4.220216	0.308465
C	-14.662426	-3.855960	0.780740
C	-13.844310	-4.804733	1.384733
C	-14.289947	-6.120499	1.525092
H	-15.898650	-7.521217	1.166711
H	-17.357497	-5.827049	0.069810
H	-14.323873	-2.822711	0.672618
H	-12.857807	-4.517781	1.754587

H	-13.647555	-6.864365	2.002181
C	-16.784635	-3.236624	-0.336855
H	-17.800095	-3.493599	-0.623477
H	-16.485311	-2.194445	-0.394506
Cl	-16.075589	-3.498930	-2.574443
P	-18.043712	-2.368675	1.961769
C	-19.565953	-3.264134	2.457080
C	-20.697767	-3.102850	1.641599
C	-19.644510	-4.115567	3.565090
C	-21.880354	-3.776945	1.933231
H	-20.664018	-2.435023	0.776368
C	-20.829639	-4.796273	3.849387
H	-18.784916	-4.247789	4.224463
C	-21.948415	-4.630316	3.035836
H	-22.754191	-3.635261	1.295593
H	-20.875560	-5.455426	4.719419
H	-22.876148	-5.161554	3.260372
C	-18.567689	-0.615801	1.968297
C	-19.583213	-0.128460	2.803778
C	-17.896442	0.269817	1.118626
C	-19.913117	1.224149	2.787099
H	-20.117652	-0.807667	3.472224
C	-18.230942	1.623606	1.100882
H	-17.109822	-0.098200	0.458994
C	-19.239129	2.101293	1.935296
H	-20.709324	1.594915	3.436315
H	-17.706002	2.302124	0.424653
H	-19.510371	3.159280	1.916012
C	-16.905643	-2.502061	3.389863
C	-16.538200	-1.394971	4.167029
C	-16.320554	-3.748194	3.666652
C	-15.617287	-1.535422	5.205066
H	-16.971850	-0.413049	3.966875
C	-15.409772	-3.887426	4.711793
H	-16.578082	-4.623067	3.064481
C	-15.053657	-2.780522	5.482419
H	-15.342226	-0.663099	5.802513
H	-14.969283	-4.865962	4.916331
H	-14.334035	-2.887788	6.297424
B	-20.588780	-1.558548	-3.497650
C	-21.418545	-1.239949	-2.099695
C	-22.460559	-2.094105	-1.732761
C	-21.299887	-0.104281	-1.299332
C	-23.304082	-1.875306	-0.652126
C	-22.130528	0.159691	-0.209467
C	-23.128008	-0.741777	0.131622
C	-19.965590	-3.097213	-3.564714
C	-19.823864	-3.988191	-2.503529
C	-19.427692	-3.573112	-4.760773
C	-19.255034	-5.255024	-2.622722
C	-18.843051	-4.823303	-4.932062
C	-18.747227	-5.678138	-3.840669
C	-19.235640	-0.612594	-3.682353
C	-18.869343	0.105054	-4.822841
C	-18.296124	-0.574405	-2.647654
C	-17.682750	0.839128	-4.920416
C	-17.099208	0.133069	-2.704328
C	-16.787945	0.850461	-3.856718

C	-21.747039	-1.275659	-4.645121
C	-22.219601	0.027766	-4.812860
C	-22.433651	-2.234604	-5.386933
C	-23.257049	0.379619	-5.666760
C	-23.482189	-1.929302	-6.255482
C	-23.899101	-0.613974	-6.397377
F	-22.696604	-3.199153	-2.447296
F	-24.260390	-2.749617	-0.348318
F	-23.912688	-0.519354	1.176239
F	-21.986881	1.277597	0.492874
F	-20.381416	0.833245	-1.549712
F	-18.539862	-1.246986	-1.524243
F	-16.240755	0.118710	-1.692070
F	-15.653004	1.522212	-3.940104
F	-17.395017	1.502933	-6.029933
F	-19.638152	0.127002	-5.908641
F	-19.415060	-2.773693	-5.848368
F	-18.331138	-5.173974	-6.106467
F	-18.169750	-6.860996	-3.959751
F	-19.155949	-6.040613	-1.557564
F	-20.217427	-3.668869	-1.269754
F	-21.654893	1.029726	-4.129555
F	-23.643532	1.645240	-5.784978
F	-24.895155	-0.307323	-7.217050
F	-24.090323	-2.892832	-6.939445
F	-22.127879	-3.532850	-5.304466
Na	-16.981776	-2.314303	-4.654410

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C	-13.371852	-5.526655	10.044847
C	-13.983043	-4.362774	9.593366
C	-13.369947	-3.115758	9.794439
C	-12.125389	-3.056840	10.445396
C	-11.518321	-4.220941	10.899368
C	-12.142809	-5.455931	10.702432
H	-13.857978	-6.491550	9.888645
H	-14.943770	-4.414122	9.081450
H	-11.639596	-2.089922	10.591145
H	-10.554394	-4.169742	11.409726
H	-11.665688	-6.369893	11.063613
C	-14.027118	-1.901268	9.354935
H	-15.030814	-1.940138	8.932890
H	-13.606369	-0.929466	9.588952
Cl	-13.101709	-1.632700	7.179652
P	-15.286612	-1.528399	11.790551
C	-15.537095	-3.257773	12.314639
C	-16.506929	-4.013145	11.637828
C	-14.687779	-3.904670	13.220992
C	-16.656406	-5.373473	11.894558
H	-17.143981	-3.539436	10.888642
C	-14.827543	-5.271405	13.463746
H	-13.904425	-3.347741	13.738813
C	-15.815314	-6.006930	12.809894
H	-17.421680	-5.941780	11.361437
H	-14.155830	-5.762995	14.171308
H	-15.923082	-7.076303	13.005649
C	-16.849762	-0.624711	12.134570

C	-18.074198	-1.228420	12.439209
C	-16.796370	0.772875	12.008132
C	-19.225012	-0.451850	12.592026
H	-18.147063	-2.309742	12.562891
C	-17.941264	1.544600	12.171018
H	-15.851901	1.264610	11.762915
C	-19.164506	0.932346	12.452877
H	-20.175376	-0.939820	12.820584
H	-17.883540	2.628205	12.052688
H	-20.069710	1.535842	12.552009
C	-14.155766	-0.806137	13.038101
C	-12.929300	-0.274145	12.628117
C	-14.508710	-0.748331	14.395380
C	-12.059032	0.295831	13.559735
H	-12.650054	-0.292247	11.573289
C	-13.639748	-0.182286	15.323597
H	-15.470520	-1.148965	14.726531
C	-12.411954	0.338888	14.906539
H	-11.104764	0.710436	13.227214
H	-13.922113	-0.143204	16.378149
H	-11.732170	0.784995	15.636321
B	-17.760651	0.276394	6.757356
C	-18.908349	0.761640	7.848323
C	-20.133197	0.091232	7.872893
C	-18.848826	1.872230	8.688547
C	-21.198691	0.435009	8.695822
C	-19.900535	2.269045	9.512923
C	-21.078648	1.539313	9.530788
C	-17.375720	-1.335630	6.874922
C	-17.741309	-2.238360	7.874434
C	-16.522072	-1.884264	5.924951
C	-17.362798	-3.581676	7.864904
C	-16.074852	-3.195105	5.894757
C	-16.508250	-4.065347	6.883756
C	-16.288106	1.006091	6.978790
C	-15.484710	1.605365	6.012592
C	-15.690740	0.924250	8.235272
C	-14.212299	2.119422	6.274016
C	-14.447005	1.453101	8.551697
C	-13.683792	2.045227	7.554651
C	-18.461249	0.669666	5.310020
C	-18.667805	2.018504	5.013509
C	-18.999803	-0.212689	4.376109
C	-19.319436	2.477762	3.875608
C	-19.663058	0.201264	3.220444
C	-19.826139	1.555387	2.966891
F	-20.326855	-0.966196	7.076198
F	-22.323504	-0.272959	8.686812
F	-22.071550	1.886303	10.339583
F	-19.774623	3.334012	10.299840
F	-17.759405	2.643132	8.757444
F	-16.335987	0.295859	9.216773
F	-13.951156	1.341595	9.782188
F	-12.472102	2.506690	7.814234
F	-13.481472	2.622303	5.279345
F	-15.861629	1.677094	4.727141
F	-16.061798	-1.104110	4.913988
F	-15.228075	-3.595900	4.952198

F	-16.106305	-5.327006	6.906148
F	-17.785492	-4.406950	8.816654
F	-18.493836	-1.870555	8.912502
F	-18.212523	2.958313	5.849688
F	-19.467010	3.779262	3.652355
F	-20.454898	1.965080	1.873517
F	-20.146966	-0.694213	2.365554
F	-18.914213	-1.536956	4.535637
Na	-13.812313	-0.619181	4.916606

[Bn-PPh₃]⁺NaCl⁻[BAr^F₂₀]⁻

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C	-14.762069	-7.106330	7.271629
C	-15.824243	-6.214225	7.132605
C	-15.599446	-4.907533	6.683315
C	-14.294629	-4.512306	6.363629
C	-13.234416	-5.407232	6.495750
C	-13.464166	-6.703573	6.956276
H	-14.951151	-8.122955	7.623807
H	-16.839196	-6.536773	7.377117
H	-14.106055	-3.494012	6.014940
H	-12.221987	-5.090723	6.241836
H	-12.631238	-7.402292	7.062550
C	-16.732355	-3.919870	6.576453
H	-17.655727	-4.380377	6.193216
H	-16.467174	-3.106020	5.890381
Cl	-16.066192	-2.518305	0.155594
P	-17.184344	-3.128030	8.159780
C	-17.952162	-4.340970	9.254981
C	-18.973860	-5.159877	8.750274
C	-17.582304	-4.428196	10.601774
C	-19.605161	-6.072275	9.589325
H	-19.283034	-5.088152	7.704756
C	-18.221181	-5.345569	11.435045
H	-16.800145	-3.784121	11.008058
C	-19.226852	-6.167477	10.930127
H	-20.397505	-6.711295	9.194634
H	-17.929000	-5.414575	12.484704
H	-19.723356	-6.886315	11.585668
C	-18.371427	-1.810655	7.822486
C	-19.427373	-1.573539	8.711492
C	-18.186775	-0.976343	6.712554
C	-20.293738	-0.506706	8.482643
H	-19.576743	-2.216851	9.581450
C	-19.054966	0.088308	6.492753
H	-17.358119	-1.137621	6.026157
C	-20.108061	0.322974	7.376809
H	-21.117835	-0.323265	9.174857
H	-18.902607	0.739391	5.629447
H	-20.788630	1.159361	7.203302
C	-15.732686	-2.418133	8.959167
C	-15.675821	-1.040119	9.191734
C	-14.663301	-3.243210	9.347031
C	-14.548959	-0.483771	9.792486
H	-16.501266	-0.391987	8.898921
C	-13.541832	-2.677229	9.943724
H	-14.705956	-4.323348	9.195510
C	-13.483536	-1.299312	10.164673

H	-14.507732	0.593791	9.961146
H	-12.706143	-3.316048	10.235617
H	-12.598777	-0.860381	10.629365
B	-13.650624	0.866318	4.336268
C	-14.299885	1.992693	5.358443
C	-14.199703	3.376975	5.244718
C	-15.163807	1.557944	6.364009
C	-14.875988	4.265095	6.083005
C	-15.856434	2.401631	7.220855
C	-15.711232	3.777303	7.077566
C	-12.474052	1.474292	3.342329
C	-11.366133	2.101284	3.918824
C	-12.373533	1.316740	1.966065
C	-10.271332	2.565958	3.200658
C	-11.298201	1.755463	1.197040
C	-10.234176	2.389385	1.821199
C	-15.019729	0.347769	3.548896
C	-15.703560	-0.843598	3.788107
C	-15.710195	1.238473	2.720650
C	-16.956085	-1.147557	3.257485
C	-16.953667	0.974850	2.156560
C	-17.588283	-0.231815	2.430864
C	-12.828600	-0.346342	5.116319
C	-12.390517	-1.449860	4.389167
C	-12.371189	-0.324196	6.434355
C	-11.595906	-2.472826	4.885497
C	-11.559478	-1.319025	6.981244
C	-11.172619	-2.403290	6.207180
F	-13.444251	3.946808	4.303902
F	-14.733369	5.576432	5.926620
F	-16.362227	4.607685	7.879879
F	-16.655836	1.916523	8.168904
F	-15.350625	0.244065	6.540239
F	-15.177405	2.429985	2.443454
F	-17.538554	1.863036	1.364866
F	-18.767241	-0.504928	1.901504
F	-17.537151	-2.306003	3.538488
F	-15.176535	-1.795759	4.572268
F	-13.341211	0.684783	1.261405
F	-11.281526	1.558010	-0.114961
F	-9.197360	2.817337	1.116782
F	-9.260627	3.165547	3.816942
F	-11.325451	2.289063	5.240602
F	-12.738658	-1.570459	3.085727
F	-11.246257	-3.501512	4.124222
F	-10.408550	-3.358240	6.719070
F	-11.130670	-1.225204	8.233736
F	-12.664227	0.683258	7.257605
Na	-14.198221	-1.442029	1.326763

Na[BAr^F₂₀]⁺Na[BAr^F₂₀]⁻BnCl⁻PPh₃

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C	-25.126088	-8.048867	5.818847
C	-24.920042	-7.158216	4.768381
C	-23.721737	-6.439813	4.675515
C	-22.729538	-6.629713	5.643358
C	-22.934116	-7.524288	6.692294
C	-24.132352	-8.232958	6.781837

H	-26.067730	-8.597833	5.889628
H	-25.696259	-7.011184	4.013062
H	-21.796102	-6.064607	5.578268
H	-22.157938	-7.661535	7.448121
H	-24.295280	-8.927886	7.608940
C	-23.522840	-5.455819	3.571510
H	-24.454537	-4.956151	3.299156
H	-22.748980	-4.716140	3.801564
Cl	-22.957989	-6.276821	2.016806
P	-25.252140	-2.840816	6.093722
C	-26.948018	-3.552725	6.135115
C	-27.291678	-4.461930	5.128150
C	-27.900956	-3.235560	7.114127
C	-28.553257	-5.057321	5.103125
H	-26.569320	-4.696937	4.345710
C	-29.162974	-3.826171	7.088808
H	-27.655203	-2.521302	7.904146
C	-29.490633	-4.740498	6.085027
H	-28.804553	-5.761564	4.306440
H	-29.896394	-3.571096	7.857471
H	-30.481919	-5.199776	6.066032
C	-25.544321	-1.175323	6.835413
C	-26.370969	-0.297700	6.114639
C	-24.934730	-0.711249	8.005745
C	-26.583719	1.006325	6.552326
H	-26.855210	-0.634863	5.196080
C	-25.143885	0.599776	8.440916
H	-24.287727	-1.370238	8.589244
C	-25.964431	1.462476	7.717262
H	-27.225779	1.672546	5.971282
H	-24.655610	0.947318	9.354650
H	-26.114841	2.491465	8.051086
C	-24.381960	-3.757282	7.433971
C	-24.996989	-4.672491	8.296597
C	-22.998794	-3.548676	7.550230
C	-24.250528	-5.343124	9.266633
H	-26.067741	-4.870555	8.215686
C	-22.256666	-4.204637	8.530136
H	-22.496674	-2.854404	6.872834
C	-22.882620	-5.105401	9.392719
H	-24.745834	-6.056787	9.929392
H	-21.183386	-4.017503	8.612993
H	-22.302359	-5.628286	10.156703
B	-24.797658	-0.719227	1.062772
C	-26.134871	0.267114	1.092472
C	-27.125686	0.007454	2.044964
C	-26.489239	1.238082	0.152207
C	-28.347086	0.664843	2.113536
C	-27.704163	1.930353	0.181742
C	-28.635657	1.649388	1.173517
C	-23.983660	-0.815926	2.512155
C	-24.072083	0.067438	3.582632
C	-22.975513	-1.762926	2.681462
C	-23.257941	0.036007	4.711210
C	-22.135796	-1.855199	3.781177
C	-22.270618	-0.931281	4.810052
C	-23.595426	-0.197796	0.046836
C	-22.900317	-0.959290	-0.886119

C	-23.094752	1.095413	0.173039
C	-21.844168	-0.487876	-1.661175
C	-22.063315	1.636301	-0.580323
C	-21.422899	0.826441	-1.513002
C	-25.492722	-2.146133	0.588164
C	-25.977918	-2.285853	-0.715576
C	-25.818788	-3.200497	1.440415
C	-26.668037	-3.405103	-1.170096
C	-26.508470	-4.343611	1.030244
C	-26.933953	-4.449485	-0.288042
F	-26.921763	-0.943143	2.956494
F	-29.224920	0.349856	3.049528
F	-29.784413	2.300268	1.211026
F	-27.975185	2.849680	-0.729510
F	-25.661246	1.575725	-0.837845
F	-23.642640	1.929102	1.088621
F	-21.686206	2.892254	-0.418906
F	-20.428458	1.300004	-2.242596
F	-21.239295	-1.286574	-2.526937
F	-23.211995	-2.260726	-1.102312
F	-22.753911	-2.685513	1.712386
F	-21.219849	-2.810605	3.859643
F	-21.480041	-0.982462	5.869157
F	-23.416818	0.919874	5.677281
F	-24.979919	1.069200	3.586506
F	-25.780016	-1.311138	-1.601303
F	-27.073246	-3.485306	-2.427290
F	-27.582727	-5.523364	-0.699121
F	-26.761896	-5.323694	1.888551
F	-25.480667	-3.156121	2.728436
Na	-23.287416	-4.198902	0.123385
B	-25.739862	6.289715	2.996425
C	-25.705981	6.666039	1.380970
C	-25.865251	5.659446	0.435075
C	-25.635107	7.943357	0.824715
C	-25.887428	5.835401	-0.939907
C	-25.664059	8.185050	-0.549331
C	-25.788847	7.128321	-1.440475
C	-27.302602	5.781177	3.219703
C	-27.753382	4.506846	3.535626
C	-28.335989	6.695408	2.994317
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C	-30.073121	5.099707	3.450474
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C	-24.087150	8.173265	3.787811
C	-25.576015	9.033859	5.920626
C	-23.588017	9.186679	4.595519
C	-24.343579	9.622628	5.678394
C	-24.583300	5.172647	3.444113
C	-24.578577	4.707180	4.765716
C	-23.465165	4.785731	2.701120
C	-23.570399	3.926069	5.317732
C	-22.438087	3.984674	3.207656
C	-22.489305	3.553543	4.524740
F	-25.986648	4.371946	0.852881
F	-25.998385	4.803608	-1.764217

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F	-25.582641	9.426394	-1.010714
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F	-23.305987	7.792718	2.770266
F	-22.402379	9.733433	4.349663
F	-23.890728	10.586341	6.468305
F	-26.304966	9.430188	6.958673
F	-27.218974	7.497397	5.419711
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F	-30.609919	7.317676	2.883804
F	-31.354006	4.786290	3.562868
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F	-26.884802	3.480201	3.725224
F	-25.581461	5.030810	5.582616
F	-23.628181	3.541604	6.582131
F	-21.517509	2.804384	5.016717
F	-21.412714	3.640829	2.442864
F	-23.313585	5.159441	1.427952
Na	-25.361062	2.784234	2.230870

TS^D

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C	-24.698716	-7.499480	5.084348
C	-23.906778	-6.379121	4.782581
C	-22.569543	-6.339994	5.210962
C	-22.035675	-7.401133	5.932479
C	-22.831618	-8.508900	6.232321
H	-24.780055	-9.426614	6.043515
H	-25.736656	-7.531807	4.745749
H	-21.956046	-5.468365	4.972946
H	-20.997433	-7.364879	6.268290
H	-22.412298	-9.340629	6.803163
C	-24.462115	-5.265759	4.037829
H	-25.500234	-5.260013	3.723934
H	-23.871674	-4.369414	3.870156
Cl	-23.975231	-5.993088	1.795581
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C	-26.978195	-4.844165	6.733730
C	-27.693475	-5.566411	5.773073
C	-27.522866	-4.684678	8.017265
C	-28.928012	-6.135943	6.091937
H	-27.298754	-5.679647	4.761981
C	-28.751064	-5.256725	8.335330
H	-26.982391	-4.107112	8.771963
C	-29.454547	-5.985566	7.372667
H	-29.478404	-6.695263	5.332149
H	-29.165629	-5.129308	9.337905
H	-30.420040	-6.431313	7.623198
C	-25.727026	-2.301959	6.681910
C	-26.598598	-1.619077	5.821490
C	-25.231099	-1.641047	7.813320
C	-26.982399	-0.307745	6.095863
H	-26.989984	-2.116800	4.932116
C	-25.610659	-0.325760	8.079452
H	-24.555461	-2.150351	8.502699
C	-26.489721	0.341045	7.227336
H	-27.662121	0.207498	5.414682

H	-25.214230	0.180156	8.962605
H	-26.777628	1.373741	7.436285
C	-24.180336	-4.637392	7.518774
C	-24.387860	-5.783993	8.294493
C	-22.933153	-3.996051	7.575557
C	-23.375085	-6.265337	9.124597
H	-25.339919	-6.316287	8.250789
C	-21.928997	-4.469980	8.415170
H	-22.741035	-3.116057	6.959012
C	-22.147394	-5.608816	9.191789
H	-23.550907	-7.163264	9.721380
H	-20.968518	-3.951325	8.454587
H	-21.357884	-5.986822	9.845364
B	-24.989878	-0.384543	1.279134
C	-26.255620	0.686178	1.150240
C	-27.354994	0.516927	1.998304
C	-26.451538	1.636748	0.145211
C	-28.545058	1.225844	1.896241
C	-27.626573	2.381838	0.007689
C	-28.681913	2.173560	0.886142
C	-24.311124	-0.467082	2.793039
C	-24.456936	0.434927	3.840393
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C	-23.758888	0.374478	5.043069
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C	-22.862761	-0.661352	5.258976
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C	-23.076970	1.264841	0.514316
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C	-26.983916	-2.984633	-0.940351
C	-26.966886	-3.880529	1.281632
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F	-27.296312	-0.395315	2.969033
F	-29.536289	0.996493	2.740702
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F	-25.500815	1.897302	-0.753715
F	-23.600035	2.133725	1.412665
F	-21.483526	2.936475	0.035373
F	-20.285133	1.272840	-1.763973
F	-21.318625	-1.219035	-2.156061
F	-23.435360	-2.035637	-0.848563
F	-23.104236	-2.392685	2.119497
F	-21.817477	-2.600320	4.420913
F	-22.201415	-0.752948	6.400439
F	-23.941251	1.299074	5.968867
F	-25.305318	1.484422	3.745487
F	-25.912340	-0.982769	-1.387736
F	-27.363532	-3.056328	-2.206525
F	-28.101698	-4.998085	-0.449387
F	-27.333524	-4.807658	2.155860
F	-25.840856	-2.799719	2.976570

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C	-25.337105	6.983442	1.074950
C	-25.441537	5.915816	0.189871
C	-25.117678	8.208717	0.445789
C	-25.291421	5.988784	-1.186553
C	-24.969134	8.346579	-0.934826
C	-25.054405	7.233162	-1.758982
C	-27.215728	6.345582	2.735608
C	-27.799265	5.129698	3.065583
C	-28.139465	7.306948	2.313952
C	-29.166869	4.872844	3.047560
C	-29.512555	7.101177	2.257080
C	-30.036337	5.866137	2.625422
C	-25.232575	8.049550	3.630354
C	-26.043115	8.627620	4.604895
C	-23.940069	8.575026	3.569435
C	-25.624426	9.670777	5.431594
C	-23.479502	9.611831	4.370483
C	-24.333894	10.166284	5.317218
C	-24.594024	5.589229	3.360615
C	-24.806075	5.196508	4.688247
C	-23.408500	5.100606	2.804330
C	-23.949682	4.371017	5.408194
C	-22.517851	4.270167	3.489852
C	-22.788617	3.903266	4.800187
F	-25.689031	4.672000	0.677981
F	-25.369777	4.905926	-1.946427
F	-24.911325	7.352497	-3.070071
F	-24.754754	9.542678	-1.467639
F	-25.042273	9.345099	1.137827
F	-23.064280	8.078232	2.688355
F	-22.238188	10.068985	4.247242
F	-23.919878	11.153923	6.098805
F	-26.450788	10.182984	6.337510
F	-27.291242	8.202705	4.818447
F	-27.714938	8.522725	1.963654
F	-30.325790	8.069134	1.856635
F	-31.340686	5.646817	2.581873
F	-29.631970	3.687129	3.416959
F	-27.043610	4.063809	3.437265
F	-25.885737	5.629111	5.339345
F	-24.226892	4.036324	6.658312
F	-21.947990	3.123643	5.458087
F	-21.415215	3.833092	2.900897
F	-23.055824	5.396078	1.551903
Na	-25.370164	3.166756	2.265084

[BAr^F₂₀]⁻...Na[BAr^F₂₀]

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B	-24.909623	-0.217520	1.427812
C	-26.225741	0.780367	1.199792
C	-27.351641	0.598820	2.012185
C	-26.423168	1.673186	0.143494
C	-28.565977	1.248904	1.825788
C	-27.620922	2.359616	-0.075746
C	-28.700984	2.142913	0.767951
C	-24.279693	-0.179307	2.963179
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C	-23.249287	-1.070591	3.277225
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C	-22.590481	-1.104807	4.500159
C	-22.945943	-0.200400	5.495856
C	-23.600194	0.196810	0.497837
C	-22.880310	-0.645366	-0.349246
C	-23.046699	1.467082	0.619676
C	-21.742850	-0.240290	-1.048540
C	-21.926491	1.928825	-0.054567
C	-21.260984	1.053134	-0.904685
C	-25.562247	-1.684819	1.029847
C	-25.997234	-1.891654	-0.280928
C	-25.860943	-2.725671	1.906227
C	-26.641439	-3.041703	-0.718149
C	-26.506565	-3.898570	1.513088
C	-26.901493	-4.059309	0.193118
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F	-29.585912	1.019996	2.637094
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F	-27.736057	3.207885	-1.086111
F	-25.450336	1.937084	-0.730648
F	-23.635784	2.369012	1.446830
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F	-20.183360	1.448176	-1.565609
F	-21.109400	-1.091834	-1.845479
F	-23.235701	-1.916226	-0.538301
F	-22.862638	-1.977471	2.377050
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F	-22.333019	-0.215498	6.669033
F	-24.331976	1.578047	6.169808
F	-25.508392	1.679310	3.834557
F	-25.787950	-0.947212	-1.205023
F	-27.014957	-3.173990	-1.986417
F	-27.518803	-5.166886	-0.195238
F	-26.757226	-4.857264	2.398858
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B	-25.774652	6.874672	2.504707
C	-25.421261	7.047691	0.893911
C	-25.480558	5.937936	0.057430
C	-25.164745	8.240932	0.219574
C	-25.253556	5.944508	-1.310461
C	-24.938511	8.311800	-1.155454
C	-24.981041	7.159829	-1.928032
C	-27.384025	6.466875	2.473833
C	-27.973312	5.259031	2.823281
C	-28.290908	7.395598	1.954147
C	-29.334846	4.983257	2.735991
C	-29.655617	7.168723	1.824100
C	-30.187780	5.944971	2.217397
C	-25.469842	8.232701	3.399652
C	-26.339845	8.845907	4.298585
C	-24.181314	8.770895	3.386408
C	-25.979566	9.933310	5.095228
C	-23.778036	9.852103	4.159240
C	-24.690511	10.441033	5.027471
C	-24.796280	5.766139	3.275657
C	-25.075039	5.434942	4.607372
C	-23.587587	5.249595	2.800900

C	-24.259730	4.639657	5.404889
C	-22.740704	4.439343	3.562327
C	-23.078253	4.131722	4.872744
F	-25.759792	4.721197	0.591960
F	-25.292242	4.827292	-2.021534
F	-24.764705	7.215466	-3.233540
F	-24.692241	9.481161	-1.732981
F	-25.128195	9.410322	0.858646
F	-23.251019	8.242627	2.583377
F	-22.536501	10.319331	4.083156
F	-24.331927	11.471435	5.781176
F	-26.860671	10.477297	5.928333
F	-27.592844	8.414078	4.464200
F	-27.859044	8.600034	1.572902
F	-30.453225	8.106602	1.330269
F	-31.485252	5.707577	2.106967
F	-29.809166	3.810779	3.133967
F	-27.230358	4.222354	3.287887
F	-26.183300	5.900558	5.183500
F	-24.594860	4.371440	6.656415
F	-22.280628	3.372310	5.604203
F	-21.616512	3.968288	3.045338
F	-23.169606	5.493553	1.557761
Na	-25.491581	3.270274	2.251607

[Bn-PPh₃]⁺

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C	-23.702387	-8.628455	4.450823
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C	-23.713045	-6.232970	4.824634
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C	-21.616433	-7.450350	4.745073
C	-22.309133	-8.641613	4.528769
H	-24.250384	-9.556432	4.272496
H	-25.491900	-7.427072	4.533537
H	-21.770523	-5.322495	5.072588
H	-20.525539	-7.451752	4.800670
H	-21.763101	-9.580809	4.414535
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H	-23.798577	-4.077925	4.849511
P	-25.079436	-4.731641	6.741836
C	-26.364199	-5.953406	7.083253
C	-27.406552	-6.090488	6.153806
C	-26.375516	-6.698165	8.267591
C	-28.440046	-6.987304	6.402544
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C	-27.416673	-7.594160	8.508193
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C	-28.443025	-7.741955	7.577461
H	-29.248504	-7.095844	5.676894
H	-27.422621	-8.177015	9.431245
H	-29.255356	-8.446287	7.769481
C	-25.808283	-3.089013	6.914033
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C	-26.779881	-2.891298	7.905302
C	-25.935400	-0.752231	6.316905
H	-24.622525	-2.150954	5.348519
C	-27.322309	-1.623759	8.096852

H	-27.116978	-3.724907	8.526242
C	-26.901680	-0.555979	7.303060
H	-25.606798	0.082667	5.694874
H	-28.079806	-1.471135	8.868069
H	-27.331865	0.436658	7.453169
C	-23.708223	-4.904747	7.899716
C	-23.094920	-6.155955	8.072191
C	-23.220848	-3.782019	8.580410
C	-21.999832	-6.274843	8.922381
H	-23.470643	-7.038243	7.550065
C	-22.122865	-3.912481	9.428582
H	-23.693716	-2.805892	8.454341
C	-21.513347	-5.154854	9.598344
H	-21.524881	-7.248655	9.056307
H	-21.745053	-3.036807	9.959966
H	-20.653906	-5.252655	10.265255

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