

Electronic Supplementary Information

For

Partner Effect in Accelerating Pincer-Co Catalyzed Nitrile Hydroboration Reactions

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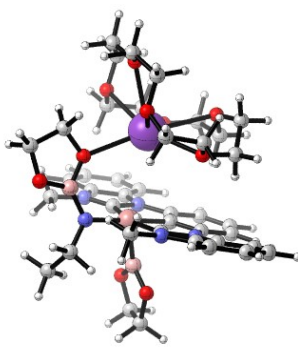
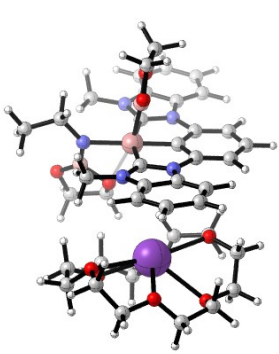
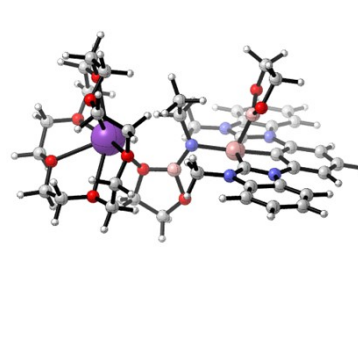
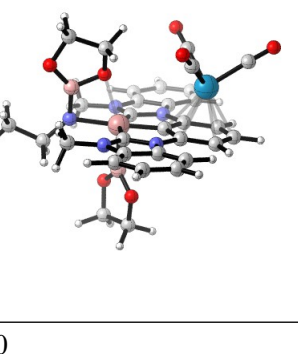
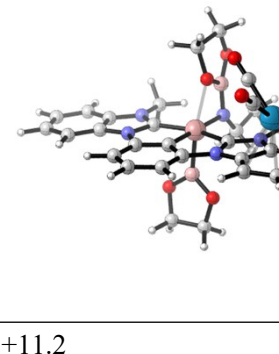
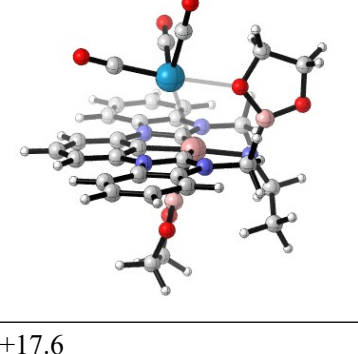
Table of Content

Binding Configuration between Partner and Catalyst	S2
Ion-pairing behavior of [K] in benzene	S3
Spin density isosurface of LCo	S5
The potential energy curve for the binding of LCo with Borate	S6
The Gibbs free energy for the binding of explicit THF molecules to [K] in THF	S6
Absolute energies for the species involved in this work	S8
Geometries for the involved species	S10

Binding Configuration between Partner and Catalyst

With ${}^1\mathbf{6K}$ as an example, the binding configuration of $[\mathbf{K}]$ and the cobalt complex is explored (Table S1). It is shown that the $[\mathbf{K}]$ partner strongly favors binding with the centroid phenyl ring over the NHC part of the ligand. Meanwhile, in comparison to the K–O bounded structure ${}^1\mathbf{6K}_3$, the K–ligand bounded ${}^1\mathbf{6K}_1$ is more stable by 2.9 kcal/mol.

Table S11. The geometries and relative Gibbs free energies (kcal/mol) for the representative binding configurations.

${}^1\mathbf{6K}_1$ (shown in Figure 4)	${}^1\mathbf{6K}_2$ ($[\mathbf{K}]$ binds at the NHC side)	${}^1\mathbf{6K}_3$ ($[\mathbf{K}]$ does not bind the Pincer ligand)
		
0.0	+8.4	+2.9
${}^1\mathbf{6W}_{\text{CO}_1}$ (shown in Figure 6)	${}^1\mathbf{6W}_{\text{CO}_2}$ (W binds at the NHC side)	${}^1\mathbf{6W}_{\text{CO}_3}$ (W binds with Co)
		
0.0	+11.2	+17.6

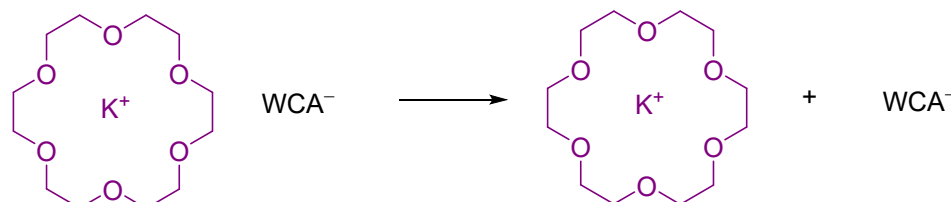
Similarly, $\text{W}(\text{CO})_3$ also favors binding with the centroid phenyl ring, with a much larger preference of 11.2 kcal/mol, which should be attributed to the much stronger covalent nature of binding. On the other hand, the geometry with W–Co bonding is significantly higher in energy. Although the metal-metal bonding is difficult to be accurately handled by DFT calculations, the huge energy

difference prompts that the W–Co bonding is inaccessible. This is also in consistence with the well-known Effective Atomic Number (EAN) rule: W can only form 18e⁻ configuration by binding the phenyl ring, rather than the Co atom.

Ion-pairing behavior of [K] in benzene

Obviously, one major challenge for applying the [K] partner in benzene is to obtain discrete (18-crown-6)K⁺ cation, rather than an ion-pair, which is much more common in a non-polar solvent like benzene. The Gibbs free energy for the dissociation of the ion pair for various weakly coordinating anions (WCAs) were examined.

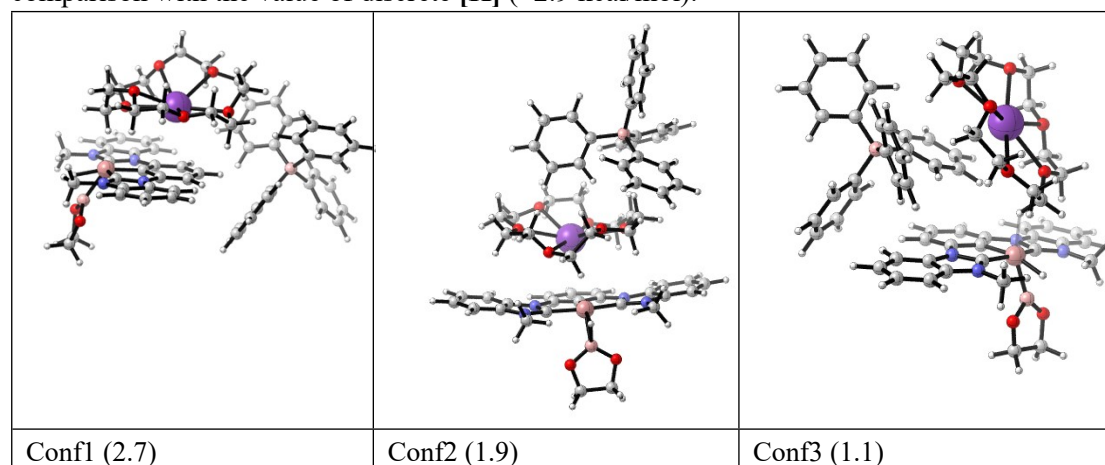
Table SI2. The dissociation free energy for the ion pair formed by [K] and WCAs in benzene.



WCA	Dissociation free energy (kcal/mol)
BPh ₄ ⁻	20.9
B(C ₆ F ₅) ₄ ⁻	15.6
Al(<i>Or</i> -C ₄ F ₉) ₄ ⁻	12.6
CHB ₁₁ Cl ₁₁ ⁻	18.1

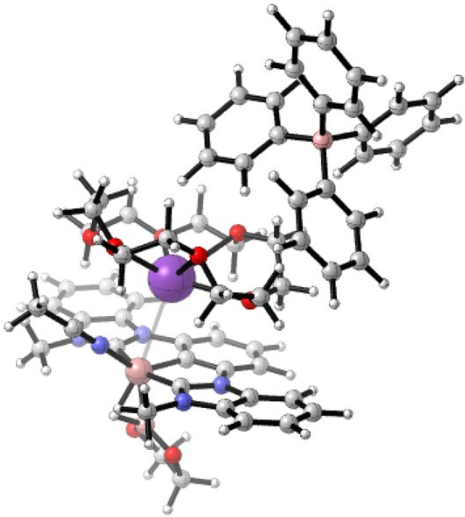
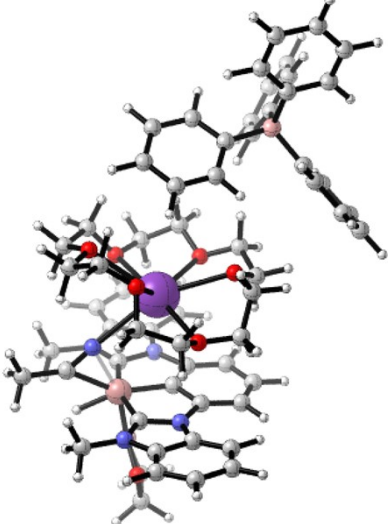
According to the above results, the dissociation of [K]–WCA ion pair is quite unfavorable in benzene, even with some of the weakest bases known yet as the counteranion. The unfavorable formation of discrete [K] might reduce the partner effect in benzene. Nevertheless, since the nature of the catalyst–[K] interaction is majorly contributed by dispersion rather than electrostatic factors, we propose that this binding does not require a dissociated cation, and an ion-pair is also able to play the role of an effective partner. This proposal is supported by the optimized binding geometry of the ion-pair with **1**.

Table SI3. The binding geometries and energetics of $[\mathbf{K}]\text{-BPh}_4^-$ ion pair with **1**. The binding Gibbs free energy (kcal/mol) describes the free energy change from **1** to the binding state, in comparison with the value of discrete $[\mathbf{K}]$ (-2.9 kcal/mol).



Among the three possible binding geometries, both Conf1 and Conf2 share a similar structure with $^1\mathbf{IK}$ in Figure 4, with the potassium atom approaches the centroid Pincer phenyl ring at a K-C distance of 3.20 Å, and there is no close contact between $[\mathbf{K}]$ and the counteranion. The distance between the counteranion and the catalytic center, described by the closest crown ether H-Pincer C distance, is as long as 6.19 Å. The three isomers are quite close in energy, and the non-covalent nature of the interaction enables rapid interchange of binding mode adapting to the requirement to stabilize the key transition states. Moreover, since BPh_4^- is the strongest coordinating anion examined in Table 2, the binding of the ion pair with the Pincer-Co fragment should be even stronger for other WCAs. These observations prompt us that WCAs might have a negligible effect on the partner effect of $[\mathbf{K}]$, although we are unable to fully explore the Gibbs energy profile in the presence of WCAs because of the large size of the system. Furthermore, in solvents with larger polar than benzene, the ion pairing will be reduced, and we believe that the partner effect of $[\mathbf{K}]$ will be further released.

Table SI4. Geometry of selected intermediate and transition state in the presence of BPh_4^- , along with their relative Gibbs free energy

	
<p>2K-BPh₄ (0.0)</p>	<p>TS1K-BPh₄ (4.3)</p>

In order to further verify the influence of counteranion, the barrier of the first migration insertion process was taken as an example and checked in the presence of BPh_4^- in the revised version. It is found that the barrier is 4.3 kcal/mol from **2K-BPh₄** to **TS1K-BPh₄**, even slightly lower than the value of 5.8 kcal/mol without the counteranion. Therefore, it can be suggested that a properly selected WCA might be not harmful to the reaction.

Spin density isosurface of LCo

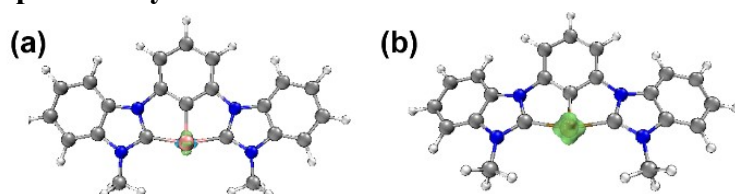


Figure S11. The spin density isosurface of 1LCo (a) and 3LCo (b), at an isovalue of 0.05.

The potential energy curve for the binding of LCo with Borate

In order to verify whether a TS exists for the binding of LCo with borate, a potential energy scan of the Co–B distance in **11** was performed. The stability of the wave-function of each point

on the curve has been ensured. It is shown that the electronic energy keeps increasing monotonously along a wide range of Co–B distance, and no maximum point appears even though the distance is similar to the sum of the van de Waals radius of Co and B ($\sim 4.0 \text{ \AA}$). As a result, we conclude that the binding process is either barrierless or very close to barrierless.

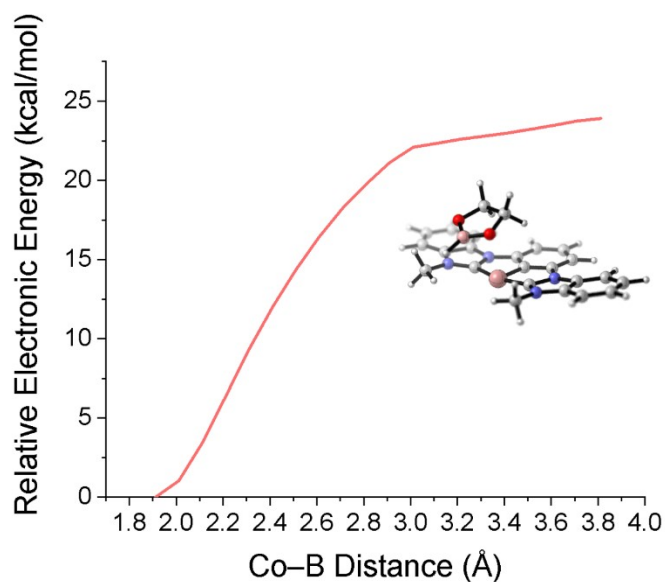


Figure SI2. The potential energy curve for the binding of LCo with Borate

The Gibbs free energy for the binding of explicit THF molecules to [K] in THF

Table SI5. The Gibbs free energy for the binding of explicit THF molecules to [K] in THF

[K]·1THF (+2.9 kcal/mol)	[K]·2THF (+8.5 kcal/mol)

The binding of explicit THF molecules with **[K]** is examined. The structures were optimized under the implicit solvation of THF, and the Gibbs free energies at room temperature were obtained at the same level used in the text. The results show that the binding of one and two THF molecules to **[K]** is disfavored by 2.9 and 8.5 kcal/mol, respectively. As a result, the implicit solvation model is sufficient to describe the solvation effect of THF, and explicit THF binding to potassium will not reduce the binding of **[K]** to the catalyst.

Absolute energies for the species involved in this work

Table SI4. Energetics for the species involved (in Hartree).

	Thermal Correction	E	G
MeCN	0.021478	-132.64870136	-132.627223
HBR₂	0.051590	-254.41586567	-254.364276
PhH	0.073836	-232.06202795	-231.988192
³LCo	0.295326	-2449.34216770	-2449.046842
¹LCo	0.296987	-2449.33936489	-2449.042378
¹1	0.373446	-2703.79768804	-2703.424242
³1	0.369622	-2703.77848180	-2703.408860
¹2	0.411375	-2836.47017077	-2836.058796
³2	0.405163	-2836.43991149	-2836.034748
TS1	0.411143	-2836.44991047	-2836.038767
³TS1	0.406102	-2836.38809910	-2835.981997
¹3	0.413558	-2836.47318196	-2836.059624
³3	0.411700	-2836.43307702	-2836.021377
¹TS2	0.417716	-2836.46586162	-2836.048146
³TS2	0.413586	-2836.42703817	-2836.013452
³4	0.414954	-2836.49273468	-2836.077781
¹4	0.420309	-2836.49944098	-2836.079132
¹5	0.490128	-3090.93968553	-3090.449558
³5	0.488942	-3090.91044626	-3090.421504
¹TS3	0.492341	-3090.92635955	-3090.434019
³TS3	0.486980	-3090.86875365	-3090.381774
¹6	0.496920	-3090.94686710	-3090.449947
³6	0.492524	-3090.94781997	-3090.455296
MECP	0.494480	-3090.9393634	-3090.444883
¹TS4	0.498455	-3090.93297532	-3090.434520
³TS4	0.495673	-3090.89443106	-3090.398758
¹7	0.496113	-3090.98155254	-3090.485440
³7	0.494550	-3090.97272481	-3090.478175
[K]	0.324451	-1522.05703488	-1521.732584
[K]PhH	0.416013	-1754.13265152	-1753.716639
¹LCoK	0.646797	-3971.42600890	-3970.779212
¹1K	0.722669	-4225.88404393	-4225.161375
¹2K	0.762520	-4358.55743070	-4357.794911
¹TS1K	0.764295	-4358.55008875	-4357.785794
¹3K	0.767010	-4358.55747800	-4357.790468
¹TS2K	0.765825	-4358.55464655	-4357.788822
¹4K	0.771696	-4358.59364195	-4357.821946
¹5K	0.847167	-4613.03515005	-4612.187983
¹TS3K	0.845069	-4613.02450243	-4612.179433

¹⁶K	0.850791	-4613.04921518	-4612.198424
¹TS4K	0.850851	-4613.02802676	-4612.177176
¹⁷K	0.848993	-4613.08171973	-4612.232727
¹W(PMe)₃PhH	0.393897	-1681.93987746	-1681.545980
¹LCoW(PMe)₃	0.617746	-3899.21015461	-3898.592409
¹1W_{PMe}	0.696604	-4153.67489558	-4152.978292
¹²W_{PMe}	0.734595	-4286.33691324	-4285.602318
¹TS1W_{PMe}	0.737053	-4286.31874956	-4285.581697
¹³W_{PMe}	0.738558	-4286.34510548	-4285.606547
¹TS2W_{PMe}	0.738855	-4286.33653815	-4285.597683
¹⁴W_{PMe}	0.741593	-4286.36669270	-4285.625100
¹⁵W_{PMe}	0.816450	-4540.80374005	-4539.987290
¹TS3W_{PMe}	0.818325	-4540.79073632	-4539.972411
¹⁶W_{PMe}	0.821233	-4540.82777112	-4540.006538
¹TS4W_{PMe}	0.822017	-4540.80655335	-4539.984536
¹⁷W_{PMe}	0.818806	-4540.84410510	-4540.025299
¹W(CO)₃PhH	0.088674	-639.04134355	-638.952670
¹LCo	0.310717	-2856.32805177	-2856.017335
¹1W_{CO}	0.386463	-3110.78641381	-3110.399951
¹²W_{CO}	0.428664	-3243.46374206	-3243.035078
¹TS1W_{CO}	0.427662	-3243.43235701	-3243.004695
¹³W_{CO}	0.430341	-3243.45762572	-3243.027285
¹TS2W_{CO}	0.431388	-3243.45191801	-3243.020530
¹⁴W_{CO}	0.434429	-3243.48638759	-3243.051959
¹⁵W_{CO}	0.508267	-3497.92765265	-3497.419386
¹TS3W_{CO}	0.510514	-3497.91671702	-3497.406203
¹⁶W_{CO}	0.513330	-3497.93898382	-3497.425654
¹TS4W_{CO}	0.515197	-3497.91905592	-3497.403859
¹⁷W_{CO}	0.513114	-3497.97813114	-3497.465017
¹LCoDipp	0.713585	-3303.92396357	-3303.210379
¹1Dipp	0.841576	-3636.95070898	-3636.109133
¹²Dipp	0.886477	-3769.63564054	-3768.749164
¹TS1Dipp	0.886484	-3769.61779316	-3768.731309
¹³Dipp	0.892284	-3769.63819046	-3768.745906
¹TS2Dipp	0.891083	-3769.62136105	-3768.730278
¹⁴Dipp	0.895530	-3769.65625184	-3768.760722
¹⁵Dipp	1.019835	-4102.67484454	-4101.655010
¹TS3Dipp	1.020173	-4102.65712187	-4101.636949
¹⁶Dipp	1.025948	-4102.67820889	-4101.652261
¹TS4Dipp	1.028832	-4102.65311844	-4101.624286
⁷Dipp	1.027615	-4102.69982948	-4101.672214
¹LCoK_{Dipp}	0.713585	-4826.01327866	-4825.299694
¹1K_{Dipp}	1.200727	-5159.03774094	-5157.837014

¹² K _{Dipp}	1.238644	-5291.72483591	-5290.486192
¹ TS1K _{Dipp}	1.242966	-5291.71984954	-5290.476884
¹³ K _{Dipp}	1.244400	-5291.72074657	-5290.476347
¹ TS2K _{Dipp}	1.244005	-5291.70643821	-5290.462433
¹⁴ K _{Dipp}	1.246650	-5291.74510243	-5290.498452
¹⁵ K _{Dipp}	1.373156	-5624.75306037	-5623.379904
¹ TS3K _{Dipp}	1.372960	-5624.74259269	-5623.369633
¹⁶ K _{Dipp}	1.379833	-5624.75774630	-5623.377913
¹ TS4K _{Dipp}	1.379500	-5624.74418945	-5623.364689
¹⁷ K _{Dipp}	1.377609	-5624.80370701	-5623.426098
[K]·1THF	0.433281	-1754.37106452	-1753.937784
[K]·2THF	0.546129	-1986.66478397	-1986.118655
TS1K-BPh ₄	1.104047	-5309.41832980	-5308.314283
2K-BPh ₄	1.103528	-5309.41087982	-5308.307352

Geometries for the involved species

¹TS4_{KDipp}

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 H -3.41677000 6.90950600 0.52689200
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 C -0.75546600 -2.51607100 -3.73578500
 C -0.11233100 -4.84842700 -3.01772200
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 H 0.23878100 -2.39832400 -4.20197900
 H -1.44953300 -2.86249400 -4.52208000
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 H -0.73131400 -5.32056100 -3.80106300
 H 0.89966800 -4.71008500 -3.44035200
 C -0.54027100 2.67108900 -2.69088000
 C -0.15967800 3.32618500 -4.01766000
 C -0.56669500 1.15134800 -2.82094000
 H 0.25575500 2.91908800 -1.97048700
 H -0.09638900 4.42471400 -3.92549200
 H 0.82274800 2.95529600 -4.35976200
 H -0.88421100 3.09440100 -4.81745300
 H -0.94914000 0.66466000 -1.90794900
 H -1.23422900 0.83545900 -3.63928000
 H 0.44893100 0.77150700 -3.02317300
 K 3.92752400 -0.15470200 -0.34894100
 O 3.80748900 -2.92002300 -0.25418500
 O 3.17114900 1.08680900 -2.71300500
 O 5.81138800 -1.57371800 1.23586300
 C 3.14420700 -3.45196200 -1.37550700
 C 4.99444400 -3.57665500 0.11014400

C 3.53835300	2.43141300	-2.88840400	H -0.03702700	-3.27522600	1.50196900
C 3.18708400	0.33875700	-3.89999200	H 0.72778500	-3.58119000	-0.07834500
C 7.08856800	-1.25256300	0.74857300	C 3.14767800	-1.63259600	0.21255800
C 5.52792400	-2.94246800	1.37473500	H 3.64003500	-0.64615400	0.17192400
C 3.81308900	-3.06681600	-2.68140200	H 3.73953100	-2.30564300	0.85987800
H 2.11582000	-3.05524700	-1.33666100	H 3.13629000	-2.04696900	-0.80930300
H 3.07236700	-4.55571600	-1.30283800	C 1.81565400	-1.12187900	2.61177900
H 4.79984500	-4.65164600	0.30331600	H 0.88923900	-1.05168400	3.20288200
H 5.75225100	-3.51748000	-0.69668500	H 2.44210100	-1.93275500	3.02728400
C 3.42718600	3.14209300	-1.56039400	H 2.36418300	-0.17077200	2.71757400
H 4.56765600	2.49462500	-3.29731100	C -2.98296100	-1.91916500	0.22242600
H 2.86545900	2.93145600	-3.61288200	H -2.37703000	-2.84149100	0.22497700
C 2.85503300	-1.09745700	-3.59842200	H -3.87683200	-2.07133400	0.85489500
H 4.18707900	0.39104000	-4.37637900	H -3.31090300	-1.73264500	-0.81364600
H 2.44351000	0.73552700	-4.62018600	C -1.89867000	-0.96862900	2.61211400
C 7.31516900	0.22359900	0.94072900	H -2.91767000	-1.09236400	3.02332500
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H 7.19554200	-1.51327400	-0.32460800	H -1.37216400	-0.19404600	3.19209700
H 4.76615100	-3.01961700	2.16709200	C -3.22046200	0.82027300	0.88642200
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H 4.84570800	-3.45398100	-2.71628200	H -2.81456400	1.69319700	1.42548300
H 3.26670400	-3.53256800	-3.52424500	C -0.19373300	3.52913600	0.18728600
O 4.27180000	2.59899600	-0.57510000	H -1.29312500	3.43722800	0.16906500
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H 2.39878700	3.03844100	-1.17938600	H 0.14647900	3.71858500	-0.84430000
H 1.88920200	-1.15114300	-3.05658200	C 0.11388000	2.14612400	2.59745800
H 2.73367000	-1.63379400	-4.56061000	H 0.49289000	3.10419000	2.99936900
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H 8.36565300	0.46925600	0.68318600	C 2.31627500	2.40929400	0.85553100
C 5.60152200	3.04413500	-0.63150100	H 2.48266400	3.40061300	1.31656000
C 6.41331100	2.32556500	0.41197100	H 2.88157700	1.65407800	1.42789800
H 6.04726600	2.85458200	-1.62792700	H 2.71152400	2.41345200	-0.17455700
H 5.65240200	4.13475300	-0.43717600	C -0.78312000	1.19182800	-2.35546200
H 7.44228100	2.73820500	0.40038800	C -1.41776400	-0.07977500	-2.32260100
H 5.98518800	2.50637900	1.41952400	C 0.64731300	1.25337400	-2.32577500
¹W(PMe)₃PhH			H -1.38030700	2.10608700	-2.36723500
W 0.00165200	-0.00489600	-0.54677700	C -0.64926800	-1.28714300	-2.35333900
P -1.94054500	-0.51195000	0.81710600	H -2.51033200	-0.13238300	-2.31991500
P 0.52894000	1.94275400	0.80398100	C 1.43089500	0.06720000	-2.35686500
P 1.41566700	-1.41833400	0.82780400	H 1.14909500	2.22532500	-2.32633700
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C -1.36851900 5.17379900 -0.21309600
C -1.15579600 5.59939400 2.17563200
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C -1.66513800 5.93986200 0.91415400
H -1.76083600 5.43637700 -1.19836700
H -1.40134500 6.22408400 3.03910700
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C 5.48729900 -3.34281100 -1.11289400
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H -3.48222200 -3.10583500 -3.02911400

13K

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C 1.17865500 1.12656900 -1.87641300
C 1.23110800 1.11576000 -3.26882600
C 0.01705200 1.08674000 -3.96870100
C -1.22287800 1.05705800 -3.31449900
C -1.22389400 1.06742900 -1.92080800
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H -2.30154700 1.49275000 2.84798900
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H 3.80436800 0.58431700 2.91096800
H 3.20950100 2.27919400 2.90680600
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H -1.37479200 5.42853400 -1.82411700
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C -0.03110200 2.66413600 3.36211000
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H 0.04543700 1.17557700 4.93698300
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H 1.92413900 -2.96097600 -3.84541400
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H 2.08708200 -3.64917200 3.25368000
H 2.84432800 -2.08132200 3.68448000
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H -2.16063600 -4.08116300 -3.14234500
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¹TSlW_{PMe}
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C 0.91489700 -0.89831600 -2.45880700
C -0.23060700 -1.56481400 -1.91590000
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C 2.81415100 5.82702500 -0.71204700
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H 4.27403700 4.87155800 -1.98656500
H 3.33792800 6.78715600 -0.72383100
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H -5.14041800 -0.23754400 2.44873000
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H -1.14805200 5.83319300 0.87544900
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C -2.65732600 2.93443800 -3.08689800
H -3.89532800 1.22414400 -3.73754800
H -4.79627500 2.47496900 -2.83053600
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H -2.98105500 3.93739200 -3.41486400
B -2.51483200 1.94195700 -1.03347200
O -3.54354200 1.28512000 -1.70016700
O -2.06699600 3.00956600 -1.80439100
N -1.29581700 1.04029200 2.65819500
C -2.20996900 1.82189300 2.63769400
C -3.09455900 2.59230300 3.54370000
H -2.82094900 2.38355200 4.59160800
H -3.00305700 3.67501300 3.35534100
H -4.15089700 2.31773100 3.38442400
W 1.31054000 -1.05693800 -0.26063200
P 0.68399400 -2.79022400 1.32743700
P 3.26103100 -2.30496500 -0.93625400
P 2.66052500 0.04339000 1.45789700
C 1.87365000 -3.92698600 2.18478100
C -0.43586000 -4.12161700 0.70338000
C -0.31395500 -2.22685100 2.77254300
C 2.90605800 -3.92341700 -1.76510500
C 4.66445900 -2.86307600 0.14229800
C 4.28594200 -1.50858500 -2.26013700
C 3.39877000 -0.86592000 2.89461500
C 1.90555100 1.42146200 2.42386700
C 4.18959200 0.91295600 0.88179900
H 1.35100900 -4.53803600 2.94381100
H 2.32094900 -4.61162300 1.44384500
H 2.68332000 -3.36977900 2.67629900
H 0.01290200 -4.60192300 -0.18285700
H -0.61898300 -4.89178500 1.47527800
H -1.40390900 -3.69003000 0.41303800
H -1.18271400 -1.65828900 2.40348600
H -0.65734200 -3.07298600 3.39701400
H 0.27612700 -1.53180300 3.39089400
H 2.20934000 -3.76127600 -2.60580700
H 3.82099700 -4.41435600 -2.14730200
H 2.41169600 -4.60104700 -1.04786700
H 4.29707900 -3.52069500 0.94549300
H 5.42310200 -3.41288200 -0.44491200

H 5.15240900 -1.99128700 0.60834200
H 4.70811400 -0.56536200 -1.87481500
H 5.11162900 -2.16232200 -2.59682300
H 3.65488600 -1.26271900 -3.12978600
H 2.59167200 -1.24647100 3.54285000
H 4.00032100 -1.71988200 2.54830200
H 4.04195000 -0.19786300 3.49630700
H 0.92371900 1.10132800 2.80940800
H 2.56513500 1.73032200 3.25552300
H 1.74202400 2.29112700 1.77003200
H 4.67014700 1.47690900 1.70302100
H 4.91784600 0.19141300 0.47601800
H 3.92059200 1.61775400 0.07896700
¹⁷W_{PMe}
C 0.00946900 0.07150400 -0.82404300
C 0.75807600 -1.03778300 -1.31232400
C 1.89663600 -0.84585300 -2.14041900
C 2.30355000 0.49781700 -2.45073800
C 1.63876500 1.61362500 -1.85729900
C 0.44320400 1.38183700 -1.10365700
H 2.42683900 -1.68460600 -2.59250700
H 3.16272000 0.66873700 -3.10235500
H 1.99332600 2.62016000 -2.08333100
C -0.72093400 3.64310600 -0.85837100
C -1.56926900 1.71183300 0.06445000
C -1.95761200 3.94480900 -0.23948400
C -0.01972900 4.63590600 -1.54366700
C -2.49520600 5.22977200 -0.26002400
C -0.56403300 5.92727700 -1.56794300
H 0.91702500 4.42393500 -2.06007200
C -1.77341900 6.22327100 -0.93346800
H -3.44978400 5.45213100 0.22379000
H -0.02620800 6.71813800 -2.09926900
H -2.16811400 7.24308500 -0.96892100
C 0.32610100 -3.55327300 -1.22469100
C -1.15020300 -2.02273100 -0.35325200
C -0.78437900 -4.25305800 -0.69641100
C 1.38630000 -4.24445300 -1.81200400
C -0.84940800 -5.64418500 -0.73130700
C 1.31458200 -5.64245000 -1.85039800
H 2.24626300 -3.72201100 -2.23093500
C 0.22031800 -6.33068500 -1.31949600
H -1.69981900 -6.18610600 -0.31032100
H 2.13753700 -6.20375400 -2.30280800

H 0.19747000 -7.42382300 -1.35907200	C 2.23852800 3.65473100 1.06427600
N 0.06244600 -2.22208900 -1.01070500	H 1.39267500 3.35057400 1.70367300
N -1.65675500 -3.30026800 -0.20840200	H 2.76897200 4.49975500 1.54128900
N -0.50683000 2.30185500 -0.62808200	H 1.82049100 4.00201400 0.10745500
N -2.43321300 2.76853300 0.29476000	C 4.62657400 3.00937100 -0.29277300
C -3.69735700 2.66111500 0.96046000	H 4.21040500 3.13409700 -1.30659300
H -3.81220300 1.62991900 1.31288100	H 4.95105800 3.99486700 0.09158200
H -3.75022300 3.34511700 1.82710400	H 5.50624100 2.34983200 -0.37557800
H -4.53364200 2.89916000 0.27684600	C 4.25779200 2.30889200 2.40331500
C -2.92444500 -3.60726700 0.38938400	H 5.03286100 1.53035600 2.47221500
H -3.65605200 -2.83184000 0.12213600	H 4.73460600 3.29863000 2.52747400
H -3.29396700 -4.56943600 0.00174100	H 3.54496800 2.16488500 3.23299100
H -2.85696900 -3.67883900 1.49145300	C 5.34396800 -0.95342500 -1.78692700
Co -1.64961300 -0.20722300 -0.00764000	H 5.62178300 0.07634600 -2.06994500
H -7.20588600 -1.22005700 -0.52681800	H 6.25947900 -1.57094600 -1.73492200
C -2.72976400 -0.71134700 2.81291600	H 4.69178600 -1.35887900 -2.57854700
C -3.91534500 -1.35480200 3.54323100	C 5.89822800 -0.50284600 0.90310600
H -1.81192800 -1.31574900 2.84376400	H 6.23518600 0.52842700 0.70505200
H -2.49588000 0.30023600 3.18491600	H 5.62571900 -0.58000500 1.96807600
H -3.75713600 -2.43275900 3.72403600	H 6.74373400 -1.18795300 0.70679500
H -4.13155000 -0.87015300 4.50882200	C 4.39196900 -2.73946800 0.16995600
B -4.54157700 -0.82518200 1.44263200	H 3.68595900 -3.21881600 -0.52755800
O -3.17385200 -0.60533800 1.46112000	H 5.38507400 -3.21705800 0.07122400
O -5.02176200 -1.19099100 2.66801100	H 4.01161000 -2.91690900 1.19016900
N -5.35557800 -0.67822200 0.29020700	C 3.15633300 -0.91410300 3.34262600
C -6.80527500 -0.84285900 0.42761100	H 2.69850600 -1.15313900 4.32058400
C -7.50442500 0.45137000 0.80500800	H 3.78907900 -1.76624900 3.04291900
H -7.33744500 1.22717100 0.03726400	H 3.80306700 -0.03219500 3.45770200
H -8.59351500 0.29277200 0.89745500	C 0.99946600 -2.23459000 2.19498200
H -7.13366200 0.83363400 1.77265000	H 1.61449800 -3.02821300 1.73646400
B -4.83258400 -0.26617300 -0.96846600	H 0.80003500 -2.49863100 3.25040800
O -3.48675500 -0.14762500 -1.22876400	H 0.04654500 -2.17390500 1.64298200
O -5.60645700 0.04328400 -2.05110200	C 0.71164100 0.45428800 3.02728700
C -3.34557300 0.45071800 -2.51507700	H 0.37601400 -0.02402600 3.96696600
C -4.72798900 0.26489800 -3.14988500	H 1.21175800 1.40710000 3.27173900
H -3.07854000 1.51276300 -2.38051400	H -0.15324400 0.67753600 2.37686200
H -2.53280900 -0.04974800 -3.06151600	¹⁵ Dipp
H -5.05960100 1.14932100 -3.71659500	C 0.03555400 1.51459700 -1.35385200
H -4.76296800 -0.61382400 -3.81823200	C -1.15435400 2.03357900 -1.86681000
H -6.99978100 -1.61219600 1.19182500	C -1.15958800 2.98389700 -2.88831300
W 2.33094800 0.23697600 -0.18125200	C 0.07468100 3.41352800 -3.39445700
P 3.35420900 2.20565000 0.78528200	C 1.29017400 2.91513600 -2.90515500
P 4.43745200 -0.91590600 -0.16812300	C 1.24555800 1.96836200 -1.88184800
P 1.86135100 -0.60723500 2.04850600	H -2.08242400 3.38528800 -3.30986300

H	0.08966500	4.15406000	-4.19941500	O	1.20121200	2.63850300	1.25091500
H	2.22859000	3.26407400	-3.33900200	O	-1.08181100	2.65950900	1.29475100
C	3.67697900	1.44648500	-1.27544100	C	0.83719700	3.97224100	1.54630400
C	1.91032400	0.36303800	-0.30897100	C	-0.68902200	4.01721100	1.31528900
C	4.17562900	0.51761000	-0.34448200	H	1.05515000	4.16001200	2.61800200
C	4.54476600	2.27768900	-1.98423900	H	-0.89224100	4.45026800	0.31477800
C	5.53651100	0.39958900	-0.08244900	H	0.03017300	0.62581400	1.57316900
C	5.91060000	2.15118900	-1.73129800	C	-3.26691700	-1.10797300	1.09169300
H	4.18105100	3.01150000	-2.70346800	C	-3.11392600	-0.89105600	2.47539200
C	6.40075000	1.23078100	-0.79430400	C	-3.67440000	-2.35195000	0.56764800
H	5.90680400	-0.30843800	0.66177000	C	-3.32250100	-1.97574000	3.33301800
H	6.61226300	2.79294900	-2.27190200	C	-3.88302300	-3.39959700	1.47270400
H	7.47744300	1.16676400	-0.61294300	C	-3.69924700	-3.22061700	2.83886000
C	-3.60505600	1.62969100	-1.24829400	H	-3.19840600	-1.84052100	4.41032400
C	-1.88999200	0.44245900	-0.30721700	H	-4.19926200	-4.37680800	1.09680800
C	-4.14647900	0.70495500	-0.33872700	H	-3.86221600	-4.05579100	3.52728000
C	-4.43280900	2.51909400	-1.93442200	C	3.18577000	-1.18029800	1.16887300
C	-5.51135800	0.64521300	-0.07668900	C	3.47210300	-2.48936400	0.73037800
C	-5.80245800	2.45375600	-1.67985000	C	3.06589300	-0.85448000	2.53334000
H	-4.03582400	3.25173800	-2.63704200	C	3.55295300	-3.49340700	1.70170700
C	-6.33533500	1.53509400	-0.76462200	C	3.14659900	-1.89751100	3.46194200
H	-5.91394700	-0.06286300	0.65059700	C	3.37310600	-3.20727300	3.05132400
H	-6.47288700	3.14259900	-2.20180200	H	3.76970400	-4.52058000	1.39429800
H	-7.41350700	1.51926100	-0.58145000	H	3.04469900	-1.67618000	4.52798100
N	-2.23871700	1.42161800	-1.21424600	H	3.43285400	-4.01023200	3.79281700
N	-3.07700400	-0.01154600	0.19169200	C	2.94900900	0.58175100	3.00016700
N	2.30231700	1.30704600	-1.23448200	C	4.31307600	1.09164000	3.47374800
N	3.07379400	-0.13375500	0.20092200	C	1.89161000	0.77781800	4.08021300
Co	0.00897000	0.21196300	-0.03447200	H	2.64011800	1.19788700	2.14455500
H	-0.14093200	-2.35791100	1.92251800	H	5.07512600	1.01145500	2.67984600
C	0.81442600	-1.72627800	-3.56312300	H	4.24435500	2.15549400	3.76489000
C	-0.68136000	-1.35261200	-3.58398400	H	4.67278500	0.52108100	4.35009300
H	0.93341700	-2.77884500	-3.89565800	H	0.91587700	0.39283700	3.74659300
H	-0.77348000	-0.26181700	-3.75977300	H	2.15842800	0.27965100	5.03043300
B	0.00213000	-1.53130400	-1.44676900	H	1.76915500	1.85370800	4.29625000
O	1.17429800	-1.65584100	-2.19594600	C	3.76806300	-2.81972800	-0.72191800
O	-1.12254700	-1.62899700	-2.26718800	C	2.97594400	-4.01722100	-1.23958600
N	-0.04759800	-1.72453200	-0.00141800	C	5.26707400	-3.06251500	-0.92204300
C	-0.11977100	-2.64881900	0.85805800	H	3.46606600	-1.95492600	-1.33019600
C	-0.18361100	-4.11314700	0.59200000	H	1.89532300	-3.84750000	-1.14255500
H	0.66343100	-4.61464300	1.09553900	H	3.19212500	-4.17094300	-2.31175200
H	-1.10970800	-4.52493800	1.03380000	H	3.24121700	-4.95231600	-0.71389500
H	-0.15861900	-4.34961500	-0.48187400	H	5.87410500	-2.20117800	-0.60085500
B	0.04946100	1.86797700	1.07063800	H	5.60627400	-3.94746900	-0.35277100

H 5.48489100 -3.24525900 -1.98977800
C -2.79307200 0.48081500 3.03118200
C -1.91904700 0.43033600 4.28035100
C -4.07704700 1.26732700 3.31109900
H -2.23823200 1.03846200 2.26477000
H -1.05913700 -0.24613900 4.14517600
H -1.52366100 1.43659800 4.50288600
H -2.48025400 0.09459400 5.17149500
H -4.68728300 1.39367400 2.40145000
H -4.69824800 0.76024200 4.07266500
H -3.82878900 2.27626600 3.68729000
C -3.93916100 -2.58260200 -0.91042200
C -5.44082200 -2.70329500 -1.18496400
C -3.21574900 -3.81284800 -1.45365100
H -3.54816700 -1.71614900 -1.46387300
H -5.99716800 -1.81176600 -0.85550600
H -5.62080500 -2.82825800 -2.26786300
H -5.86962100 -3.58192400 -0.66896200
H -2.13051300 -3.73130800 -1.30703900
H -3.57442300 -4.74680200 -0.98446400
H -3.39463700 -3.89916200 -2.53964700
C 1.62374500 4.94297800 0.69469600
H 1.34160700 5.98608800 0.92529800
H 2.70617700 4.82970400 0.87832100
H 1.43245600 4.75306500 -0.37620700
C -1.46555300 4.78634500 2.35883900
H -2.54688600 4.74690600 2.14178300
H -1.29747700 4.35600400 3.36224100
H -1.15686300 5.84677300 2.37524800
C -1.50964000 -2.10126000 -4.60046200
H -2.56959600 -1.80173900 -4.53306800
H -1.15850000 -1.88215400 -5.62434500
H -1.44335800 -3.19062100 -4.43244900
C 1.69512500 -0.83076500 -4.40371600
H 2.75456900 -1.12313500 -4.30240800
H 1.41981800 -0.90452100 -5.47103800
H 1.59090200 0.22097400 -4.08532100
¹LCoK
C 0.34927400 -0.44215700 -1.56489900
C -0.83995100 0.02970100 -2.11661500
C -0.85930100 1.11360700 -2.99732700
C 0.36723100 1.71278800 -3.32079200
C 1.58626200 1.24519300 -2.80770600
C 1.55251800 0.15355900 -1.93883100

H -1.77723400 1.47821900 -3.46284900
H 0.37551400 2.55819100 -4.01504600
H 2.51989500 1.71422700 -3.12489000
C 3.97602200 -0.31217700 -1.22747400
C 2.24786100 -1.70174300 -0.66280500
C 4.47868400 -1.35642800 -0.42494200
C 4.82761300 0.68363200 -1.70772700
C 5.82319500 -1.43490000 -0.07384800
C 6.17485900 0.60781600 -1.35193700
H 4.46838300 1.49392800 -2.34321500
C 6.66697800 -0.43039000 -0.54867600
H 6.20375600 -2.25189600 0.54393300
H 6.86367000 1.37497300 -1.71683500
H 7.73070200 -0.45827700 -0.29663400
C -3.27962500 -0.69917300 -1.78017600
C -1.51769200 -1.94605300 -1.01152100
C -3.78189000 -1.85179700 -1.14216900
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C -5.14856900 -2.08063400 -1.01041800
C -5.51796600 0.03389100 -2.16270100
H -3.78236600 1.16118400 -2.79775100
C -6.01216500 -1.11520200 -1.52988800
H -5.53147800 -2.97873000 -0.51981000
H -6.22156600 0.76932100 -2.56308000
H -7.09269200 -1.26110700 -1.44594300
N -1.90565100 -0.79807000 -1.68893300
N -2.68352000 -2.57826100 -0.71393200
N 2.62170400 -0.55544600 -1.34558500
N 3.40036400 -2.16914100 -0.11383000
C 3.49984500 -3.37235800 0.66801800
H 4.13964500 -4.11698000 0.16329300
H 3.92326300 -3.16001200 1.66496600
H 2.49080600 -3.79350300 0.78724600
C -2.77826600 -3.85430200 -0.05714300
H -3.35877200 -3.77674600 0.87773300
H -3.26410900 -4.59439500 -0.71650500
H -1.76211100 -4.20364100 0.17598800
Co 0.36517900 -2.05024400 -0.67073600
K -0.38983300 1.06735600 1.08971500
O -1.30286300 3.68357500 0.53985000
O 1.33376000 3.02883200 0.53109000
O 0.32746400 -0.56307000 3.26825200
O -2.21895300 -0.82110600 1.83226600
O 2.29290400 0.72706700 1.63978400

O	-2.99215300	1.87157600	1.95416900	H	1.63459300	2.10690800	-2.47828900
C	-0.51773400	4.03238100	-0.57029700	H	2.44871800	-0.13770100	-3.26737500
C	-2.67573400	3.59146300	0.27073700	H	1.40648400	-2.24323200	-2.45144600
C	0.91915700	4.19094900	-0.13821400	C	-0.99278700	-3.56205900	-0.87369700
C	2.72004600	2.81132800	0.55919400	C	-1.88067600	-1.75600000	0.20885100
C	-0.72219200	-1.41441500	3.65907200	C	-2.04280000	-4.00475100	-0.04168200
C	1.46952800	-1.20812600	2.75738900	C	-0.31859400	-4.46252200	-1.70112500
C	-1.57772500	-1.88178200	2.49569300	C	-2.42668100	-5.34216500	0.00546600
C	-3.44529900	-0.41084700	2.38022900	C	-0.70247700	-5.80230100	-1.65027100
C	3.06389900	1.89817200	1.70912500	H	0.46690100	-4.13810200	-2.38369400
C	2.58839600	-0.20427100	2.64627600	C	-1.73457400	-6.23961300	-0.80774500
C	-3.37864100	3.16062300	1.53662700	H	-3.24765300	-5.67653700	0.64410700
C	-3.90447200	0.83830900	1.67617700	H	-0.18946400	-6.52537300	-2.29109400
H	-0.86296900	4.98873000	-1.01474000	H	-2.01160300	-7.29768700	-0.79775100
H	-2.86931000	2.86524200	-0.54800300	C	-0.45964200	3.70763700	-0.84761300
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H	1.02896000	5.06872900	0.53008300	C	-1.53441500	4.28853900	-0.14345600
H	1.52934300	4.36958200	-1.04498900	C	0.48165300	4.50439200	-1.50066900
H	3.26970400	3.76145700	0.70827500	C	-1.71278300	5.66954600	-0.10053800
H	3.04996700	2.37063000	-0.40054000	C	0.30410500	5.88621400	-1.44958200
H	-1.33224700	-0.83933700	4.37576200	H	1.33184600	4.07187400	-2.02837700
H	-0.32485400	-2.29868600	4.19791500	C	-0.77679500	6.46099700	-0.76554600
H	1.26666000	-1.64911200	1.75575700	H	-2.55384000	6.12152300	0.43039200
H	1.78794600	-2.02132800	3.44078600	H	1.02563500	6.53412300	-1.95574100
H	-0.94791300	-2.36870400	1.72781400	H	-0.88885900	7.54897900	-0.75141000
H	-2.31364900	-2.62768200	2.85532800	N	-0.60332800	2.34810500	-0.67561500
H	-4.21178400	-1.20136300	2.25060100	N	-2.24372800	3.24334900	0.42472900
H	-3.34951600	-0.19768700	3.46295300	N	-0.90711400	-2.20454900	-0.66059200
H	2.86761000	2.41794600	2.66959700	N	-2.52696500	-2.88362800	0.60980600
H	4.14675200	1.66403500	1.66207500	C	-3.63607500	-2.91816400	1.52534700
H	2.70367300	0.30694200	3.62331900	H	-4.59489000	-2.87062400	0.98228600
H	3.53882600	-0.72971000	2.42336800	H	-3.59267000	-3.84448400	2.12062600
H	-4.47297400	3.21591400	1.38824500	H	-3.56142000	-2.05871900	2.20193000
H	-3.10776500	3.86215000	2.34491100	C	-3.43528600	3.41485600	1.21501000
H	-3.98416600	0.64744900	0.58695900	H	-3.44792200	4.42991400	1.64011300
H	-4.91451400	1.09827600	2.05087600	H	-4.33499500	3.25653400	0.59836200
H	-0.58734100	3.24887400	-1.35198600	H	-3.43023000	2.68910400	2.03864400
¹⁴W_{PMc}				Co	-2.02424100	0.16019200	0.41259900
C	-0.51160400	0.05195800	-0.67957000	H	-5.77549500	0.34536800	1.65117800
C	0.11935000	1.23301900	-1.15046700	C	-4.54526300	-0.64423200	-2.42764600
C	1.17704100	1.20106300	-2.08591500	C	-4.83893100	0.86160600	-2.41096100
C	1.63645200	-0.08320900	-2.53845000	H	-3.60658800	-0.85866600	-2.97726100
C	1.03831100	-1.28914700	-2.07494900	H	-5.35638500	-1.23917000	-2.88318600
C	-0.05570600	-1.18524100	-1.15641000	H	-4.38495600	1.38928200	-3.26904700

H -5.92930100 1.06423700 -2.42278100
B -3.92914500 0.18765500 -0.43606100
O -4.39524600 -0.98179600 -1.07129600
O -4.28468100 1.31913500 -1.20099200
N -3.81469100 0.25143500 1.04002000
C -4.70590800 0.32574700 1.93713200
C -4.40644300 0.39069300 3.39849900
H -4.82966500 1.31005400 3.84690500
H -4.87496400 -0.45703100 3.93444400
H -3.31743600 0.37125800 3.57448800
W 1.80320900 -0.10099500 -0.26195200
P 4.07667000 0.69478700 -0.43363000
C 5.26710400 -0.41227700 -1.32355100
C 5.15379200 1.18539100 0.99442800
C 4.32057400 2.22439400 -1.45189100
H 4.83548800 -0.68069300 -2.30347800
H 6.25349300 0.06350200 -1.48025600
H 5.41245600 -1.34669600 -0.75600300
H 5.27342100 0.34412100 1.69612700
H 6.15556900 1.50717100 0.65412900
H 4.68285500 2.02364800 1.53612800
H 3.72858900 3.04546700 -1.01166800
H 5.38247000 2.52880300 -1.49968600
H 3.95980300 2.05072400 -2.47999600
P 1.49509100 0.88088300 1.94771500
C -0.12295200 0.50874700 2.76811200
C 1.47935300 2.72823100 2.03667000
C 2.56161200 0.56343200 3.43288900
H -0.19220200 -0.57515000 2.95318300
H -0.24422800 1.05184900 3.72478300
H -0.94334200 0.79251600 2.07564300
H 0.82112400 3.13299600 1.25297800
H 1.13742500 3.09597300 3.02181200
H 2.49644100 3.11339900 1.84922700
H 3.61954800 0.76259100 3.20497800
H 2.25425700 1.20277400 4.28110200
H 2.46241700 -0.48981300 3.74440500
P 2.59203800 -2.12939000 0.80167300
C 1.40101000 -2.98058600 1.93276700
C 4.10977000 -2.23273200 1.86211700
C 3.00479700 -3.54531800 -0.31793000
H 0.41402400 -3.02608400 1.44471600
H 1.72532300 -4.00480100 2.19400000
H 1.29363500 -2.39480200 2.86150400

H 4.06692100 -1.49117800 2.67266200
H 4.22074900 -3.23978500 2.30506200
H 5.00337900 -2.02280700 1.25127400
H 3.71690800 -3.20710400 -1.09005600
H 3.44503900 -4.39454400 0.23638800
H 2.09164700 -3.89982700 -0.82030100
¹W_{PMc}
C -0.63845300 0.37706500 -0.61986800
C 0.45422200 1.12575300 -1.12309600
C 1.32774500 0.61378700 -2.11213800
C 1.11525600 -0.74746000 -2.52239600
C 0.02203200 -1.53710200 -2.05094000
C -0.83437000 -0.93779100 -1.08117300
H 2.14235300 1.19355400 -2.54349800
H 1.77947900 -1.18071900 -3.27518600
H -0.11490000 -2.55170200 -2.42359000
C -2.80957900 -2.55883600 -0.73992900
C -2.63465500 -0.57928100 0.38846600
C -3.89715100 -2.44338500 0.15104400
C -2.72204700 -3.64707100 -1.61085500
C -4.89253900 -3.41297300 0.22647700
C -3.72297600 -4.61578000 -1.53741800
H -1.91022400 -3.74134800 -2.33310200
C -4.78687600 -4.50893400 -0.63028100
H -5.73061200 -3.31305500 0.92039500
H -3.67657400 -5.47695700 -2.21043100
H -5.55309900 -5.28899800 -0.60329400
C 1.13893600 3.57422400 -0.75766400
C -0.72204300 2.66426400 0.21244500
C 0.50629500 4.55955600 0.02796600
C 2.31286800 3.86534100 -1.45389200
C 1.01849300 5.84952500 0.13802500
C 2.82586100 5.15756900 -1.34084000
H 2.82196000 3.11551700 -2.06025600
C 2.19207100 6.13485500 -0.55974000
H 0.52051000 6.60843800 0.74623600
H 3.74539400 5.41208500 -1.87592400
H 2.62381700 7.13788100 -0.49716000
N 0.36421300 2.44321200 -0.61457600
N -0.60457300 3.96212100 0.59852100
N -2.04112700 -1.43562700 -0.52263500
N -3.73500400 -1.24383800 0.82253500
C -4.65540800 -0.76461300 1.81953300
H -5.64399000 -0.57243900 1.37331200

H -4.74968900 -1.50722900 2.63092600
H -4.26200900 0.17532500 2.22707900
C -1.48766100 4.64134800 1.51000800
H -0.90612500 5.07193300 2.34364600
H -2.04140400 5.44081800 0.99188700
H -2.20711200 3.91155400 1.90086400
Co -1.83560800 1.14820800 0.55780700
H -3.01041800 1.88270400 1.41675700
C -5.52690100 2.33578800 -0.81545000
C -4.62619700 3.52082700 -1.16973300
H -6.03052700 1.89983100 -1.69662300
H -6.30951900 2.62545100 -0.08410600
H -4.27619200 3.45974300 -2.22011500
H -5.12229000 4.49824100 -1.03199500
B -3.45598500 2.05089500 0.12121900
O -4.65333600 1.39875500 -0.23512400
O -3.53564200 3.39663300 -0.29194300
W 1.34717300 -0.82659100 -0.28013700
P 2.25263000 0.38731800 1.64123600
P 3.56769400 -1.67180700 -0.76667900
P 0.92679600 -2.76483800 1.12698200
C 1.09915800 1.47434900 2.59758200
H 0.18260400 0.91129700 2.84300300
H 1.56870900 1.84644100 3.52685000
H 0.80779400 2.33779500 1.98303400
C 3.58842900 1.61276700 1.28322400
H 3.26449600 2.28687200 0.47439100
H 3.84281100 2.21732200 2.17338600
H 4.49593200 1.08578000 0.94427600
C 3.02740800 -0.43456900 3.11120900
H 3.85599500 -1.09405700 2.81320800
H 3.41459600 0.32074300 3.81944400
H 2.26752200 -1.03818000 3.63481100
C 4.53472400 -0.66223400 -1.98155500
H 4.68516400 0.35061700 -1.56952900
H 5.52044000 -1.11218000 -2.20070200
H 3.97692000 -0.56564700 -2.92761300
C 4.94307200 -1.94875300 0.44640000
H 5.24528200 -0.98698900 0.89374600
H 4.62132800 -2.62022900 1.25741300
H 5.82597700 -2.39103700 -0.05097200
C 3.61538400 -3.31155400 -1.62224800
H 2.87983500 -3.30970300 -2.44408400
H 4.61623300 -3.54939900 -2.02838500

H 3.32422400 -4.10728500 -0.91539700
C 2.22558800 -3.69152100 2.07061100
H 1.77157000 -4.50847900 2.66087100
H 2.94122000 -4.13739000 1.35962600
H 2.77934000 -3.03106100 2.75278500
C 0.20069400 -4.24063000 0.28555600
H 0.86561900 -4.56596900 -0.53279100
H 0.05776800 -5.08192000 0.98836400
H -0.77688600 -3.98500900 -0.14655200
C -0.32357400 -2.53916300 2.46880700
H -0.55145400 -3.48296900 2.99811200
H 0.04033400 -1.79551300 3.19752000
H -1.24805100 -2.13934100 2.02029900
¹TS_{Dipp}
C -0.10135300 -0.25659500 -2.01763900
C 1.09609900 -0.48793400 -2.67902300
C 1.15264600 -0.57518600 -4.07069400
C -0.04468500 -0.44617900 -4.78412000
C -1.27435600 -0.24758300 -4.14437800
C -1.27698300 -0.16024600 -2.75203600
H 2.08798100 -0.72028500 -4.61188200
H -0.01953400 -0.50491800 -5.87615700
H -2.18208700 -0.15576800 -4.74148500
C -3.73360500 0.01045100 -2.07307200
C -2.03873600 0.06653200 -0.53662100
C -4.29260500 0.13256700 -0.79218100
C -4.55443400 -0.08141700 -3.19839700
C -5.66790300 0.16333500 -0.58308300
C -5.93277400 -0.04936700 -2.99337600
H -4.15018100 -0.18010500 -4.20539200
C -6.48367600 0.07009000 -1.70882500
H -6.08216700 0.25758100 0.42299400
H -6.59874800 -0.12237600 -3.85795600
H -7.57046000 0.08892300 -1.58784700
C 3.42965900 -1.08554800 -1.87563200
C 1.79271400 -0.39965000 -0.42100600
C 3.94862100 -1.11174200 -0.57434700
C 4.20307000 -1.51132600 -2.95726700
C 5.23865400 -1.55646600 -0.30114900
C 5.49623900 -1.95583500 -2.68810100
H 3.82140600 -1.51420800 -3.97767300
C 6.00834300 -1.98049400 -1.38245000
H 5.62161200 -1.57981400 0.72115400
H 6.12196900 -2.29904500 -3.51697400

H 7.02568500	-2.34242400	-1.20869700	C 3.24782200	-0.38146700	1.64182700
N 2.13478500	-0.61819300	-1.74201500	C 2.88481000	-1.29671400	2.64416300
N 2.93989200	-0.65994300	0.27287200	C 3.99505300	0.78200700	1.91974900
N -2.36417000	0.00075100	-1.87404700	C 3.25981000	-1.00278100	3.95928800
N -3.23100200	0.18707700	0.10767900	C 4.36045300	1.01856700	3.24832700
Co -0.13202100	-0.07183300	-0.15371200	C 3.99093900	0.14099600	4.26131000
H -1.29022600	1.23065300	1.73128600	H 2.98093900	-1.68899600	4.76291100
C 1.35501000	5.03570200	-0.79658600	H 4.93448000	1.91600800	3.49569400
C 1.42370800	4.19565500	-2.09518900	H 4.27731800	0.34924300	5.29678700
H 2.38304100	5.22708500	-0.42826200	C -3.47786100	0.38154000	1.50412900
H 0.61675300	4.52279000	-2.78360400	C -3.56411800	1.70354500	1.99178000
B 0.60689500	2.91974900	-0.40563600	C -3.70755900	-0.73881200	2.31693500
O 0.69598900	4.20271100	0.13665200	C -3.88728600	1.87351800	3.33995200
O 1.14651000	2.87512300	-1.68388700	C -4.01642200	-0.51315100	3.66410400
N -0.02725000	1.85734100	0.21081300	C -4.10934200	0.77719700	4.17029400
C -0.24556800	1.28541300	1.39975400	H -3.95489100	2.88324000	3.75289700
C 0.67498900	1.46852700	2.57317600	H -4.19141500	-1.36787200	4.32435900
H 0.47766300	2.46707000	3.00908300	H -4.35536000	0.93426400	5.22508800
H 0.49033600	0.71449800	3.35615900	C -3.63589200	-2.15257600	1.77957100
H 1.73056900	1.43232600	2.28429900	C -4.97932900	-2.87041600	1.90573400
B -0.36593100	-1.97249500	-0.45997800	C -2.51092600	-2.93394300	2.45485300
O -1.58479700	-2.59294000	-0.69937700	H -3.37766900	-2.09735600	0.71255100
O 0.66110200	-2.89730700	-0.59928700	H -5.78351300	-2.31404200	1.39313700
C -1.38015500	-3.96084600	-1.01403800	H -4.92104200	-3.87415700	1.44735800
C 0.14760400	-4.08909800	-1.17371800	H -5.27831300	-3.00281700	2.96157400
H -1.71675600	-4.56456900	-0.14797300	H -1.54373700	-2.43429800	2.28870800
H 0.40786300	-4.07823800	-2.25074100	H -2.66904000	-3.02859700	3.54489400
H -0.19867400	-0.56112200	1.27939500	H -2.44451700	-3.95424100	2.03710000
C 0.75043300	-5.31325100	-0.52618900	C -3.30288700	2.90446000	1.09878700
H 0.36305600	-6.23260700	-1.00036400	C -2.52008000	4.00996500	1.80566200
H 1.84816600	-5.30732400	-0.63475800	C -4.60650600	3.46385700	0.52301300
H 0.50541000	-5.34644400	0.54993600	H -2.67555800	2.56055500	0.26044100
C -2.17584700	-4.35227500	-2.23774600	H -1.61695700	3.61910500	2.30179500
H -1.87312300	-3.74241400	-3.10697100	H -2.18612200	4.76031900	1.06965100
H -2.01640300	-5.41770700	-2.48252900	H -3.13319800	4.53319200	2.56155400
H -3.25457400	-4.19627000	-2.06459000	H -5.15750500	2.71202300	-0.06532400
C 0.63189400	6.35481500	-0.94860400	H -5.27212000	3.81807700	1.33162100
H 0.59176200	6.88927500	0.01608700	H -4.39372200	4.32092200	-0.14084000
H 1.14743500	7.00262800	-1.68023600	C 4.39226400	1.78541100	0.85035000
H -0.40367900	6.18926300	-1.29540800	C 5.90616700	1.79496200	0.62768100
C 2.74811600	4.26857400	-2.82072300	C 3.89776100	3.19465200	1.17846600
H 2.73107200	3.62703500	-3.71844200	H 3.91362000	1.48725100	-0.09567000
H 2.96610600	5.30359900	-3.13934700	H 6.28761700	0.79808100	0.35275500
H 3.56749800	3.92165100	-2.16609600	H 6.16746500	2.49108200	-0.18947500

H 6.44094800 2.12765400 1.53589700
H 2.80181000 3.23791100 1.28029500
H 4.34464500 3.57812800 2.11301800
H 4.18802300 3.88751100 0.36959200
C 2.16707800 -2.58783200 2.31759200
C 1.11506800 -2.96393000 3.35703500
C 3.17977900 -3.72097500 2.13318300
H 1.64955100 -2.45397800 1.35766000
H 0.43026800 -2.12313500 3.56003800
H 0.50888800 -3.81028700 2.98949900
H 1.56482900 -3.27974700 4.31597900
H 3.88602700 -3.50267600 1.31405300
H 3.76683000 -3.88486200 3.05586200
H 2.66268600 -4.66517000 1.88674600
¹⁶K_{Dipp}
C 0.77274200 0.18303000 1.35050000
C 1.42339700 1.36715800 1.71127000
C 2.61542400 1.36741000 2.43736800
C 3.15154800 0.12594700 2.81135700
C 2.53057000 -1.08234700 2.46750800
C 1.34964900 -1.02973200 1.72277800
H 3.12247500 2.28456200 2.73780700
H 4.07784500 0.09910600 3.39257800
H 2.97359700 -2.02008200 2.79667000
C 0.71487900 -3.46211100 1.40546400
C -0.64053200 -1.76229700 0.64531500
C -0.40636100 -4.02290000 0.78529900
C 1.70426100 -4.28165100 1.95614000
C -0.59349300 -5.40028200 0.69231800
C 1.52301800 -5.65926800 1.86362800
H 2.58948300 -3.87817900 2.44448700
C 0.39207200 -6.21346400 1.24317100
H -1.48355200 -5.81604700 0.21655400
H 2.27804400 -6.32398800 2.29331800
H 0.27937100 -7.30016400 1.19826400
C 1.00842500 3.80001600 1.08768700
C -0.52285400 2.14968800 0.64099500
C -0.01687400 4.33772400 0.29571800
C 2.08801500 4.59019800 1.48926700
C 0.03426200 5.64252400 -0.18640500
C 2.12022200 5.90886900 1.03968700
H 2.88913300 4.20618100 2.12002300
C 1.12043300 6.42414000 0.20130000
H -0.74410200 6.02752000 -0.84773000

H 2.95243500 6.55156100 1.34059100
H 1.19062600 7.45716600 -0.15031500
N 0.67974300 2.46523000 1.24568300
N -0.94185000 3.31806100 0.08091800
N 0.54648000 -2.09547400 1.28292900
N -1.19857200 -2.96478400 0.33755200
Co -0.95472900 0.23915600 0.60347600
H -2.92453900 2.03384700 1.49699300
C -4.15520900 -0.97940700 -2.91063400
C -5.37409400 -0.28779300 -2.26594000
H -4.28579600 -2.07483900 -2.85865100
H -5.57229300 0.66859000 -2.79438800
B -3.56397100 -0.08705600 -0.88872400
O -3.06208400 -0.62872600 -2.07808600
O -4.95849200 0.00721300 -0.95483100
N -2.82509600 0.39878500 0.19005300
C -3.59489800 1.28080700 1.05294000
C -4.33235700 0.59120500 2.19264000
H -3.65335500 -0.04517500 2.78393700
H -4.78457300 1.33491400 2.87582700
H -5.13984600 -0.04528700 1.80196700
B -1.12337700 0.21510000 2.49345400
O -1.25122600 -0.92773000 3.25714600
O -1.21560600 1.35121900 3.26779700
C -1.25383000 -0.55123000 4.63209800
C -1.50700600 0.96962600 4.60819600
H -0.23952800 -0.74840100 5.03253500
H -2.58043800 1.17148300 4.78886200
H -4.34557800 1.83412600 0.46132700
C -3.93274300 -0.57342100 -4.35032300
H -3.03895600 -1.05918700 -4.77524800
H -4.80328200 -0.87180500 -4.96195500
H -3.81130000 0.51977000 -4.43635000
C -6.63566800 -1.12113400 -2.26837600
H -7.45838000 -0.57937900 -1.77094200
H -6.95204900 -1.35155600 -3.30144300
H -6.46910700 -2.07096700 -1.73175400
C -0.66999000 1.76198500 5.58351700
H -0.87647800 2.84119500 5.48393500
H -0.89685200 1.46407700 6.62252600
H 0.40522300 1.59364100 5.39595200
C -2.26559500 -1.35135800 5.41611400
H -2.02840700 -2.42745300 5.37093200
H -2.26003400 -1.04400100 6.47682300

H -3.28221400	-1.19967500	5.01428200	H 0.16541300	-2.51464800	-4.07161800
C -2.34827900	-3.31624700	-0.44894800	H -1.50839400	-3.02021000	-4.40151900
C -2.11198600	-3.75561600	-1.76495400	H -0.10371400	-5.67550900	-2.03640600
C -3.60379100	-3.44080100	0.17256800	H -0.84022000	-5.45064100	-3.64661600
C -3.17101600	-4.34671900	-2.46021800	H 0.80233400	-4.84770600	-3.33356100
C -4.63059200	-4.03542600	-0.57029900	C -0.73252200	2.61674600	-2.70958900
C -4.41637500	-4.50054700	-1.86357000	C -0.02165500	3.72838800	-3.48718200
H -3.01384500	-4.69613700	-3.48485900	C -0.97101000	1.39650200	-3.59375600
H -5.61905600	-4.15129500	-0.12231800	H -0.06235200	2.30055200	-1.89394300
H -5.23453500	-4.97300200	-2.41535000	H 0.23928000	4.58155100	-2.83751600
C -2.09256500	3.53664100	-0.74301900	H 0.91027100	3.34933800	-3.94371900
C -3.21131200	4.20697000	-0.20772900	H -0.66233700	4.10869500	-4.30296700
C -2.00998500	3.16156400	-2.09625000	H -1.56587600	0.63396300	-3.06540500
C -4.29237200	4.43143200	-1.06647100	H -1.50381900	1.66258000	-4.52391300
C -3.12403300	3.39904900	-2.90551700	H -0.00705400	0.94877700	-3.89391300
C -4.25980200	4.01780200	-2.39360100	K 4.24205100	-0.06151300	-0.29213500
H -5.18372400	4.93521300	-0.68369900	O 3.67521700	-2.76647100	-0.27935300
H -3.09680700	3.10882900	-3.95947600	O 3.25615300	1.48564300	-2.36763000
H -5.12460600	4.19385500	-3.04037600	O 6.04839200	-1.85767700	0.95348300
C -3.83573400	-2.99067500	1.60285400	C 2.83794500	-3.10818900	-1.35784100
C -3.30204200	-4.00568200	2.61833200	C 4.72596100	-3.66192300	-0.02412100
C -5.30585000	-2.70687600	1.89497100	C 3.74174000	2.79453500	-2.52529200
H -3.27397000	-2.05108100	1.73311400	C 2.98562300	0.83842000	-3.58336900
H -2.21109000	-4.13531900	2.55636500	C 7.24674400	-1.80576100	0.22160900
H -3.53528800	-3.66741800	3.64283200	C 5.51511400	-3.14212200	1.15646700
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H -5.90006800	-3.63738300	1.94227100	H 2.62017500	-4.19402200	-1.35807900
H -5.40385800	-2.21214300	2.87577600	H 4.32821000	-4.66667700	0.22566000
C -3.27456300	4.71383300	1.22562200	H 5.38196900	-3.77832300	-0.91027600
C -4.61686300	4.42915700	1.90345000	C 4.11210800	3.34437500	-1.16761400
C -3.00406400	6.22082500	1.30120800	H 4.61012800	2.79609400	-3.21500100
H -2.48821500	4.19653600	1.79987200	H 2.96876100	3.45263400	-2.97002400
H -4.93739000	3.38449400	1.78064600	C 2.54082700	-0.57476900	-3.32105700
H -4.53957600	4.63940100	2.98464000	H 3.89423100	0.82062600	-4.21904900
H -5.41632600	5.07867800	1.50496900	H 2.18983800	1.36951100	-4.14080200
H -2.00072500	6.49121300	0.93976200	C 7.81026300	-0.41249100	0.31238100
H -3.74612000	6.78082800	0.70378100	H 7.98862800	-2.51458400	0.64103000
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C -0.76030800	-3.62374500	-2.44082200	H 4.84585400	-3.05947600	2.02797500
C -0.83164800	-2.64564600	-3.61289700	H 6.31586500	-3.86509000	1.40876600
C -0.19900900	-4.97519400	-2.88341900	O 3.61976300	-1.30056900	-2.78238800
H -0.06041900	-3.20119100	-1.70422500	H 4.41146800	-3.16034000	-2.84395000
H -1.20708900	-1.66605300	-3.27883700	H 2.76749300	-3.04882800	-3.51215100

O 5.07716500 2.57468400 -0.49058100
H 4.45100200 4.39347900 -1.27741600
H 3.21861500 3.34984300 -0.52406400
H 1.66468600 -0.57680400 -2.64023600
H 2.22087200 -1.02081300 -4.28337300
O 6.94587700 0.48820500 -0.33021000
H 7.93067500 -0.13783500 1.37971600
H 8.81311300 -0.39542900 -0.16086600
C 6.39109500 2.70827700 -0.96861600
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H 7.24209900 2.11293800 0.91772700
'TSIK
C -0.01319300 0.13384200 -1.66760600
C -1.10739100 0.69915400 -2.32785000
C -0.98331700 1.21403200 -3.61741900
C 0.27836500 1.15599100 -4.22816600
C 1.39915500 0.60680500 -3.58813600
C 1.23239700 0.10291200 -2.29808000
H -1.83054300 1.62791500 -4.16662300
H 0.38966800 1.54459200 -5.24456300
H 2.35142000 0.54932600 -4.11807700
C 3.50396200 -0.82763700 -1.55529800
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C 4.50421900 -0.42917600 -2.44123200
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C 6.09820400 -1.67204300 -1.07094200
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H 6.60858200 -0.57235100 -2.85939700
H 7.12734700 -2.00231900 -0.90504100
C -3.56764900 0.95729700 -1.64319400
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H -6.09239200 0.20480500 0.56401000
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N -3.27869600 -0.27993500 0.21313600
N 2.14439800 -0.58332900 -1.47544500
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Co -0.29268500 -0.89130300 -0.13535900
H -0.63443300 -2.13963600 0.67842700
C -0.17417600 -3.54672100 -3.34744400
C -1.54159200 -2.87321700 -3.54623700
H -0.32104600 -4.60711100 -3.06352500
H -1.44287100 -2.06086600 -4.29386100
B -0.60537500 -2.11943500 -1.60710700
O 0.37955300 -2.86816100 -2.22627500
O -1.80375600 -2.26031400 -2.28885900
N -0.06441600 0.00401600 1.71057800
C -0.37778300 -1.15183000 1.89338300
C -0.64846000 -2.13759200 2.96419600
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H 2.80088300 -0.08553200 2.02261900
H 5.18682300 -0.79616500 2.26447300

H 4.84688300	0.59417500	3.33306000	O 3.36002000	2.58392500	-1.25181900
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H 1.24353200	-0.13205600	3.96628400	O 3.17562100	2.51274700	1.60749200
H 2.62691800	-0.44499100	5.06553600	C 3.39934400	3.36455800	-2.42104500
H 2.54480200	1.06559200	4.13017900	C 4.49147800	2.74266800	-0.43753400
C 2.08201900	-4.61960000	-0.14237700	C -2.34904400	4.58077900	-0.69562700
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H 0.64693700	-5.79916500	-1.26311500	H 2.79799000	2.83299400	-3.17629800
H 0.78197100	-6.29444500	0.44001000	H 4.43362900	3.43309800	-2.81335400
H 4.22619700	-4.88730000	-0.50108500	H 5.38602500	2.30479400	-0.92638500
H 3.41099300	-6.33749500	0.14800900	H 4.70575000	3.81510500	-0.25883900
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H -2.55111200	1.35198600	1.91798200	H -0.79328600	5.92400500	-2.17182900
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H -1.83719700	2.32813900	3.99636000	C 2.21309300	4.06086400	3.13858000
H -2.74338200	1.14670400	4.97133400	H 4.28794200	3.58360600	2.98634100
H -4.97083900	1.96939300	1.99407600	H 3.64106700	4.54224300	1.61803000
H -4.98889600	1.72332900	3.76104600	H 4.04561700	0.96402700	0.65415200
H -4.02720200	3.05008400	3.05800500	H 5.19608200	2.05974800	1.46602200
C -4.07707000	-3.05493600	-0.07263800	O 1.50529500	4.77175900	-1.80076800
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C -3.28377200	-4.35945200	-0.03783800	H 2.99000700	5.35766600	-3.12179900
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H -6.08004900	-2.34039600	-0.59043000	H -3.50569600	4.21991600	1.06954800
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H -6.06092600	-3.95317500	0.17675500	H 0.62026300	3.35370100	-3.04464000
H -2.24305500	-4.17837900	0.27970700	H 0.85755900	4.97766500	-3.75876800
H -3.72963100	-5.10123600	0.64853200	O 1.12129300	4.33605100	2.30215000
H -3.25364400	-4.81456900	-1.04195800	H 1.96852400	3.22868900	3.82893300
C -2.66043900	-3.79749700	-3.95924400	H 2.46523600	4.94925300	3.75370700
H -2.77246600	-4.62799200	-3.24165300	C -1.15785000	4.96483200	2.03601600
H -3.61627800	-3.24861400	-4.01025300	C -0.02706700	4.73513600	3.00349500
H -2.45920600	-4.22481900	-4.95725900	H -0.83245300	5.70141300	1.27616200
C 0.75561500	-3.46202200	-4.53383700	H -2.01758100	5.39675300	2.58798700
H 0.32443200	-3.98547800	-5.40548600	H 0.16453300	5.67945100	3.55360900
H 0.93516000	-2.40780600	-4.80855900	H -0.31418800	3.96218300	3.74423200
H 1.72663600	-3.93068500	-4.29880900	¹⁷K		
K 0.72184600	2.49766100	0.26004900	C 0.04703000	0.19824200	-1.91182400

C 1.22750500 -0.34390500 -2.45041400
C 1.95940400 0.31997900 -3.43421800
C 1.49182300 1.56511500 -3.88421200
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C 2.48500200 -2.51455500 -1.94768500
C 0.49440400 -1.97010800 -0.93282300
C 2.12051800 -3.56406000 -1.07712300
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C 0.22060200 -4.01848700 0.46026700
H 0.66955400 -3.93901200 1.46824300
H -0.82597200 -3.69486800 0.50810100
H 0.24311100 -5.07557300 0.14862800
Co -0.97054200 -0.75770200 -0.69250800
H -4.52238100 -4.78256800 1.13543200

C -0.82533500 -0.76888700 2.39288000
C -1.53724500 -1.26674200 3.66149800
H 0.21524300 -1.12710900 2.32638700
H -0.84357700 0.32858300 2.30509200
H -0.83716900 -1.67951200 4.40606300
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B -2.46799600 -2.25040100 1.85677000
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C -4.30409100 -3.91663700 1.77973600
C -5.59124600 -3.19081700 2.12706600
H -6.09226300 -2.81827900 1.21623200
H -6.29148800 -3.86855400 2.64607800
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B -3.41307500 -2.96844600 -0.33634000
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O -4.30968900 -3.65809600 -1.09763400
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H -3.57985300 -1.26300200 -2.64680400
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H -3.48215500 -4.32230500 -2.86860700
H -3.82816800 -4.30060800 2.69582600
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C 4.82423500 2.04628200 -0.20447600
C 3.05183500 3.38432200 -1.05431400
C 4.57716500 0.70739900 -0.87566800
C 4.47215000 -1.02383300 0.75115000
C 0.01479000 4.45129200 0.69252500
C 1.99375000 4.34707200 -0.58165700
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H 1.27105900 2.61934300 5.25544600	H -7.39802300 -1.64831900 -0.69006000
H 1.54963000 -0.33628500 4.71788600	C 3.60956500 -1.61108800 -1.56710300
H 2.85049400 0.75207500 5.29576400	C 1.93459300 -0.35916700 -0.64074400
H 1.16234200 3.89541000 3.13656400	C 4.13759300 -0.86864400 -0.49913200
H -0.39338500 3.89474200 4.02890200	C 4.41037500 -2.50660200 -2.27690200
H -1.68490600 4.21214000 1.98314300	C 5.46793300 -0.98238400 -0.10813000
H -1.50085500 2.93204900 0.75029200	C 5.74298500 -2.62517500 -1.88497000
H 5.31645600 1.89655900 0.77177200	H 4.01780300 -3.10498800 -3.09942000
H 5.50969600 2.65013800 -0.83430600	C 6.26578000 -1.87563800 -0.82036500
H 2.59863900 2.64499100 -1.74408400	H 5.86171000 -0.39117000 0.72142300
H 3.81303500 3.95501900 -1.62411600	H 6.39348600 -3.32337100 -2.41952200
H 4.03848200 0.84828600 -1.82781300	H 7.31662800 -1.99616700 -0.54225300
H 5.54508900 0.22451900 -1.11078600	N 2.27651800 -1.24772900 -1.64195100
H 5.02240000 -1.77366700 0.14727700	N 3.09509600 -0.09620400 0.01103900
H 5.21655700 -0.48704800 1.37368600	N -2.28006000 -1.24335800 -1.59014100
H 0.51527900 5.17873500 1.36452400	N -3.07927000 -0.04420200 0.03627800
H -0.56471900 5.03737400 -0.04972100	Co 0.01401900 -0.09572800 -0.45641000
H 2.44727300 5.08320700 0.11322300	H -0.80498600 1.54113700 2.46578100
H 1.59586800 4.89937500 -1.45707800	C 0.15636000 2.46646600 -2.88271300
H 3.82912700 -1.15145200 4.14839700	C -0.18306700 3.86177100 -2.33381300
H 4.13723900 0.35167400 3.22164900	H 1.24798200 2.40813000 -3.08101300
H 2.76047200 -2.28565100 0.96473100	H -1.27048000 4.02118100 -2.47663800
H 4.00634100 -2.51306600 2.22843300	B -0.01839100 2.41362800 -0.58290200
H -0.01107100 1.51343200 4.66857300	O -0.16156800 1.64499900 -1.78326000
¹⁶ Dipp	O 0.07564000 3.76749700 -0.94164500
C -0.00373900 -1.40550800 -1.77502700	N 0.01491400 1.64964800 0.54911000
C 1.19357900 -1.78369900 -2.36953400	C 0.05690100 1.99692900 1.93276400
C 1.20442700 -2.56805200 -3.52373000	C 0.05688400 3.49130200 2.22399800
C -0.03068100 -2.95412200 -4.06160400	H -0.85373800 3.97354300 1.82903000
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C -1.21507400 -1.78654900 -2.33799000	H 0.92923700 3.98546100 1.76236200
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C -3.63447700 -1.52366100 -1.56275400	C -0.69607900 -3.84904300 1.18994100
C -1.91842600 -0.36692300 -0.58630900	C 0.76334300 -3.97434400 0.72857100
C -4.15098600 -0.74958000 -0.51189500	H -0.73241900 -3.85141600 2.29733800
C -4.46706600 -2.36021200 -2.30785000	H 0.78673400 -4.45440100 -0.27146100
C -5.50129500 -0.76960000 -0.17691000	H 0.95690100 1.55860000 2.40921600
C -5.81886900 -2.38710100 -1.96914700	C -3.26138100 0.83720500 1.15343100
H -4.08751500 -2.97990300 -3.12035900	C -3.43516600 2.21832700 0.92131300
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 C 3.33080000 0.29711700 2.40798900
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 C 3.84449900 2.52682100 3.21090300
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 H 3.99975600 4.07395300 1.73293400
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 H 0.31982600 5.95471900 -2.44880300
 H 1.64674500 4.86307600 -2.93814200
13
 C 0.00638600 1.08512700 -0.56094300
 C 1.20937800 1.77962000 -0.64933900
 C 1.23289200 3.15727900 -0.86537400
 C 0.00494300 3.82286700 -0.98243700
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 H 2.16432600 3.72192900 -0.94034600
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 C -5.45053400 -0.58784000 0.12127400
 C -5.88454300 1.77313300 -0.29322100
 H -4.19142300 3.05811600 -0.70950300
 C -6.33978000 0.48007000 0.00107600
 H -5.80048100 -1.59790300 0.34776200

H -6.60761600	2.58916800	-0.38092000	C 1.55213400	-1.03147300	-1.46933600
H -7.41073200	0.30447600	0.13751900	C 1.40089900	-1.12330700	-2.85240500
C 3.64833700	0.99165400	-0.33545600	C 1.04540600	0.03931000	-3.55086100
C 1.86938400	-0.42593500	-0.23562200	C 0.81530800	1.26060100	-2.89980800
C 4.11103300	-0.30641500	-0.03236100	C 0.96020500	1.29923000	-1.51156300
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C 5.46331600	-0.57711300	0.15360300	H 0.94245100	-0.00730900	-4.63904800
C 5.89631500	1.78287000	-0.26797500	H 0.54874000	2.14223400	-3.48580700
H 4.20282800	3.06528900	-0.69085900	C 0.40323800	3.68984000	-0.75420700
C 6.35195000	0.49104400	0.03116700	C 1.08719800	2.06569300	0.69894400
H 5.81361200	-1.58620700	0.38378100	C 0.47411800	4.23624200	0.54245000
H 6.61902000	2.59898800	-0.35789900	C -0.03283500	4.46410600	-1.82781100
H 7.42285600	0.31659600	0.16943800	C 0.12602400	5.55801500	0.80253500
N 2.27438500	0.87523300	-0.44921700	C -0.38535400	5.78931700	-1.56748300
N 2.99536600	-1.12782700	0.02284400	H -0.10520700	4.06058300	-2.83832500
N -2.26172600	0.86905600	-0.47248200	C -0.30623400	6.33017300	-0.27622400
N -2.98157200	-1.13543400	-0.00479700	H 0.18611400	5.97340800	1.81126300
C -3.00083200	-2.54242800	0.30387200	H -0.72725000	6.42037300	-2.39294000
H -3.53562600	-2.71518700	1.25326100	H -0.58588800	7.37460700	-0.11152900
H -3.49491600	-3.11297300	-0.50152600	C 2.22434500	-3.36796000	-0.62296800
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H 3.52738800	-3.10299200	-0.46006400	C 2.29245600	-4.28024000	-1.67519500
H 3.53636000	-2.70099700	1.29471200	C 2.83173300	-5.08810500	1.00814100
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Co 0.00749100	-0.74621600	-0.32863800	H 2.09404300	-3.98715900	-2.70664000
H 0.02198200	-4.38363600	-1.26623600	C 2.89695000	-5.99721900	-0.04775700
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H -0.83106000	0.94833000	4.22849600	N 1.91070400	-2.02254900	-0.53472600
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H -1.10828500	-1.43116400	4.07496900	N 0.79105300	2.37123100	-0.61696000
B -0.02113300	-0.42227000	1.55445900	N 0.89540600	3.21862200	1.38447200
O -0.16989400	0.74134200	2.27774800	C 1.09852000	3.38447100	2.79922300
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C 0.02395600	-3.39454400	-1.78791200	H 1.44172700	2.42775100	3.21247800
C 0.03523700	-3.48682900	-3.29167400	C 2.53747800	-2.66433000	2.92867700
H 0.92671000	-4.03919900	-3.64582300	H 1.82913000	-3.36103500	3.40642400
H -0.85086800	-4.03918300	-3.65911300	H 3.57045500	-2.96715500	3.17232600
H 0.03851800	-2.47686800	-3.73391500	H 2.34732500	-1.65304000	3.30878800
15K			Co 1.67249100	0.28739300	1.04338800
C 1.35032300	0.17027600	-0.79065800	H 3.98429600	0.51477800	3.18166800

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C 5.86195000 1.10066400 2.17380300
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H 6.44776600 0.25527300 2.57993900
H 6.22674500 1.33133100 1.15949600
B 0.15920900 -0.05696600 2.18191100
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H -2.32439300 -1.60501600 2.70041200
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O -4.01698600 1.12732500 1.35751300
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³LCo
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C 1.22656800 2.70769400 0.38107400
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C 3.23050600 -3.01772100 0.13511700
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Co 0.00004400 -1.21852300 0.18188200
¹³Dipp
C 0.00923100 1.98726900 -1.16987500
C 1.20820100 2.68664200 -1.30984400
C 1.24757600 4.04936000 -1.60631800
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C 1.89677900 0.54995200 -0.62047400
C 4.16660200 0.69327900 -0.70022300
C 4.51370000 2.98351600 -1.44662300
C 5.53102200 0.42288800 -0.71202800
C 5.88328400 2.72184900 -1.43144200
H 4.14088200 3.96211700 -1.74909900
C 6.38624400 1.46160800 -1.07793400
H 5.90947400 -0.56969800 -0.45935700
H 6.57842800 3.51723600 -1.71528400
H 7.46583400 1.28710000 -1.09539500
N 2.28034800 1.81340400 -1.02623000
N 3.06977100 -0.11769500 -0.41898800
N -2.26267500 1.84688500 -1.00880100
N -3.07106700 -0.08860500 -0.44016600
Co -0.00187400 0.26926500 -0.47577900
H -0.00972600 -2.09281700 2.69435700
C -0.77387400 2.39412000 2.61783700
C 0.75241300 2.28755800 2.84382500
H -0.96566900 3.12740000 1.80819400
H 0.95463000 2.09499900 3.91783300
B -0.00578400 0.52384500 1.61267700
O -1.15279800 1.11265100 2.15581400
O 1.14508000 1.14171100 2.11357000
N -0.00549700 -0.84710100 1.05848000
C -0.00971700 -1.99596300 1.59288400
C -0.01589400 -3.26486300 0.81786300
H 0.87232900 -3.87299900 1.06933300
H -0.91057100 -3.86360600 1.06944500
H -0.01568500 -3.04922000 -0.26170500
C -3.23787900 -1.45783000 -0.06861100
C -3.70962600 -1.76021800 1.22200700
C -3.00569000 -2.45449500 -1.03987000
C -3.98745000 -3.10171500 1.51439200
C -3.29579800 -3.77664800 -0.69408500
C -3.79491600 -4.09804700 0.56612300
H -4.36221000 -3.36687800 2.50740000
H -3.12935000 -4.57527600 -1.41992300
H -4.02349100 -5.13974700 0.81198800
C 3.23059800 -1.47648000 -0.00766500
C 3.01156200 -2.50123200 -0.95224600
C 3.68925900 -1.74105100 1.29620300

C 3.30296000 -3.81190700 -0.56577900
C 3.96581500 -3.07290200 1.63054600
C 3.78782300 -4.09622600 0.70875200
H 3.14808000 -4.63158200 -1.27025800
H 4.32976000 -3.30846500 2.63498400
H 4.01673700 -5.12981300 0.98643100
C -3.91055800 -0.70239000 2.29234500
C -3.10705700 -1.02472700 3.55241300
C -5.38773100 -0.51723500 2.64482400
H -3.51824200 0.24825900 1.90203500
H -2.03961700 -1.15416300 3.32074800
H -3.19073700 -0.19392900 4.27459200
H -3.47491400 -1.93996400 4.05083200
H -5.99000300 -0.22705700 1.76906800
H -5.81998900 -1.44452700 3.06363700
H -5.50075400 0.27686300 3.40459300
C -2.45817700 -2.09801100 -2.41193100
C -3.52690100 -1.46405000 -3.30682100
C -1.82427400 -3.28125100 -3.13382000
H -1.66271900 -1.34758100 -2.24546700
H -3.96036000 -0.55158200 -2.86906900
H -3.09252200 -1.19107100 -4.28496300
H -4.35236400 -2.17656900 -3.48697300
H -1.09049100 -3.80607400 -2.50071300
H -2.58142600 -4.01569700 -3.46226200
H -1.29922500 -2.92874000 -4.03796700
C 2.47397800 -2.18765400 -2.33855200
C 1.86531400 -3.39916100 -3.03546100
C 3.54205800 -1.56202000 -3.24013300
H 1.66682000 -1.44412900 -2.19885300
H 1.13741700 -3.92289100 -2.39413000
H 1.33998300 -3.07883700 -3.95115100
H 2.63814000 -4.12726600 -3.34089800
H 3.95774600 -0.63150300 -2.82367700
H 4.37956000 -2.26674100 -3.39320500
H 3.11319000 -1.32230300 -4.22935800
C 3.87929300 -0.65346500 2.33836500
C 5.35124500 -0.47052400 2.71292400
C 3.04881800 -0.93315200 3.59127900
H 3.50279000 0.28897500 1.91419900
H 5.97256200 -0.21596900 1.83934700
H 5.45815300 0.34790200 3.44728000
H 5.76638400 -1.38691200 3.17117200
H 1.98513100 -1.06033200 3.34187100

H 3.39834800 -1.83715200 4.12241000
H 3.12691600 -0.08365400 4.29257100
C -1.56724800 2.78237700 3.84332600
H -1.26590100 3.78294500 4.20111700
H -2.64621400 2.81304500 3.61302800
H -1.40483000 2.05502000 4.65832000
C 1.52749400 3.50509300 2.39273400
H 1.22212300 4.39859000 2.96655000
H 2.61058300 3.35373100 2.54266900
H 1.34699800 3.69632600 1.32033400
¹⁶Dipp
C 0.14764900 1.37047600 -0.53110700
C -1.01455100 2.12478100 -0.65686800
C -0.97629200 3.47075900 -1.02479200
C 0.27609500 4.04709500 -1.26782800
C 1.46636400 3.31914500 -1.14926000
C 1.37461700 1.97714800 -0.77819400
H -1.87711200 4.07614800 -1.13401400
H 0.32624300 5.10042400 -1.55938800
H 2.42073100 3.80832800 -1.35004700
C 3.78499600 1.12708500 -0.56181200
C 1.97937200 -0.23153700 -0.24751700
C 4.23353100 -0.16033600 -0.20975400
C 4.69548300 2.15447600 -0.80770400
C 5.58726300 -0.46107600 -0.09102200
C 6.05190500 1.85398700 -0.68726600
H 4.37395900 3.15949000 -1.08224100
C 6.49360700 0.56989900 -0.33539700
H 5.92406700 -1.46299000 0.18529400
H 6.78779300 2.64206600 -0.87177600
H 7.56644500 0.37406800 -0.25038100
C -3.49220900 1.57486900 -0.28981200
C -1.84680100 0.01405600 -0.02246600
C -4.07951700 0.35544100 0.09737200
C -4.27910100 2.70607100 -0.51500400
C -5.45704400 0.22691800 0.26005600
C -5.65702700 2.57668800 -0.34716800
H -3.84562900 3.66119200 -0.81095700
C -6.23837500 1.35836000 0.03260700
H -5.91314000 -0.72192600 0.55134300
H -6.29728300 3.44712100 -0.51725200
H -7.32366700 1.29300500 0.15186600
N -2.13477000 1.31870300 -0.35848900
N -3.04155000 -0.55532600 0.24991900

N 2.40591700	1.03594800	-0.58385000	H -2.17884400	5.00198500	-0.36923700
N 3.10217500	-0.94394900	-0.03730600	H -0.03381700	6.21162500	-0.14233900
C 3.13291300	-2.34072200	0.31340500	H 2.11137000	5.01181200	0.13294600
H 2.09233900	-2.69994900	0.28519000	C 3.58372100	2.22341900	0.41252200
H 3.74192500	-2.89910100	-0.41815700	C 1.81624900	0.80482400	0.11959000
H 3.56116500	-2.47444000	1.32075700	C 4.06359100	0.89595300	0.45229100
C -3.24035200	-1.92677200	0.65547200	C 4.45787000	3.29634400	0.58689000
H -2.38251900	-2.25151600	1.25367500	C 5.40599800	0.60554100	0.66838300
H -4.15309400	-1.99326000	1.26690800	C 5.80643100	3.00452000	0.79784100
H -3.33874900	-2.59138500	-0.21796200	H 4.10820200	4.32914200	0.56762900
Co 0.05824800	-0.43814400	-0.08722000	C 6.27497400	1.68428000	0.83963700
H 0.86667500	-2.78857800	2.22607400	H 5.75762700	-0.42807600	0.70706300
C -0.85902000	-2.14671300	-3.05696200	H 6.51170200	3.82878900	0.93797300
C -1.52465000	-3.50456000	-2.72616200	H 7.33813900	1.49466300	1.01300300
H -1.59792300	-1.38193100	-3.35588900	C -3.65365600	2.20928000	-0.53132000
H -0.11415600	-2.23135200	-3.87015300	C -1.88829500	0.79764900	-0.18606500
H -2.62880200	-3.43108100	-2.76419500	C -4.13611400	0.88195400	-0.52284900
H -1.22006600	-4.30035600	-3.42993300	C -4.52966900	3.27626300	-0.73320900
B -0.43974800	-2.76068600	-0.86337400	C -5.48204700	0.58416500	-0.70372900
O -0.21419600	-1.77230800	-1.86599200	C -5.88069900	2.97743700	-0.91708000
O -1.11987400	-3.84115800	-1.41930500	H -4.18101300	4.30943200	-0.75141200
N -0.03786000	-2.38246500	0.38997200	C -6.35196900	1.65731400	-0.90190800
C -0.04806100	-3.04903300	1.64867800	H -5.83536800	-0.44977500	-0.69124600
C -0.14791500	-4.56807100	1.56760500	H -6.58729100	3.79689700	-1.07762000
H 0.69729400	-4.98831000	0.99237200	H -7.41834900	1.46415000	-1.04985400
H -0.13543600	-5.02281500	2.57535900	N -2.29194800	2.11472000	-0.31911500
H -1.07606600	-4.88037000	1.05772400	N -3.03403400	0.06589200	-0.30400900
B 0.21285200	0.26971600	1.66784100	N 2.22207500	2.12423000	0.20233600
O 1.40378100	0.45748400	2.35078200	N 2.96073400	0.07289600	0.25578600
O -0.86313900	0.64450200	2.46285600	Co -0.03394000	0.52754700	-0.03027700
C 1.11425900	0.86912400	3.67408300	C 2.98320900	-1.34810200	0.13465900
C -0.37044600	1.24905600	3.64435700	C 3.54188300	-1.91889300	-1.02272700
H 1.31297500	0.03040700	4.36781000	C 2.40171100	-2.13146400	1.15540400
H 1.76870700	1.71127600	3.95706100	C 3.54695200	-3.31512000	-1.12646800
H -0.92856800	0.87802000	4.52136100	C 2.41763700	-3.51914600	0.99410800
H -0.51732300	2.34406900	3.58181000	C 2.99340900	-4.10796000	-0.12957500
H -0.87912100	-2.67974000	2.29664900	H 3.97542500	-3.78656000	-2.01579800
¹LC_{Dipp}			H 1.97124900	-4.15703400	1.75972300
C -0.03542200	2.33306400	-0.05388100	H 2.99847400	-5.19757300	-0.23096900
C -1.22799400	3.04166900	-0.21683200	C -3.06205700	-1.34597100	-0.10697100
C -1.25280100	4.43571700	-0.24884100	C -3.43827500	-1.83838200	1.15716000
C -0.03411700	5.11786600	-0.11788600	C -2.67229600	-2.19209000	-1.16033300
C 1.18428500	4.44148600	0.04277400	C -3.41089700	-3.22283800	1.35023200
C 1.15816800	3.04751700	0.07366400	C -2.64998200	-3.56903400	-0.91413800

C -3.01627100 -4.08013900 0.32686700
H -3.69056000 -3.63826900 2.32253700
H -2.34077900 -4.25390700 -1.70841400
H -2.99364800 -5.16055200 0.49962500
C 4.06681400 -1.07843200 -2.17179300
C 3.14841700 -1.20464300 -3.38912900
C 5.51278100 -1.42093700 -2.52782300
H 4.04725800 -0.02336900 -1.86079600
H 2.11384800 -0.91415900 -3.13895700
H 3.49856700 -0.54849700 -4.20608500
H 3.12649100 -2.24051000 -3.77328500
H 6.17944500 -1.32238200 -1.65387400
H 5.60850200 -2.45216000 -2.91261500
H 5.88459900 -0.73896500 -3.31294800
C 1.79143700 -1.48217000 2.38453400
C 2.87869900 -0.97246200 3.33355200
C 0.80917500 -2.37876400 3.12928300
H 1.21849100 -0.60468900 2.02680700
H 3.56720200 -0.26881700 2.83698300
H 2.42515200 -0.44652300 4.19249800
H 3.47870600 -1.81416900 3.72522200
H 0.02067800 -2.76948800 2.46222300
H 1.31166000 -3.23722600 3.61044800
H 0.31557300 -1.80150400 3.92946500
C -3.79161700 -0.90374100 2.29809900
C -2.59863300 -0.75396900 3.24473800
C -5.05111700 -1.33163800 3.04782200
H -3.99206300 0.08999500 1.86969400
H -1.70460500 -0.39703700 2.70381800
H -2.82550700 -0.02458300 4.04310000
H -2.34870900 -1.71794700 3.72319900
H -5.90790100 -1.45346300 2.36205800
H -4.91028200 -2.28402200 3.58930400
H -5.32383200 -0.56712300 3.79650400
C -2.24321000 -1.63931200 -2.50456600
C -2.85083800 -2.40435500 -3.67876600
C -0.71725100 -1.59349200 -2.60301300
H -2.60673300 -0.60066100 -2.56571100
H -3.94979300 -2.46904200 -3.59325700
H -2.61432500 -1.89044900 -4.62706700
H -2.45381000 -3.43193300 -3.75724600
H -0.29042300 -0.92081600 -1.83076500
H -0.26938800 -2.59520000 -2.47158600
H -0.40180600 -1.19919200 -3.58514400

¹⁶K

C -0.32798900 -1.01810600 -1.32230000
C 0.86180100 -1.26126300 -2.00603800
C 0.93608800 -1.16419200 -3.39684600
C -0.22849800 -0.80903800 -4.09031600
C -1.44254100 -0.55922300 -3.43615200
C -1.46823400 -0.67208600 -2.04622700
H 1.84788900 -1.39014100 -3.95168200
H -0.19278600 -0.73866900 -5.18128000
H -2.32864500 -0.31519500 -4.02304200
C -3.87621300 -0.15821100 -1.33138500
C -2.30311900 -0.91125400 0.14356900
C -4.45969900 -0.27275700 -0.05603800
C -4.62365900 0.30836400 -2.41408800
C -5.78807100 0.06758000 0.18277200
C -5.95423900 0.64994500 -2.17583100
H -4.20013600 0.41064900 -3.41339600
C -6.52971600 0.53272400 -0.90142000
H -6.23021500 -0.02899500 1.17705500
H -6.56458500 1.01490000 -3.00675500
H -7.57852400 0.80674800 -0.75749200
C 3.20357200 -1.92973500 -1.21140200
C 1.41441500 -1.86081000 0.20420700
C 3.62250000 -2.31110000 0.07641600
C 4.11929300 -1.84717400 -2.26068200
C 4.94863800 -2.62720500 0.35811600
C 5.44781100 -2.16379300 -1.98026200
H 3.82370000 -1.54325400 -3.26513100
C 5.85848200 -2.54947700 -0.69467100
H 5.26160300 -2.92469400 1.36166600
H 6.18676200 -2.11310300 -2.78508300
H 6.90919400 -2.79484100 -0.51660300
N 1.85308000 -1.66624500 -1.09009900
N 2.50376900 -2.25158600 0.89678600
N -2.56053200 -0.54922100 -1.16416700
N -3.46740100 -0.73018000 0.79980800
C -3.69238600 -1.00844300 2.19758000
H -2.74083600 -1.36247400 2.61857100
H -4.01934500 -0.09405700 2.72154900
H -4.46584600 -1.78633200 2.30787600
C 2.51973200 -2.61092400 2.29465900
H 1.49494800 -2.49204400 2.67605200
H 2.84682600 -3.65738800 2.41104500
H 3.20738200 -1.95181600 2.85178500

Co -0.46860600 -1.46092300 0.49881800
H -2.03822000 -3.66004200 2.31988900
C 0.34589100 1.19603400 3.30258500
C -0.21837000 0.68626800 4.62828600
H 1.45047500 1.23397500 3.31290400
H -0.04330200 2.18838300 3.02828800
H 0.44213300 0.91111000 5.48356600
H -1.21179900 1.13155600 4.83701000
B -0.39224100 -0.96466100 3.08740600
O -0.08709600 0.22886900 2.35806700
O -0.34335900 -0.70468100 4.45557600
N -0.66115000 -2.08795600 2.35255300
C -1.04665900 -3.40795400 2.75589600
C -1.10731300 -3.65125300 4.25752600
H -1.83333000 -2.98101500 4.74843300
H -1.40703800 -4.69453300 4.46471800
H -0.12828900 -3.47440900 4.73559400
B -0.87336500 -3.09956100 -0.35811100
O -2.15084200 -3.51112600 -0.68059600
O 0.05857100 -4.06549300 -0.68189600
C -2.08929700 -4.85042100 -1.14476500
C -0.59834700 -5.09778700 -1.40003300
H -2.49551100 -5.52121000 -0.36572200
H -2.70568100 -4.95989300 -2.05237900
H -0.25604900 -6.08182700 -1.03955500
H -0.34020000 -5.01166000 -2.47161400
H -0.35191300 -4.15155900 2.30879400
K 0.58904500 1.80702900 0.12943100
O 1.13414800 4.18430400 1.54342500
O -1.48245400 3.29407500 1.30468300
O 1.09343000 3.26802000 -2.27745400
O 2.98516000 1.30510300 -1.27153200
O -1.51007800 2.69471300 -1.40249100
O 3.01683900 2.13663300 1.44594200
C 0.06470300 4.88618900 2.11838000
C 2.32161100 4.24151800 2.28554700
C -1.17140700 4.66237200 1.28643100
C -2.66879600 2.91618800 0.65256300
C 2.42063300 3.15772900 -2.72627200
C 0.13074800 2.68146200 -3.12054600
C 2.98458800 1.75355600 -2.60751100
C 4.20177300 1.47717300 -0.58985900
C -2.67393100 3.22707200 -0.83004300
C -1.24188600 3.14100800 -2.70405900

C 3.39811800 3.48349100 1.55313500
C 3.97203400 1.26742700 0.89000800
H 0.28256100 5.97327400 2.15581100
H 2.17025500 3.80536400 3.29419500
H 2.65473200 5.29141300 2.41715300
H -0.97666900 5.01732800 0.25577800
H -2.00352800 5.26296700 1.70741200
H -3.55241100 3.39563100 1.12161200
H -2.74911300 1.82835400 0.80711500
H 3.00850800 3.85587200 -2.10636600
H 2.50309900 3.49443100 -3.78087600
H 0.17749000 1.57654500 -3.08363300
H 0.29768800 2.98954300 -4.17290900
H 2.37020000 1.04379900 -3.18616900
H 4.00490900 1.72738400 -3.03509600
H 4.95228000 0.73873100 -0.93731200
H 4.61959800 2.48604200 -0.77931300
H -2.71358900 4.32123500 -1.00486900
H -3.58640500 2.79043800 -1.28347800
H -1.28841300 4.24829100 -2.74302800
H -1.98687700 2.74155200 -3.42159600
H 4.34980500 3.57706300 2.11460500
H 3.54401300 3.94273300 0.55563200
H 3.58179200 0.25066300 1.05792900
H 4.94133000 1.35395300 1.42137800
H -0.11268000 4.54133900 3.15767800
¹⁵W_{Co}
C -0.01680800 -0.23106100 -0.63568100
C -1.22716800 0.32665300 -1.09774500
C -1.26021700 1.26767000 -2.16234800
C -0.01255800 1.70131500 -2.68657500
C 1.24057800 1.21928600 -2.20079400
C 1.20353700 0.29687500 -1.12826100
H -2.18632700 1.66216900 -2.57762900
H -0.01219500 2.43522100 -3.49529300
H 2.16729400 1.57492300 -2.64852200
C 3.62801600 -0.16534300 -0.44400500
C 1.85290800 -1.32692400 0.41833200
C 4.10084700 -1.10497200 0.49134700
C 4.50139500 0.70934800 -1.08482000
C 5.45315900 -1.21328300 0.79808800
C 5.85803700 0.60151100 -0.77578300
H 4.14987600 1.46680100 -1.78630600
C 6.32786600 -0.34476500 0.14468600

H 5.81443600 -1.94167300 1.52775900
H 6.56753400 1.27916500 -1.25897500
H 7.39824000 -0.39706400 0.36334500
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C -1.88906500 -1.25904800 0.47815400
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H 2.03366800 -3.14250700 2.19952600
C -3.09339500 -2.66020700 2.11972000
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H -2.07772400 -3.03563700 2.30096200
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C -0.95616700 -2.21625900 -3.59925000
H 0.94960300 -1.10524300 -3.70956800
H 1.02216700 -2.72806700 -4.45644200
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O 1.00910500 -2.69496300 -2.39260500
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H 0.82378300 -6.44077200 -0.56714400
H -0.94868100 -6.44788000 -0.51021700
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H 1.05482300 -0.04952800 4.99795900
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O 0.44504900 5.28560900 -1.13134100
C -1.40396000 2.81999800 0.82797700
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¹TS2K
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C 1.12678300 0.20663200 -3.44127400
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17
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Co -0.04838800 -0.17704200 -0.56896900
H 0.30096900 5.55890800 -0.03366600
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C -0.25494300 1.71448900 3.50054200
H -1.58150800 0.39406400 2.33331400
H 0.03337500 -0.30997900 2.63499000
H -1.07871300 1.80932400 4.22593200
H 0.68318400 1.54059800 4.05761100
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O -0.03774000 1.21558900 1.23952100
O -0.13103200 2.92047000 2.75509400
N 0.35392300 3.51345200 0.41794300

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H 2.71980200 4.93461100 0.25282700
H 2.23930600 6.20493200 1.41277200
H 2.40423500 4.51414400 1.96449300
B 0.45293800 3.14977500 -0.94910000
O 0.22641500 1.87042100 -1.42887400
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¹W(CO)₃PhH
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O 1.95740100 0.78582900 2.40214700
C 1.28242200 -1.54533400 -0.32745300
O 1.94220800 -2.47221800 -0.52952600
C 1.28542800 1.05032200 -1.17777800
O 1.94832200 1.67468200 -1.88907600
C -1.82219600 1.04923100 0.95838000
C -1.82607600 -0.31504600 1.38459600
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C -1.81523500 0.30705200 -1.38459000
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¹TS3W_{Co}
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H 1.72195500 -2.18193300 -2.45055300
H -0.50443700 -2.38679800 -3.53727100

H -2.42968400 -0.95471900 -2.90205700
 C -3.56264600 1.16481100 -0.83408400
 C -1.63268900 1.82830400 0.19803300
 C -3.85809400 2.18489200 0.08725300
 C -4.57116400 0.55523100 -1.57622100
 C -5.15754100 2.64010400 0.28439600
 C -5.87461500 1.00967400 -1.37725500
 H -4.36632500 -0.25351200 -2.27830400
 C -6.16448000 2.03568900 -0.46728100
 H -5.38057500 3.43417000 1.00067500
 H -6.68882600 0.54858800 -1.94326100
 H -7.19966600 2.36451700 -0.33961300
 C 3.36032800 -0.93741500 -0.06945700
 C 1.95781000 0.74028600 0.60904300
 C 3.96954000 -0.22224200 0.97570400
 C 3.99259700 -2.03189200 -0.65421700
 C 5.22589600 -0.56676800 1.46370100
 C 5.25318700 -2.37661800 -0.16696700
 H 3.52767200 -2.61146400 -1.45205800
 C 5.86164100 -1.65735000 0.87105900
 H 5.69283300 -0.00994300 2.27931700
 H 5.77420600 -3.23329700 -0.60354500
 H 6.85018000 -1.96040400 1.22746000
 N 2.13892800 -0.31659000 -0.26468700
 N 3.08166600 0.77840200 1.35357200
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 H -1.55313500 3.44978000 2.18490300
 C 3.29089300 1.60731800 2.51292000
 H 3.46731200 0.96713900 3.39272200
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 H 2.38445800 2.19865200 2.68536400
 Co 0.24517800 1.60641800 0.50049000
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 C 3.70247200 3.26107800 -2.94987600
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 H 3.93013700 3.98599300 -3.75032700
 H 4.64477700 3.03974100 -2.41219400
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11
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H 3.59899600	2.96233600	-0.53000300	C -5.53103500	3.59929800	-1.75896000
H 3.74368200	2.36931600	-2.22582200	H -3.64156200	4.63801000	-1.69370200
H 2.12619100	2.68949900	-1.50700900	C -6.21929300	2.39101400	-1.59730900
C -3.14337400	2.30982600	-1.31064400	H -6.06961200	0.28228500	-1.08418900
H -3.75330600	2.35056500	-2.22945900	H -6.07696000	4.49288800	-2.07511900
H -3.59748700	2.95033600	-0.53715300	H -7.29328700	2.34719800	-1.79973200
H -2.13120900	2.67548700	-1.52480000	N -2.15631500	2.22687900	-0.89704000
Co 0.00018400	0.57423900	-0.76470800	N -3.25598800	0.37911600	-0.55013400
H -0.00557500	2.19783800	-0.93693300	N 2.36136800	1.71773700	-0.97642400
C 0.73095400	3.05892700	2.32612800	N 2.91839700	-0.38316200	-0.67860800
C -0.76970200	3.32588600	2.17510400	Co -0.04132700	0.47160700	-0.21140000
H 0.92833400	2.29014300	3.09954700	H -1.13711000	2.58816700	2.13186100
H 1.30695400	3.96347200	2.58956400	C -0.17944100	-2.74068800	1.15763200
H -1.34356200	3.06775800	3.08260200	C -1.36571200	-2.65605900	2.13719200
H -0.97349700	4.38856500	1.93320600	H 0.65740000	-3.28739000	1.62520400
B -0.01477800	2.07421900	0.41918800	H -2.31238100	-2.63672900	1.57050000
O 1.12669200	2.57860700	1.06304000	B -0.34448900	-0.64140100	2.02473900
O -1.16414800	2.50914900	1.09695900	O 0.24895500	-1.37786900	1.01652900
¹⁷ Dipp			O -1.22034700	-1.37680000	2.76416900
C 0.13283400	2.19159600	-0.85724800	N -0.11323800	0.76618000	2.14198200
C -0.98723700	2.97966300	-1.10119700	C -1.22336200	1.60439300	2.61893700
C -0.87052300	4.29685500	-1.55236000	C -1.24211700	1.76298500	4.12797200
C 0.41234000	4.80331700	-1.79117500	H -0.31874400	2.25267900	4.48476900
C 1.55940100	4.01949900	-1.61589600	H -2.09649600	2.39078600	4.43799100
C 1.39615000	2.71411700	-1.15423100	H -1.33357600	0.78482100	4.63066700
H -1.73540700	4.93331300	-1.73778600	B 1.19036800	1.37838200	2.19400100

O 2.36049300	0.70126900	2.42610200	H 3.72018900	-0.90608000	1.51041800
O 1.34020600	2.73945200	2.23496800	H 5.89415000	-2.05496200	0.91888500
C 3.41104700	1.66499800	2.41989900	H 5.70312200	-1.82936000	2.67652800
C 2.68382300	3.01025500	2.61668100	H 5.43074100	-3.43365100	1.95095100
H 3.88526500	1.64769600	1.42133300	H 1.98130800	-2.02707400	2.78868500
H 2.67845000	3.26841300	3.69482100	H 3.00024100	-3.48848700	2.99872200
H -2.16574500	1.15920800	2.26983300	H 3.46710600	-1.94060100	3.75027500
C -0.50419400	-3.33734500	-0.18027000	C -4.71992300	-0.04697500	1.96964800
H 0.39392200	-3.38896300	-0.81251600	C -4.23924600	-0.41127500	3.37580500
H -0.90795900	-4.35728900	-0.05727400	C -6.21134300	0.29770800	2.02360800
H -1.26103800	-2.71805200	-0.68088200	H -4.17684000	0.85603200	1.64866700
C -1.40699500	-3.75638200	3.16656100	H -3.17805200	-0.70043700	3.38547800
H -2.27193700	-3.62699800	3.83889600	H -4.37164700	0.45163600	4.05260800
H -1.50461200	-4.73720100	2.66925600	H -4.82848700	-1.24623800	3.79667000
H -0.48587600	-3.76024500	3.77534800	H -6.60445700	0.62327300	1.04874700
C 3.25815400	4.15878900	1.82516500	H -6.80553400	-0.57084300	2.36079700
H 2.66319400	5.07378000	1.98382700	H -6.38199300	1.11849700	2.74290100
H 4.29750400	4.36057300	2.13875900	C 2.24766900	-1.52816500	-3.23286500
H 3.25187000	3.92698100	0.74793400	C 0.82110300	-1.75197100	-3.72511200
C 4.44180900	1.34930300	3.47551400	C 3.27529900	-1.76669800	-4.33963200
H 4.93206200	0.38316400	3.27026800	H 2.31901700	-0.47074300	-2.93987500
H 5.22403100	2.12840300	3.49019200	H 0.09918300	-1.49929400	-2.93111400
H 3.97391500	1.30057100	4.47437000	H 0.60484500	-1.10365700	-4.59322000
C 2.87714000	-1.80691200	-0.76501500	H 0.65463800	-2.79952600	-4.03396600
C 2.55155500	-2.37648000	-2.01320100	H 4.30217700	-1.57879400	-3.98000100
C 3.27488200	-2.60066500	0.32772100	H 3.23268200	-2.80228800	-4.72322600
C 2.55253300	-3.77079200	-2.12311500	H 3.08569100	-1.08715200	-5.18978800
C 3.24531700	-3.99167600	0.17278100	C -2.91093800	-1.69559200	-2.55359700
C 2.87999900	-4.57524900	-1.03592400	C -3.83891200	-0.90464800	-3.48219200
H 2.29481900	-4.23444600	-3.08029500	C -2.45505200	-2.95863700	-3.27883200
H 3.53830200	-4.62997000	1.01227200	H -2.02004800	-1.07017600	-2.36362800
H 2.86885600	-5.66494700	-1.13734100	H -4.11568500	0.07742000	-3.07171600
C -3.71465600	-0.93870000	-0.24171100	H -3.33863600	-0.72920700	-4.45102800
C -4.43537800	-1.14491800	0.95612100	H -4.77004800	-1.46758100	-3.67634100
C -3.56625100	-1.96172400	-1.20676000	H -1.79328300	-3.59073200	-2.66374100
C -4.94472500	-2.42631200	1.20108800	H -3.31334700	-3.57331800	-3.60486800
C -4.08661000	-3.22344500	-0.90260700	H -1.89735900	-2.67826200	-4.18761000
C -4.76312500	-3.45892300	0.29084000	¹²W_{CO}		
H -5.49754500	-2.61416200	2.12603100	C 0.00103000	-0.19729700	-0.62047900
H -3.97107300	-4.04082600	-1.61694200	C -1.21615800	0.32592600	-1.10741500
H -5.16433200	-4.45458700	0.50364100	C -1.25700900	1.31956500	-2.11678800
C 3.81144100	-1.99581500	1.60940900	C -0.01175200	1.82731900	-2.58067700
C 5.28977200	-2.34877000	1.79307200	C 1.23956000	1.33849700	-2.11354000
C 3.01602100	-2.39310900	2.84991200	C 1.21133400	0.34254900	-1.10574500

H -2.18577100 1.70305200 -2.53619500
H -0.01663300 2.60839700 -3.34380000
H 2.16358900 1.73618000 -2.53021800
C 3.65376200 -0.25844000 -0.60356000
C 1.88176100 -1.38702300 0.31409600
C 4.13857300 -1.30377500 0.20498500
C 4.52815200 0.60702000 -1.25598000
C 5.50151000 -1.53094300 0.36578400
C 5.89538400 0.38198400 -1.09020500
H 4.17262100 1.44026900 -1.86334200
C 6.37530500 -0.66995700 -0.29865700
H 5.87204100 -2.34800300 0.98915500
H 6.60644300 1.04733000 -1.58796200
H 7.45421800 -0.81578100 -0.19422200
C -3.65071300 -0.30462100 -0.60330300
C -1.86447800 -1.41215300 0.31275000
C -4.12238200 -1.35423500 0.20741500
C -4.53575500 0.55064500 -1.25481200
C -5.48246400 -1.59584600 0.37148900
C -5.90010300 0.31107800 -1.08580300
H -4.19070400 1.38726300 -1.86357800
C -6.36690100 -0.74507600 -0.29202500
H -5.84286900 -2.41595600 0.99677300
H -6.61938000 0.96827100 -1.58258700
H -7.44395700 -0.90228400 -0.18497000
N -2.26978300 -0.38483700 -0.52500400
N -3.00716600 -1.98590100 0.74257700
N 2.27396400 -0.35389100 -0.52273500
N 3.03153700 -1.94814000 0.74173200
C 3.11160400 -3.08849400 1.61678200
H 3.51936700 -3.95867900 1.07641900
H 3.75277700 -2.85678500 2.48407700
H 2.09710500 -3.32506600 1.96342200
C -3.07341400 -3.12409900 1.62191100
H -3.70885300 -2.89334100 2.49368000
H -3.47992300 -3.99842400 1.08749700
H -2.05473900 -3.35410700 1.96043400
Co 0.01035600 -1.58075600 0.60490700
H 0.02184800 -3.10608300 1.09986600
C 0.79355500 -5.03975000 -1.57585600
C -0.70888900 -4.85303400 -1.80209100
H 1.36694700 -5.09289800 -2.51795800
H 1.00756300 -5.95873700 -0.99395600
H -0.91690800 -4.39616400 -2.79011300

H -1.27577800 -5.79851700 -1.73884100
B 0.02888500 -3.30042400 -0.30096400
O 1.17810300 -3.90507600 -0.83291900
O -1.10784200 -3.97367800 -0.77640900
N 0.00389000 -0.65099000 2.31305900
C 0.00124100 0.10115900 3.18987000
C -0.00212000 1.09840200 4.23956700
H 0.88555300 1.74438400 4.13207500
H -0.90584000 1.72390200 4.14599200
H 0.01113900 0.62310400 5.23442700
W -0.01734100 2.26616400 -0.25806600
C 1.34102500 2.52742700 1.13614000
O 2.16620000 2.62868900 1.95063700
C -1.37350900 2.49678000 1.14392800
O -2.19646500 2.57902700 1.96280600
C -0.03799100 4.21546200 -0.50895800
O -0.04982900 5.36065700 -0.70001300
³¹
C -0.00323500 -1.25024600 -0.00418700
C -1.21218000 -1.90793800 0.23441700
C -1.23414400 -3.22279800 0.69864200
C -0.00646700 -3.86194400 0.92291600
C 1.22281400 -3.22506200 0.70088800
C 1.20418400 -1.91020700 0.23650400
H -2.16455400 -3.75998700 0.89072300
H -0.00774400 -4.89415700 1.28549700
H 2.15182700 -3.76402700 0.89476000
C 3.65255800 -1.18204300 -0.01896500
C 1.89571100 0.20221000 -0.51576000
C 4.15627900 0.05457800 -0.47492700
C 4.51995000 -2.20898100 0.34936600
C 5.52386700 0.29723000 -0.57144300
C 5.89216100 -1.96490900 0.25080100
H 4.15363900 -3.17286900 0.70349400
C 6.38736400 -0.73551200 -0.20053200
H 5.90664100 1.25945500 -0.91964300
H 6.59281400 -2.75545700 0.53469000
H 7.46823800 -0.57912100 -0.26237600
C -3.65845900 -1.17365600 -0.02239000
C -1.89751100 0.20673900 -0.51640000
C -4.15862900 0.06527000 -0.47589700
C -4.52880900 -2.19872100 0.34422000
C -5.52549100 0.31212400 -0.57213600
C -5.90031500 -1.95034600 0.24631100

H -4.16532500 -3.16438200 0.69645600
C -6.39197400 -0.71874000 -0.20289100
H -5.90535800 1.27599400 -0.91897000
H -6.60326700 -2.73934500 0.52882700
H -7.47239900 -0.55917400 -0.26448300
N -2.28265700 -1.04956600 -0.06391600
N -3.06631400 0.86180900 -0.76824000
N 2.27707700 -1.05427700 -0.06071700
N 3.06613100 0.85332900 -0.76958900
C 3.18617900 2.18230400 -1.30613900
H 3.55568500 2.88545800 -0.54192000
H 3.87693900 2.17611000 -2.16701100
H 2.19678800 2.51813800 -1.64181000
C -3.18328000 2.19231300 -1.30164600
H -3.85831500 2.18710500 -2.17506100
H -3.57010100 2.89025700 -0.54123600
H -2.18959200 2.53506300 -1.61618200
Co 0.00020000 0.53678400 -0.51360900
H 0.00011300 2.13176900 -0.97025400
C 0.76820300 4.04639000 1.74163600
C -0.74425000 3.85794300 1.91177700
H 1.32248800 3.94067400 2.68923900
H 1.01897700 5.03063300 1.30271000
H -0.98828100 3.30814600 2.84002400
H -1.30181800 4.80944500 1.91664900
B 0.00856400 2.48102300 0.29122100
O 1.15451000 3.02388100 0.83903000
O -1.13106600 3.07948400 0.79340300

HBR₂

C 0.89301200 0.77105700 -0.01485300
C 0.89287700 -0.77121200 0.01487500
H 1.40631300 1.21407800 0.85510700
H 1.35544900 1.17763900 -0.93057400
H 1.35525600 -1.17791400 0.93057300
H 1.40607700 -1.21430200 -0.85510900
B -1.22128500 0.00010600 -0.00003400
H -2.42916600 0.00022200 0.00017400
O -0.48153100 -1.14032600 -0.01387600
O -0.48132300 1.14041000 0.01386000

³TS1

C 0.00607700 1.49394300 -0.16171600
C 1.20594200 2.10314200 0.16679600
C 1.24131000 3.39299400 0.70158000
C 0.01331500 4.02845300 0.93483700

C -1.21811400 3.39823600 0.70598700
C -1.19009000 2.10846000 0.17048500
H 2.16947600 3.90075500 0.97287200
H 0.01621800 5.03931200 1.35407000
H -2.14312900 3.90972600 0.98099300
C -3.64036400 1.38268100 -0.09294900
C -1.92430800 -0.11412800 -0.22546100
C -4.16820100 0.10590100 -0.36396400
C -4.47873400 2.49275600 0.01130700
C -5.53467600 -0.10466100 -0.52556600
C -5.84738000 2.28142700 -0.14982800
H -4.08820300 3.49334600 0.19921000
C -6.36941500 1.00575800 -0.40980600
H -5.93640400 -1.09725900 -0.74185500
H -6.52838200 3.13418500 -0.07557700
H -7.44917800 0.88045500 -0.53114200
C 3.65320400 1.36585400 -0.09588900
C 1.93104900 -0.12384500 -0.22358700
C 4.17597100 0.08525200 -0.35849200
C 4.49629500 2.47287800 0.00300700
C 5.54172200 -0.13249300 -0.51671800
C 5.86416400 2.25448200 -0.15485500
H 4.10978100 3.47630100 0.18401300
C 6.38107500 0.97495600 -0.40643000
H 5.93911300 -1.12829400 -0.72618100
H 6.54881400 3.10467600 -0.08483200
H 7.46046500 0.84433700 -0.52542300
N 2.28336900 1.19471400 -0.01941100
N 3.09315300 -0.78003800 -0.41790200
N -2.27143300 1.20525200 -0.01520500
N -3.08923500 -0.76391900 -0.42645700
C -3.21396700 -2.17541700 -0.69025200
H -4.06347400 -2.58251600 -0.11849900
H -3.37429300 -2.35838600 -1.76664300
H -2.29870300 -2.67289300 -0.35075100
C 3.21230800 -2.19441000 -0.66885900
H 3.39310500 -2.38612200 -1.74050100
H 4.04658400 -2.60423500 -0.07690100
H 2.28647300 -2.68324500 -0.34554000
Co 0.00044500 -0.45580100 -0.33364100
H 0.00334700 -2.37694300 -0.39564500
C -0.78409600 -3.22924000 2.79829100
C 0.71872700 -2.98773100 2.96477200
H -1.36282800 -2.99183700 3.70733900

H -1.00350400 -4.27786900 2.51649200
H 0.93287200 -2.28361100 3.79153700
H 1.28679300 -3.91573200 3.15054200
B -0.01579100 -1.95819000 1.06292200
O -1.16375100 -2.36696700 1.74349500
O 1.12009700 -2.40854900 1.73906100
N -0.00309900 -1.30775700 -2.33849500
C -0.00138000 -2.41343700 -1.85603800
C -0.00424300 -3.85324600 -2.23197800
H -0.00890900 -3.95496300 -3.33230400
H 0.88733500 -4.35930800 -1.82253700
H -0.89360000 -4.35732400 -1.81524100
¹W_{Co}
C -0.00045200 0.11474400 0.63409000
C -1.22242700 -0.45504300 1.04688000
C -1.26788600 -1.59025300 1.89437300
C -0.02126800 -2.16927900 2.26806800
C 1.23786400 -1.61303400 1.89399600
C 1.21242400 -0.47992000 1.04621800
H -2.19679100 -2.04612100 2.23256700
H -0.02956200 -3.06268700 2.89583600
H 2.15801100 -2.08619000 2.23235000
C 3.65920200 0.11939200 0.56929600
C 1.90157800 1.28810600 -0.33157600
C 4.15794000 1.14273200 -0.25805900
C 4.52498500 -0.74325400 1.23885900
C 5.52324900 1.34045900 -0.43855200
C 5.89354900 -0.54657800 1.05558900
H 4.16294300 -1.54538500 1.88247200
C 6.38656700 0.47644700 0.23372300
H 5.90254000 2.13873700 -1.08050100
H 6.59705300 -1.21006600 1.56637600
H 7.46696900 0.59844400 0.11604000
C -3.65909700 0.18756500 0.57061600
C -1.88133500 1.32948500 -0.32453900
C -4.13989600 1.22059400 -0.25538900
C -4.54008500 -0.66397900 1.23474300
C -5.50151300 1.43889900 -0.44014900
C -5.90485000 -0.44666800 1.04721900
H -4.19240400 -1.47376500 1.87674600
C -6.37987000 0.58576000 0.22647100
H -5.86668100 2.24399700 -1.08175200
H -6.61980800 -1.10156200 1.55318400
H -7.45793400 0.72353500 0.10486400

N -2.28093800 0.29174800 0.50600700
N -3.02931600 1.87268300 -0.77578000
N 2.28293200 0.24518700 0.50144700
N 3.05918900 1.81056400 -0.78322700
C 3.17233400 2.91965300 -1.69677300
H 3.65405300 3.77681700 -1.19946500
H 3.76407300 2.61932500 -2.57779700
H 2.16412400 3.21162800 -2.01439100
C -3.12187800 2.98520800 -1.68770400
H -3.70027600 2.69100900 -2.57964800
H -3.60780000 3.84291600 -1.19552100
H -2.10696800 3.27452100 -1.98548700
Co 0.01381300 1.53741200 -0.53509800
H 0.03571300 2.95501400 -1.33224400
C 0.82632000 5.23561000 1.05323600
C -0.68007200 5.08412900 1.28564200
H 1.39417900 5.36403000 1.99117400
H 1.05445300 6.09723000 0.39463600
H -0.89744200 4.71216600 2.30635500
H -1.23722700 6.02578800 1.13928000
B 0.04810200 3.39258900 -0.04385100
O 1.20429400 4.03695400 0.41257100
O -1.08366300 4.12626000 0.33335200
W -0.02462800 -2.20133200 -0.08494000
C 1.32802400 -2.17557400 -1.52666000
O 2.15099200 -2.11170600 -2.33922900
C -1.43465000 -2.23540200 -1.46758100
O -2.29133400 -2.21075400 -2.24700000
C 0.00923000 -4.17280700 -0.19565900
O 0.02931500 -5.33164800 -0.22094900
¹7
C 0.32395100 -2.00732200 -0.01725100
C 1.61259100 -2.56669100 0.02216600
C 1.81626200 -3.94494500 0.00306700
C 0.69075800 -4.78110500 -0.05877600
C -0.61353200 -4.26461000 -0.09953400
C -0.77528200 -2.88077900 -0.07691000
H 2.81411600 -4.38691700 0.03618300
H 0.83407700 -5.86572600 -0.07531400
H -1.46196800 -4.95009800 -0.14948800
C -3.29995800 -2.43189600 -0.12505000
C -1.73365000 -0.74831300 -0.09077300
C -3.97224800 -1.18838300 -0.12477800
C -4.02071400 -3.62442100 -0.13816700

C -5.36245400	-1.10971200	-0.13240900	H -2.88480400	4.79286200	0.51830500
C -5.41731900	-3.54364500	-0.14930000	H -2.44904200	6.34233800	-0.25604100
H -3.52377900	-4.59487400	-0.13781100	H -2.53687200	4.85290600	-1.23745800
C -6.07805300	-2.31080100	-0.14631400	B -0.57718400	2.83818200	1.25824800
H -5.87724900	-0.14570500	-0.12332100	O -0.28361000	1.49430100	1.38195200
H -6.00189500	-4.46829000	-0.15841600	O -0.97342100	3.39718600	2.44006800
H -7.17175700	-2.28356200	-0.15231600	C -0.66015700	1.08983100	2.69814700
C 3.93363800	-1.47581300	0.10511300	C -0.80919600	2.41340500	3.45508400
C 1.98194400	-0.26036000	0.10351800	H -1.60526600	0.52513600	2.63305700
C 4.25686300	-0.10017800	0.14600700	H 0.11485000	0.42582200	3.10811700
C 4.94163900	-2.43788500	0.09379100	H -1.68241300	2.42406400	4.12663400
C 5.57763200	0.33981000	0.16997800	H 0.09046000	2.65755200	4.04765300
C 6.26819600	-1.99443800	0.12130400	H -0.15097500	5.48107200	-0.73382300
H 4.71681200	-3.50436700	0.06295100	3		
C 6.58285700	-0.63196300	0.15816100	C -0.12758200	-1.55759700	-0.06037300
H 5.82099400	1.40504600	0.19333800	C 1.03532500	-2.31088300	-0.15817600
H 7.07467100	-2.73353600	0.11180000	C 0.99988800	-3.68810100	-0.38379800
H 7.63120800	-0.31956700	0.17609100	C -0.25570900	-4.29485800	-0.51050600
N 2.55393100	-1.53147600	0.08126400	C -1.44876000	-3.56792000	-0.41722700
N 3.06281800	0.59246500	0.15395800	C -1.35560000	-2.19385200	-0.18966600
N -1.95370500	-2.12512400	-0.10634000	H 1.90081000	-4.29859600	-0.45845700
N -3.00110900	-0.20726800	-0.11505300	H -0.30622200	-5.37327100	-0.68747800
C -3.28960300	1.19779800	-0.11589500	H -2.40304100	-4.08582800	-0.52261300
H -2.37847700	1.74322900	-0.38819500	C -3.78152000	-1.33475600	-0.15749600
H -4.07007400	1.43014800	-0.86083800	C -1.99663700	0.05225900	0.15215200
H -3.63753900	1.54766900	0.87436200	C -4.24814000	-0.01634800	0.00806100
C 2.97506300	2.02374600	0.19964800	C -4.68084000	-2.38363000	-0.36034500
H 3.24360100	2.48264500	-0.77049200	C -5.60422800	0.29762400	-0.02358800
H 1.94721600	2.30548200	0.45762500	C -6.03814400	-2.06940600	-0.39152400
H 3.65237500	2.42565500	0.97306000	H -4.34997100	-3.41420200	-0.48919000
Co 0.08125400	-0.17026500	0.00839100	C -6.49583400	-0.75321200	-0.22658300
H -0.49680300	5.41623500	1.00571100	H -5.95338300	1.32446500	0.10734000
C 0.49377900	1.30325800	-2.64529100	H -6.76381900	-2.87275000	-0.54784800
C 0.21057100	2.61141500	-3.39077700	H -7.56989200	-0.54914500	-0.25658400
H 1.57031700	1.07108100	-2.58376000	C 3.53082500	-1.70041200	-0.01831700
H -0.02809100	0.42961600	-3.06230800	C 1.88272000	-0.14996900	0.27497400
H 1.03319500	2.90635200	-4.06146300	C 4.11985600	-0.44813400	0.24216200
H -0.72108600	2.55947700	-3.98183400	C 4.32771800	-2.82386700	-0.24740200
B -0.13764600	2.92173800	-1.19010100	C 5.50074100	-0.27492700	0.28437000
O 0.00817200	1.55554900	-1.32653000	C 5.70982700	-2.65072100	-0.20466300
O 0.05280800	3.58763700	-2.36757300	H 3.90110800	-3.80458700	-0.45695300
N -0.46198000	3.55868300	0.03860700	C 6.28995300	-1.40010300	0.05686200
C -0.77565800	4.98973400	0.02907700	H 5.94607100	0.70248000	0.48425200
C -2.24405400	5.25717400	-0.25211900	H 6.35712400	-3.51442200	-0.38191400

H 7.37936700 -1.30649300 0.08036500
 N 2.16724400 -1.47364400 0.01563000
 N 3.08033300 0.45241900 0.41895800
 N -2.40447800 -1.24659700 -0.06556600
 N -3.12949900 0.78301000 0.18837900
 C -3.19075200 2.21391500 0.36724600
 H -3.73254600 2.67270000 -0.47696200
 H -3.70919000 2.46235100 1.30849500
 H -2.15924000 2.59062600 0.39909000
 C 3.28424100 1.85009100 0.71417100
 H 3.95282800 1.95387100 1.58488500
 H 3.73586000 2.36283600 -0.15216000
 H 2.30669100 2.29620100 0.94015700
 Co -0.04273500 0.29434100 0.29461800
 H -0.23305900 3.78046500 2.14349400
 C 0.76409900 4.86426400 -1.66653700
 C 1.15889900 3.59008400 -2.42773800
 H -0.17057000 5.30293600 -2.07022200
 H 1.54570400 5.64369300 -1.70348400
 H 0.73216500 3.55004200 -3.44545500
 H 2.26006400 3.49747500 -2.51976100
 B 0.39102400 3.05255000 -0.36389200
 O 0.55782600 4.43786700 -0.34060100
 O 0.65450300 2.53949000 -1.63964700
 N 0.04670600 2.22952700 0.70899900
 C -0.18744600 2.69481200 1.97629800
 C -0.69252900 1.77424600 3.03022600
 H -0.55002900 2.19789800 4.04139300
 H -1.77864400 1.53007400 2.94263000
 H -0.16246900 0.79776200 3.00343600
¹³K_{Dipp}
 C -1.11203600 0.25202400 -1.96267000
 C -0.69054700 1.39331400 -2.64701700
 C -0.62032200 1.41745700 -4.03975200
 C -0.99004600 0.25790500 -4.73691100
 C -1.42073200 -0.90369000 -4.08224300
 C -1.47490900 -0.88322000 -2.68881500
 H -0.30420600 2.29895700 -4.59913400
 H -0.94678400 0.26310000 -5.82997200
 H -1.69595800 -1.78193700 -4.66714600
 C -2.39001900 -3.16114200 -1.96710800
 C -1.78941300 -1.54963500 -0.45514000
 C -2.61007500 -3.65226600 -0.66985100
 C -2.69507200 -3.94200900 -3.08293300
 C -3.11611000 -4.92731000 -0.43749300
 C -3.21389500 -5.21548400 -2.85326900
 H -2.54726900 -3.58264300 -4.10144100
 C -3.41804600 -5.70399800 -1.55421500
 H -3.26404200 -5.29713900 0.57931000
 H -3.46814200 -5.84655900 -3.70960000
 H -3.82315600 -6.71023300 -1.41518500
 C -0.00965100 3.72690500 -1.83684900
 C -0.64408300 2.06691100 -0.39476400
 C 0.02757600 4.22836800 -0.52361300
 C 0.34016400 4.54201200 -2.91456700
 C 0.40781500 5.53605900 -0.23970900
 C 0.72316900 5.85331500 -2.63311800
 H 0.31373300 4.18579500 -3.94431700
 C 0.75721200 6.34486800 -1.31987200
 H 0.42187100 5.90666400 0.78780000
 H 0.99652800 6.51446100 -3.46040200
 H 1.05620800 7.38140800 -1.14054800
 N -0.41362900 2.40911100 -1.71508400
 N -0.35963600 3.18799000 0.31453200
 N -1.86497200 -1.89289900 -1.79287900
 N -2.21623300 -2.64879600 0.21311300
 Co -1.26185500 0.27341900 -0.09876700
 H -2.31766400 0.52275800 3.24510600
 C -5.11907400 0.67315600 -1.53061700
 C -4.50588900 2.00821200 -1.98508100
 H -5.82624700 0.85294600 -0.69693900
 H -4.23964900 1.93743100 -3.05907100
 B -2.94660300 0.81756200 -0.83008900
 O -4.00928900 -0.05071800 -1.01228400
 O -3.29070300 2.09381300 -1.24872900
 N -1.06075800 0.18194200 1.65988500
 C -1.30232600 0.23176500 2.88708400
 C -0.34246800 -0.06450800 4.00588200
 H 0.66178500 -0.29662700 3.62153500
 H -0.27521100 0.80315700 4.68654000
 H -0.70765800 -0.92157100 4.60045600
 K 3.63593600 -0.89524700 -0.15448800
 O 3.02144900 0.94249100 -2.10075300
 O 5.74383100 -0.15976500 1.55024300
 O 2.70770800 -1.87070100 -2.52349000
 C 3.80255800 2.11139500 -2.03386200
 C 2.86139600 0.40791600 -3.39407300
 C 6.17727700 -1.06835200 2.52862700

C 6.76215900 0.68723900 1.08463300	H -0.46946400 3.88025200 5.55757000
C 3.71258800 -2.60557600 -3.17164000	C -2.29582300 -2.83053000 1.62846800
C 2.07210900 -0.87584300 -3.29524100	C -3.54750700 -2.69560500 2.24655300
C 5.28974100 1.81685100 -2.08664000	C -1.13554300 -3.21779200 2.32925700
H 3.54148400 2.60231500 -1.08030900	C -3.63093800 -2.98481600 3.61416000
H 3.53070300 2.81231600 -2.84804900	C -1.27614600 -3.50389000 3.68885300
H 2.30037300 1.11580300 -4.03530000	C -2.51183800 -3.39670500 4.32514900
H 3.84324100 0.22754000 -3.87496900	H -4.59159000 -2.88329500 4.12753100
C 5.07707200 -2.07499200 2.78656800	H -0.40397600 -3.80607200 4.27229200
H 7.10596100 -1.57207200 2.19335700	H -2.59561100 -3.62630700 5.39184600
H 6.41476000 -0.54677600 3.47856000	C 2.10353100 2.84677400 1.78642400
C 6.20401700 1.67062900 0.09275300	C 2.54188700 1.43069800 2.16283600
H 7.56332800 0.09006800 0.60364800	C 3.19134500 3.87520000 2.09414800
H 7.21511200 1.25369000 1.92329600	H 1.94074300 2.85590300 0.69643600
C 4.09385100 -3.77066500 -2.29653300	H 1.79072700 0.69630600 1.82246300
H 3.34511800 -2.99601200 -4.14172700	H 3.52922400 1.19869200 1.72528300
H 4.60827100 -1.98265900 -3.37403700	H 2.64665300 1.32049100 3.25693800
H 1.11188500 -0.67009200 -2.79924400	H 2.86770000 4.89525800 1.82473800
H 1.85838600 -1.25306000 -4.31313200	H 3.46478700 3.87821400 3.16395500
O 5.70667000 0.98421900 -1.02693900	H 4.10978400 3.65111200 1.52216000
H 5.54750300 1.29232500 -3.02245300	C 0.21611300 -3.29361700 1.63718400
H 5.85393600 2.76931100 -2.08378600	C 0.36555000 -4.54949700 0.77457000
O 4.64220000 -2.72981500 1.62073700	C 1.39355300 -3.20316700 2.60272900
H 5.42002300 -2.80400500 3.54745800	H 0.26834100 -2.41070900 0.97492900
H 4.18955800 -1.55896000 3.19068600	H -0.41306000 -4.63041300 0.00070200
H 5.41497100 2.28235100 0.57428800	H 1.34486300 -4.54192800 0.26141200
H 7.02237000 2.35593900 -0.20599900	H 0.31591700 -5.46019400 1.39858900
O 4.64561400 -3.28845300 -1.09780400	H 1.31826000 -2.32141100 3.25989400
H 3.19194200 -4.38052200 -2.08789800	H 1.46741300 -4.10017800 3.24366100
H 4.82433000 -4.40891200 -2.83396700	H 2.34168000 -3.13689000 2.04229500
C 5.53405500 -3.66509900 1.06725600	C -4.77555500 -2.22708200 1.49126900
C 4.89187600 -4.28819500 -0.14377700	C -5.26260900 -0.88593600 2.03771800
H 6.48388500 -3.18371000 0.76417600	C -5.88993900 -3.27286900 1.50345000
H 5.76974600 -4.46043800 1.80246200	H -4.48564300 -2.04921900 0.44520300
H 5.57544300 -5.06091700 -0.55032500	H -4.46571300 -0.12834800 1.97603000
H 3.94514900 -4.78955200 0.14331400	H -6.12364400 -0.52247500 1.44909900
C -0.40654300 3.33718300 1.73409800	H -5.58640100 -0.96488000 3.09141600
C 0.79083400 3.20171700 2.45712600	H -5.54835600 -4.23526400 1.08515800
C -1.62221400 3.67904500 2.34637400	H -6.26592900 -3.46107100 2.52553800
C 0.74390900 3.40105700 3.83937500	H -6.74413800 -2.92700400 0.89414000
C -1.61935700 3.86346000 3.73316100	C -2.90980900 3.82612500 1.56406000
C -0.45042900 3.72807800 4.47410600	C -3.52800100 5.21241700 1.73737300
H 1.65749100 3.29571700 4.43192700	C -3.88420300 2.71307800 1.94385900
H -2.55302800 4.12238600 4.24103800	H -2.68328300 3.69046800 0.49623900

H -2.81932000 6.00913600 1.44973500
H -4.42360000 5.31195600 1.09841300
H -3.84151500 5.39868500 2.78032200
H -3.43753500 1.73258800 1.71578900
H -4.14176200 2.74138300 3.01822200
H -4.82233900 2.80339900 1.37044600
C -5.37099300 3.22524900 -1.76626800
H -4.82831300 4.14067900 -2.05737800
H -6.28843200 3.16327400 -2.37757200
H -5.66468900 3.31716400 -0.70666100
C -5.80625100 -0.11711000 -2.61812000
H -6.66540300 0.44358700 -3.02691700
H -5.10245000 -0.33362800 -3.44097200
H -6.18058600 -1.07644200 -2.22139100

¹TS3

C -0.24815500 0.39996200 -1.07390400
C 0.94506100 0.56440000 -1.76255800
C 0.98092700 1.20630200 -3.00032800
C -0.22777300 1.68114800 -3.52628400
C -1.44682400 1.53322300 -2.85187900
C -1.43010900 0.88450400 -1.61630200
H 1.90640200 1.35376500 -3.55955300
H -0.21895600 2.18687600 -4.49639200
H -2.36283300 1.92601300 -3.29675800
C -3.87014900 0.72678100 -0.81618600
C -2.12017100 -0.04048200 0.42471300
C -4.36883000 0.13142200 0.35887100
C -4.73758900 1.27623500 -1.75929900
C -5.73270800 0.06736300 0.62716800
C -6.10471900 1.21219100 -1.49020600
H -4.37248500 1.74099200 -2.67558500
C -6.59643300 0.61920900 -0.31868500
H -6.11176800 -0.39448400 1.54190300
H -6.80806200 1.63645500 -2.21257300
H -7.67548500 0.58946400 -0.14218700
C 3.33381400 -0.23549400 -1.26457500
C 1.60612900 -0.56687300 0.18519200
C 3.79366400 -0.99650900 -0.17235700
C 4.20105200 0.11830000 -2.29792700
C 5.11264100 -1.42991100 -0.08048300
C 5.52492600 -0.31121000 -2.20355300
H 3.86907200 0.70862900 -3.15230700
C 5.97575500 -1.07305700 -1.11617700
H 5.45776900 -2.02378900 0.76927900

H 6.22641800 -0.04585600 -2.99977700
H 7.02124600 -1.39230100 -1.07842400
N 1.99371700 -0.00886300 -1.01352600
N 2.71049100 -1.17882000 0.67388000
N -2.49516500 0.59936200 -0.73460700
N -3.27057700 -0.32107900 1.07524400
C -3.37480700 -1.09110000 2.28664900
H -3.73941100 -0.46782300 3.12135200
H -4.06797400 -1.93453100 2.13185000
H -2.38311800 -1.49434300 2.52681500
C 2.74122100 -2.06499100 1.80765000
H 3.06783500 -3.06732000 1.48340100
H 3.42853100 -1.69142600 2.58533900
H 1.72549400 -2.14088900 2.21344900
Co -0.23739600 -0.31765500 0.65000300
H -1.16670200 0.35905700 3.01814300
C 2.77619200 3.70502900 2.05078600
C 2.48458400 3.77932900 0.54418200
H 2.79607500 4.69805400 2.53285300
H 3.74460100 3.20778600 2.25572400
H 2.00081100 4.73601200 0.26672400
H 3.39317800 3.66651400 -0.07275100
B 1.09778700 2.28193100 1.51600100
O 1.72589100 2.92527000 2.57841700
O 1.59777100 2.71333800 0.30042000
N 0.03776300 1.37520600 1.66686300
C -0.14624300 0.42879700 2.60215200
C 0.91045000 0.11766400 3.63385200
H 0.91539900 0.93084300 4.38253600
H 0.71155000 -0.83211100 4.15967500
H 1.91483000 0.08478600 3.18624800
B -0.53295800 -2.15168100 0.12962800
O -1.77936200 -2.75555200 -0.00078000
O 0.46395400 -3.07141900 -0.17924200
C -1.61793300 -4.04129400 -0.56631200
C -0.12181400 -4.33584000 -0.41989400
H -2.25524700 -4.77059000 -0.03709400
H -1.93310900 -4.01715000 -1.62644200
H 0.08718900 -5.00586600 0.43633700
H 0.31832600 -4.79041900 -1.32376800
H -0.25661200 -1.17525700 1.91244500

³TS2

C 0.04909100 -1.52520700 -0.05865700
C -1.14430700 -2.21232800 0.14977800

C -1.15729900 -3.56241200 0.50132700
C 0.07655000 -4.20391500 0.67280200
C 1.29573300 -3.52640300 0.54094100
C 1.25440500 -2.17736400 0.18665800
H -2.08147800 -4.11842600 0.66824300
H 0.08751900 -5.26218700 0.95026000
H 2.23004700 -4.05366300 0.74204100
C 3.69251500 -1.41100000 -0.00723100
C 1.94428300 0.06272400 -0.04215900
C 4.19321100 -0.11009700 -0.20276100
C 4.55232400 -2.50851800 0.02838000
C 5.55519400 0.13495700 -0.35775900
C 5.91648700 -2.26226100 -0.12561500
H 4.18389200 -3.52605500 0.16007500
C 6.41206900 -0.96406200 -0.31233000
H 5.93745900 1.14592800 -0.51568800
H 6.61357600 -3.10491100 -0.10363700
H 7.48851100 -0.81027200 -0.43066700
C -3.60030800 -1.50782500 -0.08762300
C -1.88299900 0.00021900 -0.15565000
C -4.12454600 -0.22480400 -0.33292700
C -4.44158100 -2.61742800 -0.01205000
C -5.48976200 -0.00742800 -0.49604200
C -5.80979600 -2.40007200 -0.17663400
H -4.05791600 -3.62289500 0.16204000
C -6.32793300 -1.11873200 -0.41117700
H -5.88800500 0.99248600 -0.68313500
H -6.49241100 -3.25300500 -0.12179200
H -7.40708800 -0.98795900 -0.53243500
N -2.23285200 -1.32750300 0.00881400
N -3.05019000 0.65026000 -0.37325700
N 2.32162900 -1.26151100 0.08623600
N 3.10187300 0.74547600 -0.20967900
C 3.22600200 2.16871200 -0.40523800
H 4.08721500 2.54054600 0.17373900
H 3.38035800 2.40037200 -1.47342600
H 2.31661700 2.65357100 -0.03376400
C -3.21000200 2.05708200 -0.63745600
H -3.71248300 2.19715700 -1.60999300
H -3.80967400 2.52941400 0.15776600
H -2.22015900 2.52033400 -0.66689500
Co 0.02081100 0.38042300 -0.13556000
H 0.21660700 3.88836700 -0.98141700
C 0.35479200 3.75386000 2.42251800

C -1.16486700 3.61047400 2.31034700
H 0.72087100 3.50812200 3.43686300
H 0.71528100 4.76346800 2.16213500
H -1.67266900 3.61763200 3.28956500
H -1.61357200 4.40671400 1.68573600
B -0.15246600 1.93751000 1.12825900
O 0.86496300 2.80605500 1.49970100
O -1.35362300 2.35578100 1.67816700
N 0.04781700 1.84605100 -1.26598800
C 0.14818000 3.02092600 -1.68597000
C 0.20203100 3.40135100 -3.14196600
H -0.62872600 4.08617300 -3.39807400
H 1.14223800 3.93997700 -3.36735800
H 0.13895900 2.50335600 -3.77822400
¹³K_{Dipp}
C 0.94893100 -0.11003300 -1.39709700
C 1.39774200 -1.37009800 -1.78951100
C 2.51355200 -1.53472700 -2.61451200
C 3.17104400 -0.38011500 -3.06514700
C 2.73278900 0.90683000 -2.72000400
C 1.62428800 1.01294100 -1.87790500
H 2.86791400 -2.51474300 -2.93825500
H 4.04531700 -0.48798700 -3.71252900
H 3.24230600 1.78141500 -3.12691600
C 1.33203500 3.51536900 -1.35729800
C -0.23815000 1.94991000 -0.79938500
C 0.29399300 4.14791900 -0.64860300
C 2.45103900 4.23525900 -1.77854100
C 0.34427100 5.49958400 -0.32172900
C 2.49360600 5.59296100 -1.46581600
H 3.27444800 3.75975300 -2.31072300
C 1.46136500 6.21594900 -0.74741600
H -0.45743900 5.96964700 0.25130300
H 3.35650000 6.18486400 -1.78451900
H 1.53492400 7.28205400 -0.51518200
C 0.54198700 -3.73830400 -1.30285500
C -0.64412600 -1.86708800 -0.72151200
C -0.66860200 -4.13706500 -0.71409400
C 1.48537500 -4.68468300 -1.70672600
C -0.98936500 -5.47911200 -0.52588700
C 1.16803200 -6.02755100 -1.51592000
H 2.43880700 -4.39442900 -2.14765600
C -0.05016900 -6.42091400 -0.93867900
H -1.93607800 -5.77289700 -0.06768800

H 1.88484800 -6.79302100 -1.82638500	H -5.87525400 -3.55423100 -0.96394700
H -0.26497700 -7.48525600 -0.80885200	H -4.42100600 -3.18156500 3.05362600
N 0.51182400 -2.35568700 -1.29865000	H -6.28775100 -3.54952700 1.47796900
N -1.36014100 -2.97186300 -0.38081900	C -2.97076300 4.45721000 -1.59629800
N 0.96779900 2.18102300 -1.42474400	C -3.03389000 5.96998100 -1.80941600
N -0.64664700 3.16246700 -0.35032000	C -4.15374300 3.76225100 -2.27434000
Co -0.76151000 0.08263600 -0.65993500	H -2.04836900 4.09191500 -2.07576300
C -5.41845000 0.85094300 1.29057600	H -2.16793400 6.48616200 -1.36162800
C -6.13706900 0.40014200 0.00392600	H -3.04415800 6.20445700 -2.88873600
H -5.51795400 1.95102400 1.38400600	H -3.95047800 6.39966600 -1.36685100
H -6.48479800 -0.64648700 0.12935600	H -4.16169100 2.67944000 -2.07073500
B -3.88941100 0.40929900 -0.32037200	H -5.11445000 4.17733300 -1.91999400
O -4.05769200 0.54803900 1.05743500	H -4.11192900 3.91162000 -3.36794700
O -5.12141200 0.41708000 -0.98077400	C -3.54162200 -3.27796700 -2.28944100
N -2.66982500 0.29968700 -0.94656500	C -4.49280600 -2.33274000 -3.02718400
C -2.05249800 0.07414300 -2.12063700	C -3.68022800 -4.70456000 -2.82628900
C -1.95253300 1.10215400 -3.21506100	H -2.51204400 -2.94580500 -2.49649700
H -1.83991700 2.12140700 -2.81767400	H -4.52765200 -1.33430600 -2.56143200
H -1.10266600 0.88080600 -3.88515900	H -4.17627800 -2.22312400 -4.07965700
H -2.87404000 1.07833800 -3.83126100	H -5.52363700 -2.73039400 -3.03821300
H -2.09740700 -0.94738100 -2.54110100	H -2.95150800 -5.39211000 -2.36561700
C -5.91818200 0.20373400 2.56036200	H -4.69322400 -5.10205900 -2.63431000
H -5.34434600 0.56686200 3.43070300	H -3.51469700 -4.71986000 -3.91846500
H -6.98246400 0.44597200 2.73009400	C -0.60075300 2.27870900 2.36280400
H -5.80915000 -0.89245900 2.50466500	C -0.82083000 0.77091800 2.21772700
C -7.30190100 1.27227600 -0.40235400	C -0.28631500 2.64468700 3.81051400
H -7.74201500 0.91614200 -1.34947200	H 0.28254500 2.54660600 1.75702500
H -8.09212200 1.25793300 0.36923200	H -1.27148600 0.51944300 1.23076900
H -6.97017600 2.31560000 -0.54751600	H 0.12102200 0.21350300 2.35610800
C -1.81077000 3.41899600 0.44314800	H -1.56151600 0.41753200 2.95122000
C -1.78124700 3.04197200 1.79803500	H -0.12256400 3.73012100 3.92858000
C -2.90546000 4.08928400 -0.12763600	H -1.09696700 2.34702000 4.49741700
C -2.89001700 3.35320100 2.58651000	H 0.62419800 2.12371900 4.15149400
C -3.98464000 4.39442900 0.70844800	C -1.77745500 -2.80712100 2.50349100
C -3.97784000 4.03558400 2.05082400	C -1.10921400 -4.14348200 2.84054000
H -2.90711500 3.06288700 3.63947200	C -2.21587000 -2.10877300 3.78945400
H -4.85098300 4.91704900 0.29287900	H -1.03106300 -2.16012500 2.01079100
H -4.83377100 4.28136500 2.68647300	H -0.68838600 -4.63641200 1.94987100
C -2.70199500 -3.02996100 0.12836500	H -0.29174400 -3.99911800 3.57019600
C -3.75175200 -3.22890900 -0.78807400	H -1.84152500 -4.83588200 3.29317500
C -2.91581900 -3.00186600 1.51951000	H -2.83697900 -1.22246500 3.58024300
C -5.04034100 -3.40606400 -0.27384200	H -2.79370200 -2.78421200 4.44469500
C -4.22039800 -3.19584900 1.98034800	H -1.33166000 -1.78283200 4.36537300
C -5.27352300 -3.40155300 1.09508800	K 3.84812200 -0.26259900 0.24845800

O 4.82386600 2.33127400 -0.14372800
O 2.53006600 -0.77408500 2.62043300
O 6.12655600 0.08861900 -1.32710800
C 4.52569600 3.17147600 0.94707700
C 6.14082500 2.42902100 -0.62420100
C 2.26354000 -2.10704600 2.97423000
C 2.79499600 0.05756800 3.71909100
C 7.19450800 -0.53714000 -0.66362200
C 6.33508000 1.41712800 -1.73149900
C 5.00680800 2.59555100 2.26592700
H 3.42916000 3.29282200 0.95278600
H 4.96249100 4.17890200 0.79864100
H 6.32934800 3.44258700 -1.03441700
H 6.87855000 2.26212500 0.18580000
C 2.03612200 -2.91204900 1.71403300
H 3.10704100 -2.51476500 3.56742700
H 1.35542900 -2.16971000 3.60846100
C 3.18462500 1.42884900 3.23599800
H 3.62128600 -0.36192400 4.32764300
H 1.90039100 0.14040500 4.36863400
C 6.90919400 -2.01458000 -0.59360200
H 8.14184900 -0.38481800 -1.21845800
H 7.33239600 -0.13331100 0.36033500
H 5.59991600 1.60967600 -2.52946000
H 7.34844800 1.54217200 -2.16244400
O 4.41720400 1.35153200 2.56518000
H 6.09600500 2.42246500 2.23746700
H 4.81355900 3.32459400 3.07748900
O 3.12545000 -2.86689400 0.82579900
H 1.79248600 -3.95694100 1.98294600
H 1.17587000 -2.49380200 1.16927300
H 2.38936900 1.83620500 2.57872300
H 3.26695900 2.09776800 4.11574900
O 5.78497500 -2.23954500 0.21720100
H 6.72628100 -2.39259700 -1.61935200
H 7.79612800 -2.54107500 -0.18575600
C 4.18292000 -3.73466900 1.14298000
C 5.29479600 -3.55328100 0.14474200
H 4.57460600 -3.53639900 2.16021400
H 3.84116600 -4.78878900 1.10740200
H 6.09556800 -4.28467000 0.37573800
H 4.92535500 -3.76748800 -0.87900000
¹³W_{Co}
C -0.00143200 -0.09848400 -0.66235300

C 1.21714800 -0.70972700 -1.04314300
C 1.26409800 -1.88245100 -1.83208200
C 0.01744500 -2.48275600 -2.17811300
C -1.23390800 -1.91057400 -1.82355500
C -1.20558100 -0.72914800 -1.03683600
H 2.19340600 -2.35106200 -2.15031400
H 0.02525300 -3.40632100 -2.76043000
H -2.15633500 -2.39908300 -2.13194100
C -3.65488800 -0.11120800 -0.63230700
C -1.91037700 1.13582200 0.19308300
C -4.17255900 0.97696400 0.09508400
C -4.50399400 -1.03570800 -1.23869000
C -5.54358600 1.18138400 0.22455100
C -5.87680300 -0.83248600 -1.10340700
H -4.12545700 -1.89192600 -1.79714400
C -6.38975900 0.25744700 -0.38705100
H -5.94473000 2.03149700 0.78095000
H -6.56647700 -1.54332200 -1.56720400
H -7.47266200 0.38619600 -0.30443300
C 3.65365900 -0.04864600 -0.64173400
C 1.88905300 1.16940500 0.18561600
C 4.15356500 1.04921200 0.08300400
C 4.51706000 -0.95961800 -1.24818400
C 5.52116200 1.27708500 0.20989600
C 5.88648900 -0.73288500 -1.11569300
H 4.15199300 -1.82334800 -1.80401500
C 6.38180100 0.36680700 -0.40195300
H 5.90891900 2.13465000 0.76429400
H 6.58740700 -1.43254300 -1.57960500
H 7.46248800 0.51423900 -0.32149000
N 2.27819800 0.06609700 -0.56060700
N 3.05309600 1.73996500 0.57369400
N -2.28182700 0.02700400 -0.55316700
N -3.08318900 1.68577500 0.58463100
C -3.20587300 2.88881200 1.36835800
H -3.18935600 3.77912000 0.71838500
H -4.14793100 2.85973200 1.93637600
H -2.37077400 2.93923900 2.07664500
C 3.15703400 2.94292000 1.36050000
H 4.10323400 2.93039500 1.92208700
H 3.11966200 3.83531200 0.71419400
H 2.32603600 2.97455000 2.07466100
Co -0.01265200 1.43228000 0.36798600
H -0.04984200 5.19879800 1.58279700

C -0.82804500 3.88869000 -2.55289900
C 0.67453800 4.20253900 -2.50576400
H -1.02315900 2.93704700 -3.08453700
H -1.42137400 4.68334700 -3.03636000
H 1.23660700 3.69878300 -3.31133500
H 0.87132100 5.28989800 -2.57777000
B -0.04103900 3.40614400 -0.51167300
O -1.20278600 3.75986300 -1.19831300
O 1.10080300 3.73274200 -1.24386800
N -0.02584500 3.24230600 0.95195900
C -0.03317800 4.12810300 1.86043900
C -0.02170200 3.81582800 3.31766100
H 0.85701300 4.27515600 3.80934600
H -0.91119700 4.24604200 3.81629300
H -0.00368800 2.72613900 3.48450200
W 0.02670000 -2.40457900 0.18400700
C 1.31855600 -2.19639000 1.65856800
O 2.10653400 -2.02026800 2.49140300
C -1.41435800 -2.47198900 1.52818600
O -2.29222300 -2.46643900 2.28633600
C 0.21365700 -4.35594400 0.38545400
O 0.32670600 -5.50865400 0.46154700

PhH

C -0.96030800 -1.01266900 -0.00000100
C 0.39697800 -1.33784000 0.00011300
C 1.35718000 -0.32528100 -0.00008500
C 0.96023000 1.01273800 0.00001800
C -0.39687400 1.33786700 0.00008000
C -1.35720700 0.32518700 -0.00008300
H -1.71322300 -1.80674100 -0.00007100
H 0.70802900 -2.38701800 0.00005700
H 2.42131000 -0.58031700 -0.00019400
H 1.71334100 1.80661300 -0.00001300
H -0.70816600 2.38696400 0.00004300
H -2.42128300 0.58048700 -0.00007700

³³

C 0.02230300 1.49052600 -0.05372800
C 1.22679600 2.14440700 0.17572400
C 1.26236700 3.49855000 0.51254000
C 0.03715000 4.16717700 0.64451900
C -1.19591100 3.51658500 0.49600200
C -1.17558500 2.16190900 0.16027000
H 2.19384400 4.03702600 0.69931300
H 0.04313100 5.22933000 0.90717500

H -2.12167800 4.06906700 0.66952700
C -3.62826000 1.39068700 -0.02751900
C -1.88184200 -0.07342900 -0.06322200
C -4.12684800 0.08588900 -0.21600800
C -4.49333900 2.48325200 0.01476300
C -5.48803900 -0.16725100 -0.35630700
C -5.85760000 2.22918000 -0.12610800
H -4.12740000 3.50219800 0.14495300
C -6.34936200 0.92828400 -0.30558500
H -5.86502100 -1.18195900 -0.50464800
H -6.55896000 3.06808100 -0.09808500
H -7.42632100 0.76981200 -0.41213000
C 3.66932000 1.34134400 0.00599700
C 1.90549100 -0.10217400 -0.02739200
C 4.15293000 0.02949700 -0.17189100
C 4.54656900 2.42448900 0.04125400
C 5.51147200 -0.23994700 -0.30830700
C 5.90799200 2.15392800 -0.09553700
H 4.19147600 3.44843500 0.16205600
C 6.38508400 0.84609000 -0.26433200
H 5.87734200 -1.25965800 -0.44994500
H 6.61879000 2.98503600 -0.07346700
H 7.46027400 0.67464200 -0.36865500
N 2.29408100 1.21745300 0.08902000
N 3.04654400 -0.80705500 -0.18132000
N -2.25465100 1.25000700 0.05890300
N -3.03048600 -0.76347400 -0.22892100
C -3.10989900 -2.19107700 -0.40403800
H -3.79519900 -2.62677500 0.34304400
H -3.47287600 -2.43612700 -1.41670900
H -2.10235900 -2.60947600 -0.27075800
C 3.10976000 -2.23645000 -0.35057300
H 3.41653700 -2.49090600 -1.37945800
H 3.83402000 -2.66754200 0.36128300
H 2.11076600 -2.65178600 -0.15621500
Co 0.00826400 -0.42309500 -0.13934300
H 0.01668100 -3.44063700 -1.81048600
C -0.07117100 -3.06158800 3.16401800
C -0.22558000 -4.06074600 2.01330500
H 0.91199300 -3.14878200 3.66325300
H -0.85512400 -3.16526200 3.93322700
H 0.50398100 -4.88697700 2.05545900
H -1.24000600 -4.50046500 1.97718800
B -0.05726100 -1.94045900 1.17669400

O -0.16965900 -1.78817300 2.54409400
O -0.01190900 -3.28749900 0.84090600
N 0.02101200 -1.38505900 -1.72366900
C 0.02581800 -2.46444400 -2.35541100
C 0.04385800 -2.57974300 -3.85863100
H 0.93483700 -3.14246100 -4.19696400
H -0.84208900 -3.13682800 -4.21882000
H 0.05274000 -1.57952900 -4.32226600
¹⁶W_{PMe}
C 0.24755100 -0.01859800 -0.98337300
C -0.64084200 1.01055200 -1.38498400
C -1.80477200 0.73905900 -2.14887800
C -2.12433900 -0.64492500 -2.36235600
C -1.27993600 -1.72065700 -1.94312700
C -0.10355400 -1.36296200 -1.22400300
H -2.46071800 1.51670100 -2.53724700
H -3.02674400 -0.89290000 -2.92785200
H -1.56301500 -2.75021000 -2.15732000
C 1.30689000 -3.50072400 -1.09557100
C 1.99115700 -1.54125800 -0.15298900
C 2.58109800 -3.68809300 -0.52552500
C 0.68042700 -4.54126800 -1.78398700
C 3.25265900 -4.90478400 -0.60341300
C 1.35618000 -5.75750100 -1.86912300
H -0.30012600 -4.41807500 -2.24387200
C 2.61870900 -5.94215900 -1.28550700
H 4.24074900 -5.03625100 -0.15581400
H 0.88774000 -6.58710300 -2.40671100
H 3.11648700 -6.91214000 -1.37327100
C -0.45172000 3.56365500 -1.27734400
C 1.15259800 2.19380200 -0.40961100
C 0.55946700 4.35536100 -0.69795700
C -1.55866700 4.15978300 -1.88464500
C 0.49789800 5.74631300 -0.70064800
C -1.61870500 5.55253500 -1.88886500
H -2.35332500 3.56886800 -2.34076900
C -0.61041400 6.33576400 -1.30657400
H 1.28875400 6.35001300 -0.24906700
H -2.47477700 6.04477700 -2.35945000
H -0.69387500 7.42604700 -1.33091100
N -0.05835000 2.26007300 -1.06494600
N 1.50007300 3.48111800 -0.17830400
N 0.96233200 -2.19714400 -0.79811600
N 2.94307600 -2.47878300 0.04234100
C 4.20607400 -2.24761000 0.69476900
H 4.21093600 -1.19547800 1.01690200
H 4.30963500 -2.91084100 1.57079100
H 5.03751500 -2.43726400 -0.00485500
C 2.66519800 3.90707400 0.55550400
H 3.11679900 3.00595300 0.99763800
H 3.38520700 4.41034800 -0.11174500
H 2.36548200 4.60454400 1.35614100
Co 1.82093800 0.39950800 -0.08191100
H 4.95833100 0.35132200 -0.50695100
C 2.22032600 0.39771000 4.20999900
C 3.71432100 0.57592000 4.50388800
H 1.63989500 1.29572000 4.50753900
H 1.78221400 -0.47521200 4.72627500
H 3.90772900 1.28865300 5.32570600
H 4.18514100 -0.39090700 4.77690300
B 3.36333600 0.73903800 2.26226700
O 2.16622000 0.22636100 2.81893300
O 4.25854100 1.05259100 3.29960000
N 3.48956200 0.85725800 0.89729200
C 4.64516800 1.21377100 0.12493300
C 5.86844600 1.69926600 0.89370500
H 6.24280300 0.93181000 1.59161200
H 6.68231100 1.95559800 0.19004900
H 5.63904200 2.59538200 1.49651100
B 2.30051200 0.36681700 -1.90707800
O 2.79628100 -0.74930700 -2.57237000
O 2.25439700 1.45285300 -2.77357100
C 3.15873700 -0.38068100 -3.88757900
C 2.52144100 0.99854900 -4.08534300
H 4.26190400 -0.34312100 -3.96720100
H 2.78782700 -1.13259300 -4.60497800
H 3.18476300 1.71078200 -4.60532700
H 1.57147900 0.93629600 -4.64963800
H 4.37274500 1.99615700 -0.61602700
W -1.91974900 -0.41408100 -0.13281000
P -2.13777600 1.27580800 1.63297200
P -4.33674200 -0.64073700 -0.16652400
P -1.74969800 -2.15086200 1.57417500
C -0.62019900 2.13957300 2.24308500
H -0.81507100 2.64776600 3.20531400
H 0.20902600 1.42178500 2.35806200
H -0.31420700 2.90364600 1.51377800
C -3.16475100 2.75340300 1.21046700

H	-3.11139100	3.52763000	1.99817900	C	3.94488500	3.89410500	-1.02948200
H	-2.80779600	3.18636200	0.26222900	C	5.30934700	1.46207400	-0.44698500
H	-4.21919000	2.45703200	1.07860500	C	5.33387700	3.84269600	-0.94057600
C	-2.87767300	0.90448000	3.29157300	H	3.45134100	4.83439000	-1.26845100
H	-2.99981500	1.83176100	3.88064700	C	6.00959900	2.64660500	-0.65656400
H	-3.85997800	0.42188500	3.18387000	H	5.82167500	0.52184300	-0.23394600
H	-2.21402800	0.22632900	3.85319200	H	5.90838200	4.75899700	-1.10404100
C	-5.52036000	-0.42221500	1.24264900	H	7.10187400	2.64290100	-0.60126100
H	-5.26234000	-1.09521500	2.07433200	C	-4.01548400	2.11762800	-1.00091100
H	-5.48231000	0.61624200	1.61129700	C	-2.22231400	0.81429100	-0.44605900
H	-6.55595300	-0.63853000	0.92168200	C	-4.45699900	0.79196300	-0.85876400
C	-5.20019700	0.47090300	-1.36869300	C	-4.89701900	3.12704600	-1.39105900
H	-4.79796400	0.32560100	-2.38424500	C	-5.76792000	0.42592400	-1.14630000
H	-6.28968700	0.28517500	-1.39235400	C	-6.21891700	2.76546900	-1.64253700
H	-5.01951300	1.52044500	-1.08078800	H	-4.57300900	4.16020700	-1.51388600
C	-4.92432500	-2.28767900	-0.76739200	C	-6.64757200	1.43485600	-1.53147400
H	-6.00886300	-2.29985800	-0.98429400	H	-6.08391500	-0.61618500	-1.09526100
H	-4.36605100	-2.55976200	-1.67908700	H	-6.93137300	3.53639900	-1.94957000
H	-4.70786400	-3.05289200	-0.00210300	H	-7.68652700	1.18132700	-1.76042800
C	-3.08881400	-2.57704300	2.78261000	N	-2.65537000	2.07913800	-0.75518200
H	-3.95387200	-2.99444000	2.24001500	N	-3.34196700	0.03361200	-0.49969200
H	-2.73481900	-3.33758300	3.50272800	N	1.90088400	2.35493900	-0.84413600
H	-3.42207600	-1.69089800	3.34129900	N	2.95862000	0.52147200	-0.38054100
C	-1.47619700	-3.86892700	0.95756400	Co	-0.28856700	0.59708700	-0.32964600
H	-1.47975500	-4.60287600	1.78394500	H	-2.05722300	-0.18290000	2.08180200
H	-2.27286100	-4.13114600	0.24031200	C	1.43149000	-3.61848400	-0.35630500
H	-0.50958900	-3.93758200	0.44010700	C	0.64466400	-4.23935500	0.80602100
C	-0.33118200	-1.98176000	2.73936300	H	2.48751700	-3.52325900	-0.05597700
H	-0.52118400	-1.13136400	3.41497600	H	-0.25694000	-4.74958500	0.40677100
H	-0.17608600	-2.89380800	3.34553300	B	0.29814300	-1.98572200	0.74684300
H	0.58385800	-1.73912700	2.17569000	O	0.89600100	-2.30525200	-0.47155200
¹TS_{Dipp}				O	0.22756000	-3.12339300	1.55930900
C	-0.39142900	2.36153400	-0.94226300	N	-0.27680200	-0.75960100	1.12941100
C	-1.62478700	3.01606600	-0.96486900	C	-1.29218500	-0.96837800	2.16405800
C	-1.74465400	4.39402600	-1.12852700	C	-0.72809000	-0.97025500	3.57939800
C	-0.56828800	5.13818600	-1.27036500	H	-0.12123700	-0.07016400	3.77087600
C	0.69056400	4.53203200	-1.21328800	H	-1.53892200	-1.00312800	4.33144500
C	0.75224900	3.14772200	-1.03312600	H	-0.08388100	-1.84972900	3.73627400
H	-2.71010200	4.90188400	-1.12545800	B	-0.07276100	1.31545200	1.38361500
H	-0.63257500	6.22127100	-1.40900300	O	1.12821500	1.71940100	1.96268400
H	1.58074100	5.15431000	-1.29338700	O	-1.14178400	1.87087400	2.07475500
C	3.23699300	2.70779200	-0.81234200	C	0.86023600	2.75801200	2.88925100
C	1.69538300	1.01729000	-0.55227200	C	-0.65605000	2.65197300	3.15221900
C	3.91927700	1.52300100	-0.51745300	H	1.07364300	3.72290100	2.38656500

H -0.83431300 2.09733400 4.09517400
H -1.80785400 -1.93035500 2.00416900
C 1.36360500 -4.41248300 -1.63821000
H 1.89793900 -3.89971500 -2.45339400
H 1.84831200 -5.39373000 -1.48734800
H 0.32187000 -4.59106600 -1.95249100
C 1.43367800 -5.21162900 1.65256200
H 0.82331100 -5.56878700 2.49974300
H 1.73951300 -6.08998800 1.05691700
H 2.34085500 -4.73074400 2.05755700
C -1.37144800 3.98192400 3.20920500
H -2.45436400 3.83280100 3.35983300
H -0.98929600 4.59633700 4.04411200
H -1.22555600 4.53651300 2.26562300
C 1.72985800 2.63639100 4.11794100
H 2.79618600 2.70949700 3.84588900
H 1.50288900 3.44707900 4.83304600
H 1.56318900 1.66833600 4.62207200
C 3.47716900 -0.81427300 -0.28803200
C 3.91958900 -1.39956300 -1.49361300
C 3.77853500 -1.35902500 0.96975900
C 4.66288500 -2.57960900 -1.41090900
C 4.54136900 -2.53571000 0.99729100
C 4.98373200 -3.13713800 -0.17479900
H 5.02276900 -3.05867300 -2.32425500
H 4.80049700 -2.98280000 1.96041700
H 5.58218000 -4.05210000 -0.12771700
C -3.34369300 -1.39388700 -0.42198900
C -4.05475800 -2.04962800 0.60155000
C -2.63703900 -2.09790900 -1.42424900
C -3.97129900 -3.44725900 0.64949900
C -2.58405900 -3.48832200 -1.31974400
C -3.23081800 -4.15817300 -0.28356700
H -4.49739700 -3.98666100 1.44226500
H -2.03448800 -4.06550200 -2.06529900
H -3.16864000 -5.24859800 -0.21661000
C 3.36615900 -0.68201200 2.26204200
C 4.50439900 0.18143900 2.81292200
C 2.90144500 -1.67880600 3.32163100
H 2.52043600 -0.01457900 2.03683000
H 4.77257600 0.99944900 2.12448000
H 4.20562000 0.63595100 3.77399600
H 5.41194400 -0.42413500 2.99438000
H 2.11822800 -2.34821700 2.93090500

H 3.73401900 -2.29599000 3.70628700
H 2.47858700 -1.13423400 4.18349100
C -4.95059300 -1.34240800 1.60944700
C -4.51705200 -1.53026200 3.06482900
C -6.40044500 -1.82260200 1.46387800
H -4.92434100 -0.26244400 1.39752700
H -3.55693100 -1.04186000 3.27830100
H -5.27461000 -1.08851000 3.73665500
H -4.42269300 -2.59886800 3.32713200
H -6.75306700 -1.81020300 0.41989500
H -6.51266000 -2.85705900 1.83515400
H -7.07648100 -1.18202800 2.05746300
C 3.63205800 -0.73028400 -2.82680200
C 2.20384500 -1.00630500 -3.29702300
C 4.63823300 -1.07643300 -3.91880100
H 3.71251500 0.35688700 -2.65980700
H 1.47205900 -0.82554300 -2.49462000
H 1.95202500 -0.36329800 -4.15948100
H 2.09537800 -2.05746600 -3.61489800
H 5.67727100 -0.89384700 -3.59290600
H 4.55767600 -2.13026900 -4.24008600
H 4.44993200 -0.45226800 -4.80992000
C -2.02440300 -1.37595200 -2.61536400
C -3.11220400 -0.84692300 -3.55527000
C -1.03185000 -2.21525200 -3.40460900
H -1.46269800 -0.50295700 -2.22886700
H -3.82301300 -0.17219400 -3.05364400
H -2.65405600 -0.28763200 -4.39016100
H -3.68989500 -1.68641800 -3.98322400
H -0.23004200 -2.59016500 -2.75444000
H -1.52045600 -3.06866400 -3.90893200
H -0.57002700 -1.59442000 -4.19072300
¹²D_{Dipp}
C 0.04537600 -1.82001900 -1.19240100
C -1.14484100 -2.44614800 -1.57325300
C -1.15310000 -3.67319300 -2.23679900
C 0.07930800 -4.26887800 -2.53695300
C 1.29568900 -3.65513800 -2.20811100
C 1.25321800 -2.43069000 -1.54228300
H -2.07827100 -4.16776500 -2.53752100
H 0.09234600 -5.23005000 -3.05922000
H 2.23537500 -4.13417100 -2.48844800
C 3.68386100 -1.70085100 -1.19884000
C 1.89655300 -0.39786000 -0.58386200

C 4.17318800 -0.49473300 -0.66336300	C -3.63804900 3.94535000 1.43460400
C 4.56591000 -2.68640800 -1.64137500	H -3.78372600 4.72356500 -0.56915300
C 5.53453200 -0.22610400 -0.57110000	H -3.44524900 2.92235300 3.31880500
C 5.93337300 -2.42380600 -1.54044500	H -3.82014200 4.91819300 1.90228200
H 4.21300200 -3.63340400 -2.05044700	C 3.17175500 1.56202500 0.26223600
C 6.41227600 -1.21479600 -1.01832800	C 3.12668300 1.69428000 1.65984900
H 5.89460200 0.72060700 -0.16126600	C 3.36962100 2.65817100 -0.59838600
H 6.64519100 -3.18204800 -1.87943700	C 3.26392100 2.98075000 2.19423900
H 7.49079800 -1.04273700 -0.95779700	C 3.50282900 3.92268000 -0.01668000
C -3.59438100 -1.75226000 -1.29935500	C 3.44962900 4.08331300 1.36607800
C -1.84621500 -0.42896300 -0.61855000	H 3.23378100 3.11922900 3.27865300
C -4.11813100 -0.56608800 -0.75289200	H 3.65731700 4.79795800 -0.65351200
C -4.44723100 -2.74117800 -1.78951700	H 3.56091800 5.08099900 1.80274900
C -5.48642900 -0.32550200 -0.68601400	C 3.40754100 2.47764400 -2.10527900
C -5.82109100 -2.50447700 -1.71935500	C 4.45091000 3.36161200 -2.78407700
H -4.06724400 -3.67101700 -2.21309500	C 2.02044300 2.68510900 -2.71901200
C -6.33480700 -1.31798300 -1.17896300	H 3.69272000 1.43227600 -2.30326100
H -5.87495300 0.60183400 -0.25868300	H 5.44723600 3.24034600 -2.32340700
H -6.51022600 -3.26556600 -2.09667600	H 4.53667400 3.09040100 -3.85095400
H -7.41741500 -1.16663500 -1.14068600	H 4.18353900 4.43279800 -2.74255900
N -2.22156400 -1.62547800 -1.20728900	H 1.28664900 1.97543600 -2.30235400
N -3.03145200 0.20276200 -0.35490300	H 1.65689800 3.71364900 -2.53676900
N 2.30728500 -1.59547600 -1.14708800	H 2.05854200 2.53152300 -3.81251300
N 3.06369400 0.26304600 -0.31017500	C 2.97766500 0.48739700 2.56311400
Co 0.02219500 -0.20567300 -0.26373700	C 1.95365400 0.71140800 3.67121200
H -0.01660800 -0.28767600 1.39052800	C 4.33445600 0.07297500 3.13672600
C 0.80125300 -3.50018200 2.19835000	H 2.60688500 -0.35075900 1.95489100
C -0.70378700 -3.63076400 1.88466000	H 0.99435100 1.05982100 3.25446600
H 0.94416700 -3.41753000 3.29558300	H 1.76115500 -0.23588800 4.20441000
H -0.83203600 -4.25549000 0.97749900	H 2.29684100 1.44905800 4.41952700
B 0.02623100 -1.58113400 1.22882200	H 5.05914300 -0.15195300 2.33526800
O 1.17580100 -2.26250900 1.61799000	H 4.76437400 0.87002100 3.77141600
O -1.10932000 -2.31129900 1.56904900	H 4.22679500 -0.83548600 3.75639400
N 0.00201700 1.68391500 -0.05235000	C -3.36420300 2.49871100 -2.08545500
C -0.00748300 2.81801000 0.16856500	C -2.18111000 3.26631500 -2.67736400
C -0.02949100 4.24023800 0.43249600	C -4.68778700 2.95165900 -2.70202400
H 0.52764500 4.78064200 -0.35041300	H -3.22342200 1.43904700 -2.34737100
H -1.07351800 4.59394100 0.44888600	H -1.22311800 2.86794300 -2.30365900
H 0.43949400 4.45115000 1.40761700	H -2.17541700 3.17146600 -3.77793400
C -3.19008200 1.48023400 0.25412700	H -2.23194700 4.34400400 -2.43538200
C -3.39004300 2.60031700 -0.57228100	H -5.53919200 2.38353800 -2.28900300
C -3.20701900 1.56470700 1.65806700	H -4.87718700 4.02567700 -2.52353300
C -3.61806000 3.83432000 0.04716100	H -4.67543800 2.79277700 -3.79495400
C -3.42668600 2.82229100 2.22996500	C -3.04088400 0.33174300 2.52298100

C -4.40158100 -0.18156800 2.99939000
C -2.09859900 0.56217000 3.70010000
H -2.58811600 -0.45797100 1.90577500
H -5.06861100 -0.40745300 2.14990100
H -4.27554500 -1.11082400 3.58382300
H -4.90803300 0.56157500 3.64296200
H -1.13753000 0.98284300 3.36149500
H -2.52788200 1.24351600 4.45729700
H -1.88370300 -0.39716200 4.20227200
C -1.54095900 -4.19648200 3.00759900
H -1.44402300 -3.57449700 3.91533100
H -2.60562000 -4.22339600 2.71829100
H -1.22517200 -5.22628900 3.25194400
C 1.65255400 -4.62854800 1.66339600
H 1.36516300 -5.58905100 2.12765000
H 1.53210700 -4.71476700 0.56933100
H 2.71862700 -4.44553400 1.88248500
'TS4
C -0.01016100 1.63077800 -0.36463800
C -1.21033600 2.33702500 -0.35896900
C -1.24582100 3.73201500 -0.36481500
C -0.02714800 4.42067900 -0.36788200
C 1.20052200 3.74786100 -0.35788300
C 1.18109500 2.35323900 -0.35590300
H -2.18049200 4.29427600 -0.36549900
H -0.03450300 5.51456800 -0.37215600
H 2.12932700 4.32007300 -0.34919300
C 3.64093100 1.61805400 -0.28760500
C 1.91224100 0.12590300 -0.28644100
C 4.16281700 0.31154500 -0.23423000
C 4.49333000 2.72257100 -0.29863200
C 5.53209900 0.06602400 -0.18928100
C 5.86543200 2.47697500 -0.25295800
H 4.11652700 3.74461100 -0.34134300
C 6.37924800 1.17313400 -0.19871000
H 5.92506800 -0.95257700 -0.14923600
H 6.55594500 3.32534000 -0.25976700
H 7.46199400 1.02197200 -0.16392100
C -3.65821800 1.58855300 -0.21465900
C -1.92614400 0.09892100 -0.30880900
C -4.17505200 0.28194700 -0.14089200
C -4.51194700 2.69160100 -0.17095500
C -5.53942100 0.03332800 -0.02045000
C -5.87896700 2.44354800 -0.05105100

H -4.14091100 3.71484500 -0.22573000
C -6.38749900 1.13873900 0.02350300
H -5.92860800 -0.98562800 0.04066700
H -6.56955600 3.29101400 -0.01342600
H -7.46627600 0.98550300 0.11901400
N -2.28915700 1.42936800 -0.32272900
N -3.09351200 -0.58109300 -0.21102400
N 2.26830000 1.45651600 -0.32273200
N 3.08000000 -0.55227000 -0.23771200
C 3.21148300 -1.98308400 -0.15079500
H 3.65517500 -2.38974600 -1.07633600
H 3.85163400 -2.24739500 0.70698300
H 2.20888100 -2.39828300 0.01011800
C -3.24450500 -2.01023700 -0.12207300
H -3.66174300 -2.28712200 0.86058300
H -3.91603200 -2.37325600 -0.91861600
H -2.25826600 -2.47194700 -0.23027700
Co 0.00179800 -0.21514900 -0.34090000
H -0.88511900 -2.87334200 2.14453100
C -0.24328500 -2.20951600 -3.22766900
C -0.29774400 -3.71615500 -2.95901600
H -1.24853200 -1.79046300 -3.42306200
H 0.41882300 -1.93710200 -4.06578600
H -1.14852800 -4.20856800 -3.45968200
H 0.63318000 -4.21854400 -3.28516900
B -0.03504200 -2.61463400 -0.99741300
O 0.26420100 -1.68224700 -2.01626300
O -0.42985300 -3.82493400 -1.55523100
N 0.00165400 -2.25471100 0.34254400
C -0.30149400 -3.29845300 1.31015500
C 0.93719100 -3.99183800 1.86350200
H 1.62655700 -3.26172700 2.31851000
H 0.65784600 -4.73625000 2.63236300
H 1.48244200 -4.52401700 1.06351600
B 0.05544100 -0.63089600 1.48782000
O 1.20116000 -0.66242200 2.29577000
O -1.08653800 -0.60094500 2.30305200
C 0.81000000 -0.76497200 3.64581900
C -0.68598100 -0.42633500 3.64259000
H 0.99746300 -1.79237000 4.01624700
H 1.40296200 -0.07029500 4.26657500
H -1.27495700 -1.08206900 4.30862700
H -0.86763200 0.62211500 3.94924200
H -0.95196600 -4.06833300 0.84993100

¹TS2_{Dipp}

C 0.00381000 -2.04166900 -1.16405200
C -1.18011900 -2.77307900 -1.25908700
C -1.18526700 -4.13355800 -1.56644600
C 0.04966200 -4.76327700 -1.77130800
C 1.26285800 -4.07158000 -1.65430200
C 1.21258400 -2.71286900 -1.34286300
H -2.10579300 -4.71508900 -1.63963500
H 0.06793800 -5.82916300 -2.01675800
H 2.20336500 -4.60696200 -1.79352500
C 3.64825700 -1.92092900 -1.19286700
C 1.88095000 -0.55997800 -0.68639300
C 4.14409700 -0.66004500 -0.81838600
C 4.51849600 -2.93883100 -1.58623700
C 5.50274800 -0.36321400 -0.85612900
C 5.88228200 -2.65031600 -1.59995000
H 4.15786200 -3.92282900 -1.88636000
C 6.36861600 -1.38263800 -1.24803900
H 5.86679000 0.63445300 -0.60248000
H 6.58635000 -3.42986000 -1.90481200
H 7.44410200 -1.18771900 -1.28753200
C -3.63773600 -2.07506100 -0.99919700
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14
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 H 1.38390800 3.32297900 4.40980800
 H -2.68756500 4.57048800 3.90631300
 H -0.73503900 4.17787800 5.36449500
 C -2.39382000 -2.82370400 1.53256800
 C -3.75404600 -2.80542900 1.89156200
 C -1.36964100 -3.02695100 2.47398500
 C -4.06448300 -2.94983600 3.24831900
 C -1.73092300 -3.15224400 3.81820600
 C -3.06704000 -3.11071100 4.20351300
 H -5.11202300 -2.94041400 3.56233100
 H -0.95766900 -3.29694900 4.57704000
 H -3.33399200 -3.21617000 5.25949800
 C 1.96041800 2.74268900 1.82998000
 C 2.42257800 1.44474700 2.48810900
 C 3.01905200 3.83749200 1.97255100
 H 1.82920700 2.53955600 0.75412000
 H 1.69380900 0.63907600 2.30949000
 H 3.41277900 1.13430300 2.10942900
 H 2.53072300 1.55720100 3.58131900
 H 2.70344800 4.77412600 1.48432300
 H 3.22696200 4.06081500 3.03410500
 H 3.96941400 3.52026500 1.50693400
 C 0.08275100 -3.08687600 2.04893500
 C 0.89460000 -4.13523000 2.80503700

C 0.72325400 -1.70649300 2.17071200
 H 0.10579100 -3.36437000 0.98172400
 H 0.43875200 -5.13770900 2.72476400
 H 1.91724400 -4.18152400 2.39191400
 H 0.99172900 -3.89089800 3.87765500
 H 0.17483600 -0.95862500 1.57069200
 H 0.71599500 -1.36001400 3.21980800
 H 1.77396400 -1.75725300 1.83770600
 C -4.86682400 -2.68889900 0.86754200
 C -5.88788300 -1.61490900 1.23640900
 C -5.56535600 -4.03534300 0.66289800
 H -4.41323500 -2.38024600 -0.08545800
 H -5.40287500 -0.63707400 1.38091900
 H -6.63230000 -1.51069800 0.42767800
 H -6.44260800 -1.86626800 2.15830400
 H -4.86174900 -4.82049300 0.34163400
 H -6.05446500 -4.37696800 1.59341300
 H -6.34533300 -3.94750400 -0.11477000
 C -2.90840700 4.20257100 1.20777100
 C -2.77815700 5.56325900 0.51526600
 C -4.24202900 4.14299900 1.94817000
 H -2.93220500 3.42736500 0.42566400
 H -1.88807900 5.62481600 -0.12984200
 H -3.66115400 5.74999800 -0.12202700
 H -2.71880300 6.38027100 1.25772700
 H -4.35194700 3.21640700 2.53525900
 H -4.37870300 5.00046600 2.63144500
 H -5.06981900 4.17823300 1.21972700
 C -5.67657400 2.90074800 -1.53636400
 H -5.26108200 3.91463200 -1.66554000
 H -6.57057100 2.81386600 -2.17899500
 H -5.99077700 2.78070000 -0.48505000
 C -5.54961900 -0.30959300 -2.97090700
 H -6.40026100 0.20886700 -3.44797000
 H -4.70899400 -0.34230000 -3.68638800
 H -5.85868900 -1.34613100 -2.75177100
¹TS4_{PMe}
 C 0.13815200 0.03751900 -0.77731700
 C -0.49808500 1.19580200 -1.25957100
 C -1.64823000 1.11139200 -2.09950600
 C -2.08413800 -0.16900200 -2.55048300
 C -1.44991200 -1.35587600 -2.05844600
 C -0.32668200 -1.23185400 -1.19960700
 H -2.15484800 1.99918400 -2.47525700
 H -2.92465800 -0.24366900 -3.24309900
 H -1.79179800 -2.32819600 -2.41221400
 C 0.61476000 -3.59528000 -0.92061900
 C 1.75339100 -1.74573500 -0.22421700
 C 1.85394200 -3.99826900 -0.38545300
 C -0.28276200 -4.53975100 -1.42217300
 C 2.22998100 -5.33807000 -0.33224500
 C 0.09271100 -5.88144700 -1.36511900
 H -1.24488000 -4.25297800 -1.84634600
 C 1.32733700 -6.27715500 -0.82912700
 H 3.19237000 -5.64172900 0.08639200
 H -0.59415800 -6.64127900 -1.74911700
 H 1.58669200 -7.33943500 -0.80106000
 C -0.00799500 3.69585800 -0.95383200
 C 1.34767200 2.07441400 -0.10411700
 C 1.00871300 4.30880500 -0.19421200
 C -0.96861300 4.47111200 -1.60581500
 C 1.08918500 5.69115300 -0.05052300
 C -0.88739500 5.85526100 -1.46334800
 H -1.75405100 4.02184600 -2.21324500
 C 0.12115500 6.45887700 -0.69670500
 H 1.88204500 6.15605300 0.54030700
 H -1.62827300 6.48422300 -1.96545900
 H 0.15261100 7.54871300 -0.60984600
 N 0.22249500 2.34143000 -0.84477400
 N 1.79320300 3.28717800 0.31254900
 N 0.59894400 -2.22202400 -0.80151100
 N 2.50879800 -2.84816400 0.01431800
 C 3.86884700 -2.85522700 0.48922900
 H 3.92282500 -3.22193500 1.52828400
 H 4.47551700 -3.50612500 -0.16146000
 H 4.25950400 -1.83233400 0.42605800
 C 2.88819900 3.51910100 1.21739500
 H 2.53984700 4.11060200 2.08135800
 H 3.26217200 2.55031900 1.56679400
 H 3.70615500 4.06120800 0.71480700
 Co 1.81556800 0.18682500 0.02777400
 H 4.68741300 1.99800800 -0.74359400
 C 2.91674000 -0.59683900 3.72761700
 C 4.36787400 -0.14765200 3.92610300
 H 2.20350700 0.14027000 4.14248900
 H 2.69997400 -1.57870200 4.18187000
 H 4.48947400 0.54407100 4.77771400
 H 5.04170800 -1.01162100 4.08895500

B 3.79552200 0.08738900 1.74111600
O 2.76594500 -0.66602600 2.32688200
O 4.70525300 0.49668300 2.71947400
N 3.86750900 0.42586000 0.39049000
C 4.99137400 1.28782100 0.04312200
C 6.20570200 0.49482200 -0.42605000
H 5.95062400 -0.16119000 -1.27478100
H 7.02591500 1.16904900 -0.73655700
H 6.58541500 -0.14713600 0.38924000
B 3.00489700 0.17601500 -1.41227700
O 3.58081600 -0.93297800 -2.05346200
O 3.16045900 1.30617400 -2.22564400
C 3.95155600 -0.56126400 -3.35953400
C 3.96965500 0.97082800 -3.33038400
H 4.93241400 -0.99762800 -3.61959000
H 3.20492600 -0.94465400 -4.08244100
H 4.99390800 1.36724000 -3.18238200
H 3.56010100 1.42300300 -4.25018500
H 5.30204600 1.89783600 0.91189600
W -2.13881500 -0.13818400 -0.24797800
P -3.65309500 1.65568200 0.41605400
P -3.83168800 -1.86332600 0.01767900
P -1.45663100 -0.40475000 2.07412000
C -4.62481700 -2.43242700 -1.55744900
H -3.87152300 -2.82825900 -2.25759400
H -5.38075100 -3.21791000 -1.37486100
H -5.11227300 -1.56581200 -2.03615900
C -5.39809300 -1.76483000 1.00860800
H -6.09535800 -1.05506100 0.53580500
H -5.88866200 -2.75453100 1.05238900
H -5.19835400 -1.42343500 2.03631400
C -3.24640600 -3.48983400 0.68262100
H -3.06890800 -3.39307000 1.76751800
H -3.98932800 -4.29323400 0.52216000
H -2.29379400 -3.77619300 0.21006400
C -5.15555300 1.48585600 1.49061600
H -5.52292300 2.48158800 1.79946500
H -5.95974400 0.97965000 0.93408900
H -4.93184600 0.89271800 2.38987000
C -4.49388000 2.55862100 -0.96901000
H -4.99298300 1.82271100 -1.62287400
H -5.24349600 3.27797400 -0.59199300
H -3.75746400 3.11294000 -1.57156200
C -2.89042100 3.09627900 1.29351000

H -1.93591300 3.36470500 0.81463500
H -3.55598600 3.97928800 1.28895100
H -2.68620300 2.81837100 2.34155000
C -2.65032500 -0.49211600 3.48755500
H -3.24303400 0.43637500 3.53607800
H -3.34484500 -1.33653400 3.34109900
H -2.13093100 -0.62720600 4.45419300
C -0.32254400 0.89240600 2.74568800
H -0.76367000 1.89472700 2.63135500
H -0.08628100 0.71902000 3.81139900
H 0.60882800 0.86530100 2.15607100
C -0.42791400 -1.88465400 2.48491200
H -0.20568500 -1.92948200 3.56693600
H -0.94402600 -2.81101700 2.18727000
H 0.52623600 -1.81905400 1.93858600
¹³W_{PMc}
C -0.39239200 0.61658300 -0.61628900
C 0.92793300 0.67181800 -1.12844200
C 1.36422000 -0.20661800 -2.15703500
C 0.45827100 -1.25990800 -2.52560100
C -0.86437400 -1.38839400 -1.99044200
C -1.25149700 -0.42842200 -1.00861100
H 2.33930000 -0.12797700 -2.63481000
H 0.77106000 -1.97156600 -3.29498200
H -1.52205500 -2.18244100 -2.34149200
C -3.79471000 -0.67071300 -0.69824200
C -2.57129200 0.88088900 0.42758600
C -4.66442000 0.12815500 0.07283600
C -4.30121700 -1.67862900 -1.51903900
C -6.04266500 -0.06338100 0.06149500
C -5.68334000 -1.86600800 -1.53485100
H -3.64870900 -2.30281400 -2.13026800
C -6.54203300 -1.07689500 -0.75607100
H -6.70601900 0.56001900 0.66600700
H -6.10479200 -2.64903900 -2.17187400
H -7.62050100 -1.25567200 -0.79307500
C 2.75926500 2.45355500 -0.85520800
C 0.76763200 2.57712100 0.23797400
C 2.72969100 3.63925300 -0.09110900
C 3.87915100 2.13002500 -1.62184100
C 3.80320600 4.52474800 -0.07002600
C 4.95349900 3.01932800 -1.60100100
H 3.92408900 1.21713400 -2.21659000
C 4.91938500 4.19659800 -0.83941800

H 3.77228800 5.43951700 0.52677800
H 5.84374200 2.78942800 -2.19363300
H 5.78238500 4.86858600 -0.84789500
N 1.55013400 1.83499900 -0.61765100
N 1.50257200 3.66645900 0.55203800
N -2.52181700 -0.20870600 -0.41660400
N -3.87395200 1.04726600 0.74103500
C -4.37586100 2.13028700 1.54553200
H -5.12029100 2.71041600 0.97385800
H -4.84121700 1.75043500 2.47160700
H -3.52088700 2.77284700 1.79988000
C 1.04704700 4.73288200 1.40464200
H 1.65008900 4.77965500 2.32807700
H 1.11575600 5.69787300 0.87409800
H 0.00029900 4.52331400 1.66480400
Co -0.96598700 1.88473400 0.61269200
H -1.75284900 3.71256900 3.80620800
C -2.67273000 3.10203800 -2.97330600
C -1.21114600 3.50430900 -3.19333400
H -3.06391000 2.44959700 -3.77263900
H -3.33961200 3.98145400 -2.89015800
H -0.69977700 2.82452700 -3.90111300
H -1.09709000 4.53727400 -3.56471200
B -1.43859100 2.59686600 -1.11148000
O -2.66272200 2.40308400 -1.74467000
O -0.61628700 3.37792000 -1.91743000
N -1.14020500 2.41286500 2.31801100
C -1.26429000 2.74516200 3.51782200
C -0.79122600 1.93682900 4.70297500
H -0.44075100 0.94332000 4.37822800
H 0.03684900 2.45294700 5.22720400
H -1.60475900 1.80689100 5.44216200
W 0.72529800 -1.44966400 -0.30192200
P -0.57970100 -2.70905600 1.31554000
P 2.04677100 -3.39326800 -0.86139200
P 2.34214100 -0.89724600 1.44459600
C 0.02219400 -4.21059200 2.22063200
C -2.13760000 -3.46412600 0.67460600
C -1.24683500 -1.73483400 2.73458400
C 1.10352400 -4.77821100 -1.64778000
C 3.09079900 -4.40175300 0.29150900
C 3.33196400 -3.11798200 -2.16788100
C 2.65089900 -1.96208700 2.93264200
C 2.17410600 0.71228100 2.34767900

C 4.09746400 -0.71287800 0.88829400
H -0.73575800 -4.56270400 2.94455300
H 0.20905500 -5.02008500 1.49413100
H 0.95856900 -4.00710700 2.76006900
H -1.89767100 -4.10427500 -0.19171300
H -2.64653200 -4.07160600 1.44533900
H -2.82900700 -2.67755400 0.34155400
H -1.67113100 -0.78940300 2.35657500
H -2.01507400 -2.29166200 3.30274400
H -0.42207000 -1.46993300 3.41751200
H 0.48506100 -4.37702800 -2.46845400
H 1.76692900 -5.56831400 -2.04650900
H 0.42305600 -5.22902400 -0.90488800
H 2.47190800 -4.81982100 1.10009300
H 3.58323700 -5.23416600 -0.24430500
H 3.87103800 -3.76992900 0.74669800
H 4.07978600 -2.39577500 -1.79841500
H 3.84545600 -4.05701900 -2.44481700
H 2.86955000 -2.69252400 -3.07356600
H 1.75044100 -1.98244700 3.56889400
H 2.89568200 -2.99417700 2.64111500
H 3.48751900 -1.55731800 3.53074000
H 1.11247900 0.96219200 2.50555000
H 2.70070400 0.67806100 3.31846000
H 2.62454200 1.52019400 1.75061400
H 4.74947400 -0.34901100 1.70426500
H 4.48761100 -1.67880300 0.52664000
H 4.13607200 0.00672300 0.05455000
13K
C -0.00460400 1.26299100 -0.92271800
C 1.19893900 1.17992400 -1.62538900
C 1.21683700 1.02781000 -3.01180100
C -0.01051500 0.98631800 -3.68525300
C -1.23523600 1.08950900 -3.01177300
C -1.21158900 1.22426300 -1.62319300
H 2.14597900 0.94859400 -3.57720600
H -0.01308800 0.88096000 -4.77383800
H -2.16663400 1.07732200 -3.57974400
C -3.65228700 1.29503800 -0.84079900
C -1.89520800 1.51023300 0.59519000
C -4.14858300 1.43251500 0.46864300
C -4.52131200 1.12870700 -1.91782900
C -5.51234000 1.39861000 0.74402100
C -5.88844300 1.09661900 -1.64304800

H -4.16047900 1.02902200 -2.94195700
C -6.37793100 1.22787600 -0.33582800
H -5.89229700 1.49825100 1.76338900
H -6.59369400 0.96983300 -2.46925100
H -7.45665100 1.19851600 -0.15895100
C 3.64582400 1.28187100 -0.85710100
C 1.89543900 1.43889100 0.59637500
C 4.14803200 1.41643200 0.45046400
C 4.50886100 1.17001600 -1.94664100
C 5.51498200 1.41983300 0.71191200
C 5.87849300 1.18158000 -1.68492800
H 4.14038900 1.07816100 -2.96869500
C 6.37490800 1.29884100 -0.37893000
H 5.90221300 1.51211500 1.72926700
H 6.57998800 1.09880900 -2.51986600
H 7.45558600 1.30061700 -0.21180700
N 2.26825400 1.26980800 -0.71940800
N 3.04882300 1.52520700 1.29266500
N -2.27530600 1.34633400 -0.71678400
N -3.04531600 1.57130200 1.30216000
C -3.13643700 1.78489800 2.72385900
H -4.02709700 2.39316100 2.94703400
H -3.20570200 0.82904800 3.27156800
H -2.24777200 2.33650000 3.05881600
C 3.14238200 1.72579600 2.71567500
H 3.19323300 0.76341900 3.25394700
H 4.04347900 2.31578800 2.94357300
H 2.26355500 2.29110700 3.05476500
Co 0.00107000 1.49773900 0.90655100
H 0.01382700 1.95776900 2.52376900
C -0.66066800 5.39421400 -0.43025400
C 0.83250400 5.23055800 -0.73416500
H -1.25070000 5.67946600 -1.31710400
H -0.84760900 6.14152500 0.36277200
H 1.02536800 5.11528000 -1.81671600
H 1.44484200 6.06889600 -0.36226700
B 0.04832000 3.33900900 0.26223500
O -1.07137500 4.11552200 0.02777900
O 1.19893300 4.03161500 -0.07097100
N -0.05379300 -0.16222800 2.09894700
C -0.02147100 0.76540100 2.91063400
C -0.01262500 0.82226100 4.40611700
H -0.04894200 -0.19756600 4.82204800
H 0.89704300 1.33041400 4.77187800
H -0.87687500 1.39831600 4.78127400
K 0.06020600 -1.92550800 -0.00251100
O 1.00565300 -3.43909900 2.13654400
O 2.82402200 -2.08371200 0.39588100
O -1.06680700 -3.47791300 -2.09041500
O -2.65830600 -1.67533200 -0.44714600
O 1.66398900 -2.72912800 -2.11087300
O -1.81110900 -3.51647900 1.49102000
C 2.21229300 -2.86384000 2.55845600
C 0.01230500 -3.46973500 3.12787400
C 3.21659000 -2.93837800 1.43882100
C 3.56503900 -2.22038700 -0.79298600
C -2.47116200 -3.41184300 -2.12839000
C -0.39884500 -3.05142800 -3.24993200
C -3.00888500 -2.04106900 -1.75971200
C -3.50399900 -2.16058100 0.56746800
C 2.94216300 -3.19482200 -1.76511500
C 1.04975800 -3.45219900 -3.14400400
C -1.20840900 -4.17210400 2.57584600
C -2.69481500 -2.46872400 1.80266300
H 2.61849800 -3.41196900 3.43399000
H -0.23260700 -2.43865900 3.45206600
H 0.36767600 -4.03559300 4.01518600
H 3.28785800 -3.98827600 1.09153200
H 4.21158500 -2.63795200 1.82633300
H 4.60729900 -2.52393700 -0.57793000
H 3.59997200 -1.22579600 -1.26234100
H -2.83064800 -4.16405100 -1.40644600
H -2.84798000 -3.70028900 -3.13085200
H -0.47173300 -1.95260800 -3.38759900
H -0.83261400 -3.53695900 -4.14779900
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H -4.28106900 -1.40748000 0.80609000
H -4.01403600 -3.08742200 0.24511500
H 2.87441000 -4.21341600 -1.32902900
H 3.59314300 -3.25878600 -2.66181300
H 1.10801700 -4.54104000 -2.94309000
H 1.55532700 -3.25333600 -4.11135700
H -1.93940300 -4.32363800 3.39546900
H -0.90446500 -5.16470600 2.20268000
H -2.14504100 -1.56539100 2.13616000
H -3.38904800 -2.77119100 2.61365900
H 2.05649100 -1.80607800 2.85257200

¹TS3K_{Dipp}

C -0.30212000 -0.46348100 -1.16996700
C 0.76201500 0.30517300 -1.63100900
C 1.73223900 -0.24070800 -2.47443200
C 1.59174400 -1.58491800 -2.85335900
C 0.52822700 -2.38055000 -2.40782700
C -0.41183100 -1.79674300 -1.55373800
H 2.58359400 0.33408100 -2.84225600
H 2.34398800 -2.02339000 -3.51375100
H 0.45659900 -3.41678600 -2.74027700
C -2.02656100 -3.66326400 -0.89235300
C -2.28373100 -1.50868300 -0.16045400
C -3.14499400 -3.60375900 -0.04680800
C -1.62916100 -4.87433500 -1.46044600
C -3.88996100 -4.73380100 0.27384600
C -2.37825400 -6.00797400 -1.14650500
H -0.76972200 -4.94976500 -2.12629900
C -3.48748300 -5.94265600 -0.29118100
H -4.75095400 -4.66862000 0.94257300
H -2.09008800 -6.97064600 -1.57826800
H -4.04694400 -6.85436900 -0.06389600
C 1.38323500 2.76250800 -1.34379900
C -0.37110700 1.81348000 -0.21089100
C 0.79106100 3.73698800 -0.52868700
C 2.45234400 3.08834100 -2.17691000
C 1.28897900 5.03391900 -0.44879200
C 2.93818600 4.39369400 -2.12117300
H 2.89867400 2.36038300 -2.85223400
C 2.38098700 5.34762700 -1.25618700
H 0.83058000 5.77200900 0.21239100
H 3.77248200 4.67908100 -2.76874600
H 2.79512000 6.35949300 -1.22937200
N 0.66878200 1.60106100 -1.09885700
N -0.28530200 3.12961500 0.11614200
N -1.54359400 -2.36727900 -0.94981500
N -3.28094800 -2.27788000 0.35861300
Co -1.54488800 0.28174800 0.00537000
H -4.06099500 0.17327700 0.04166300
C -3.10098400 -0.45362500 -4.05324200
C -1.83663000 0.40048900 -4.27600400
H -3.93666800 -0.03276600 -4.64889400
H -0.94088300 -0.24054000 -4.14126600
B -2.69357100 0.83885500 -2.22546000
O -3.40475700 -0.26524200 -2.68054400

O -1.86591700 1.34334100 -3.22137700
N -2.83825300 1.52565700 -0.99241300
C -3.46797900 1.09517100 0.11197000
C -4.10377700 2.06364000 1.07413200
H -5.03077800 2.45153400 0.61037300
H -4.38890500 1.55299800 2.00908600
H -3.45721400 2.91732900 1.30874400
B -0.27085700 -0.53858700 1.19957800
O -0.34957300 -1.84896600 1.65114500
O 0.92486600 0.02388800 1.64697000
C 0.87514500 -2.23706700 2.24257300
C 1.59483300 -0.89802300 2.49765400
H 0.65673000 -2.75630300 3.19267000
H 2.64956800 -0.94951500 2.18162500
H -2.27511100 0.62910900 1.29673700
K 4.16064500 -0.93313100 -0.01350200
O 4.44010900 0.68405500 2.35694900
O 5.04467200 -3.54928800 0.35177200
O 4.45705800 1.71187200 -0.29251000
C 5.19052000 0.11769800 3.40398100
C 4.68888600 2.04617200 2.10709200
C 5.22101300 -4.39067800 -0.75763500
C 5.88162800 -3.85661000 1.43549600
C 5.68736600 2.12936600 -0.82167400
C 3.98650100 2.42778400 0.82503900
C 6.45001600 -0.54642300 2.88273100
H 4.54121100 -0.62231300 3.90391800
H 5.45465000 0.87864300 4.16296600
H 4.29139200 2.67138000 2.93156800
H 5.77734500 2.24303800 2.03857500
C 4.44724200 -3.82781200 -1.93136500
H 6.29998100 -4.47853000 -0.99709300
H 4.85173100 -5.41531000 -0.54705400
C 5.75655100 -2.78728600 2.48876800
H 6.93597700 -3.91121300 1.09744400
H 5.61234000 -4.83681900 1.87848700
C 5.93102000 1.40353800 -2.12040500
H 5.67618900 3.21953900 -1.02047800
H 6.52082800 1.91898200 -0.12159200
H 2.91730000 2.17821300 0.91700600
H 4.07440700 3.51817100 0.65676000
O 6.18270200 -1.56348000 1.94714300
H 7.07792000 0.19264800 2.35680700
H 7.04212900 -0.94393000 3.73197100

O 4.74223700 -2.48280100 -2.20960000
H 4.62818900 -4.46617100 -2.81991300
H 3.36692200 -3.85229200 -1.71139100
H 4.70736700 -2.73042300 2.84575800
H 6.38717600 -3.07370300 3.35408700
O 5.94774300 0.01962600 -1.88765000
H 5.13531400 1.65795700 -2.84896800
H 6.89774200 1.74367700 -2.54449000
C 6.03296900 -2.21190200 -2.69376400
C 6.11514100 -0.75031400 -3.04959200
H 6.80730500 -2.44340100 -1.93609100
H 6.24611900 -2.81517700 -3.59924400
H 7.10107000 -0.54847100 -3.51549200
H 5.32994900 -0.50272300 -3.79288300
C 1.55894500 -0.43561600 3.93684900
H 2.10649500 -1.14361700 4.58437200
H 2.02862500 0.55715300 4.02948800
H 0.51953100 -0.36923100 4.29910700
C 1.61716000 -3.16942000 1.30543100
H 1.77785900 -2.67708800 0.32886800
H 2.59349800 -3.47620900 1.71904800
H 1.02217000 -4.07910900 1.11600000
C -2.94129900 -1.91892500 -4.38331600
H -3.86591900 -2.47526400 -4.15241100
H -2.72248600 -2.05228500 -5.45768700
H -2.11481500 -2.35958100 -3.80044800
C -1.76534700 1.09046500 -5.61719500
H -0.84826800 1.70003600 -5.68816600
H -1.75217700 0.35240900 -6.43858300
H -2.63437500 1.75740400 -5.75663500
C -1.22711300 3.92370000 0.84347800
C -1.20438500 3.89979900 2.24984700
C -2.09249900 4.76208600 0.11127700
C -2.08182700 4.75202700 2.92696300
C -2.93343900 5.60952200 0.84115100
C -2.93119200 5.60680900 2.23061900
H -2.10170100 4.75317700 4.01900500
H -3.61853100 6.27332300 0.30622700
H -3.60581800 6.27100300 2.77937100
C -4.40523800 -1.87602700 1.15692600
C -5.62753000 -1.60287300 0.50430400
C -4.28764400 -1.85800400 2.55692100
C -6.72730600 -1.26829800 1.29869700
C -5.41746500 -1.50504500 3.30454600
C -6.62527000 -1.20956600 2.68536300
H -7.68516700 -1.04702500 0.82002300
H -5.34838400 -1.47606100 4.39608600
H -7.49869800 -0.93998100 3.28690500
C -3.01061300 -2.24450000 3.26916000
C -3.20837200 -3.50932700 4.10598200
C -2.46884800 -1.09349100 4.11482200
H -2.25130000 -2.46129300 2.50638500
H -3.57369900 -4.34842900 3.48811400
H -2.25104800 -3.82049000 4.56246000
H -3.93333700 -3.35301200 4.92537300
H -2.25843800 -0.21239400 3.48584800
H -3.17811200 -0.79091800 4.90665200
H -1.52886500 -1.39306600 4.61076700
C -5.77941100 -1.66683500 -1.00414300
C -6.45433500 -0.41991000 -1.57509600
C -6.53770000 -2.92650900 -1.42939000
H -4.77309800 -1.70568600 -1.44637200
H -5.94503400 0.50293800 -1.25234500
H -6.41937100 -0.44794900 -2.67759700
H -7.51615400 -0.35007100 -1.27827500
H -6.03415400 -3.84490100 -1.08499400
H -7.56662400 -2.92976800 -1.02547400
H -6.60844800 -2.97565200 -2.53104100
C -2.17133100 4.76592600 -1.40554600
C -1.62599400 6.06577900 -2.00139300
C -3.60102300 4.53061400 -1.89513400
H -1.57072800 3.92354000 -1.77909800
H -0.57300300 6.24196700 -1.72908300
H -1.68412800 6.02999100 -3.10392300
H -2.21559400 6.93768100 -1.66369700
H -4.01997900 3.61664600 -1.44856300
H -4.26309000 5.38470800 -1.66340400
H -3.59971800 4.39809200 -2.99152000
C -0.24187200 3.00563600 3.00681000
C -0.78194300 2.56071200 4.36231100
C 1.11598700 3.69517400 3.16695900
H -0.08169600 2.09813000 2.40404700
H -1.78548500 2.11096800 4.27009000
H -0.11233300 1.80475900 4.80480400
H -0.84463100 3.39608500 5.08207700
H 1.54842000 3.97607500 2.19151200
H 1.02334200 4.61614900 3.77103000
H 1.83051500 3.02390100 3.67755800

¹LCoW(PMe₃)₃

C -0.14222200 -1.08338300 -0.58201900
C -1.33523200 -0.50188200 -1.05188300
C -1.29367200 0.60178500 -1.95682500
C -0.03653400 0.99143600 -2.51179500
C 1.17698700 0.35112800 -2.08790800
C 1.10009300 -0.71369300 -1.15559800
H -2.19806800 1.10978300 -2.29674700
H 0.00251500 1.80102200 -3.24332000
H 2.12486000 0.65870400 -2.53266600
C 3.45860800 -1.68703000 -0.90373200
C 1.61639600 -2.72889800 -0.03518800
C 3.88036900 -2.84285500 -0.21057500
C 4.38926500 -0.87134600 -1.54898600
C 5.22235800 -3.20385100 -0.13293300
C 5.73527100 -1.23348500 -1.46903200
H 4.08522400 0.01564600 -2.10503900
C 6.14833000 -2.37723700 -0.77262100
H 5.53954800 -4.09881600 0.40812800
H 6.48314800 -0.60770700 -1.96476200
H 7.21196100 -2.62921100 -0.73169200
C -3.80193000 -1.19339100 -0.83745200
C -2.11822200 -2.37773400 0.15679100
C -4.36917500 -2.27800600 -0.13232500
C -4.61518300 -0.35287600 -1.60097900
C -5.73864000 -2.52545100 -0.13547000
C -5.98806200 -0.60296300 -1.60622000
H -4.20132400 0.46471400 -2.19187900
C -6.54597800 -1.66456700 -0.88087600
H -6.16424100 -3.36661400 0.41737300
H -6.64168000 0.04549200 -2.19706000
H -7.62705900 -1.82855900 -0.90808500
N -2.44633300 -1.26302900 -0.60018500
N -3.31818600 -2.95482100 0.45687400
N 2.08969800 -1.64678300 -0.76262300
N 2.73910300 -3.43449400 0.29627300
C 2.73481000 -4.63905200 1.07929400
H 3.20307300 -5.47076900 0.52391500
H 3.27593200 -4.49364100 2.03105400
H 1.68908200 -4.90148800 1.29963400
C -3.46986800 -4.14860600 1.24189700
H -4.05875000 -3.94850900 2.15441200
H -3.97061100 -4.94135000 0.65850300
H -2.46799000 -4.49845400 1.53288100

Co -0.24792600 -2.68031600 0.35361400
W 0.09508000 1.19213900 -0.22914600
P 0.56337900 0.71721400 2.10998400
P -1.60614200 2.77264900 0.42875000
P 1.76710400 2.93272500 -0.23509600
C 1.83916800 -0.57123200 2.46138900
H 2.79265600 -0.29692700 1.97831200
H 2.00460300 -0.70395500 3.54635400
H 1.49234300 -1.52485800 2.02653400
C -0.84394300 -0.01053500 3.06060500
H -1.20427400 -0.89018700 2.49752300
H -0.55181300 -0.32046500 4.08179500
H -1.67232500 0.71506300 3.12997600
C 1.14572000 1.97675500 3.33907600
H 0.47259000 2.84677000 3.35189600
H 1.19913100 1.55090000 4.35801000
H 2.15340300 2.32580700 3.05732000
C -3.32102600 2.10018800 0.58607100
H -3.32494900 1.27069800 1.31282700
H -4.04249300 2.87157100 0.91324000
H -3.65628500 1.69759900 -0.38064300
C -1.61834000 3.77764600 1.98731200
H -1.71882500 3.10361800 2.85483400
H -0.68341600 4.34739600 2.09802100
H -2.46857000 4.48427100 1.99797400
C -1.93202600 4.13264600 -0.78607400
H -2.07926600 3.69067300 -1.78608000
H -2.82212500 4.73379500 -0.52084000
H -1.05725600 4.80290200 -0.84437300
C 1.68673300 4.50125900 0.74919300
H 2.58631000 5.12370400 0.58773800
H 0.80103200 5.08730100 0.45166100
H 1.60569800 4.26955500 1.82247700
C 2.08593200 3.71244900 -1.88574400
H 1.15748600 4.18969000 -2.24390200
H 2.88597000 4.47396200 -1.83729300
H 2.37802600 2.94438400 -2.62046500
C 3.49407600 2.43690100 0.20738300
H 4.22875500 3.23473500 -0.00967200
H 3.54651900 2.19672500 1.28270100
H 3.77005900 1.52556500 -0.34696800

¹TS4K

C 0.22437800 0.77629700 -1.53407200
C -0.95802800 0.99251900 -2.24092800

C -1.03700500 0.80262800 -3.62192500
 C 0.11923100 0.39065700 -4.29628300
 C 1.33359900 0.19069700 -3.62714400
 C 1.36113500 0.39705300 -2.24794600
 H -1.94851600 1.00235000 -4.18759600
 H 0.07918600 0.24468500 -5.37947400
 H 2.22204400 -0.08590700 -4.19637500
 C 3.77974700 -0.04629100 -1.51989500
 C 2.20978100 0.81203500 -0.09980500
 C 4.37578800 0.18783600 -0.26677100
 C 4.51782900 -0.60262500 -2.56572900
 C 5.70907900 -0.12431800 -0.01560700
 C 5.85361500 -0.91454200 -2.31475200
 H 4.08208200 -0.79695200 -3.54595200
 C 6.44171400 -0.68081900 -1.06279200
 H 6.16194000 0.05528200 0.96210900
 H 6.45621700 -1.35040100 -3.11663900
 H 7.49312300 -0.93741100 -0.90588700
 C -3.30208200 1.71658600 -1.49912800
 C -1.51577800 1.70675800 -0.07489000
 C -3.72785500 2.15651900 -0.23252100
 C -4.21433900 1.58156400 -2.54620200
 C -5.05526700 2.48571100 0.02774600
 C -5.54543400 1.90625500 -2.28606000
 H -3.91425200 1.23540600 -3.53544100
 C -5.96168800 2.35374700 -1.02317200
 H -5.37337600 2.83545900 1.01262800
 H -6.28066100 1.81436800 -3.09059800
 H -7.01318000 2.60693200 -0.86136500
 N -1.95065100 1.46502500 -1.36020600
 N -2.61526900 2.12718200 0.59639800
 N 2.46315500 0.34872800 -1.37299000
 N 3.38899400 0.71318300 0.55500300
 C 3.64328200 1.16362600 1.90116000
 H 2.82397700 1.83089100 2.19715700
 H 3.71528600 0.31034200 2.59782400
 H 4.58691500 1.73155400 1.92331600
 C -2.66970600 2.52135500 1.98142200
 H -1.70054900 2.31271500 2.44644500
 H -2.88008200 3.60047800 2.06597500
 H -3.46009400 1.95837600 2.50614200
 Co 0.36426100 1.33079400 0.23199400
 H -0.09411600 4.54101600 1.79657500
 C 0.05001600 -0.66292300 3.32562700
 C 0.29853400 0.19996700 4.56271300
 H -1.02512000 -0.88368300 3.19080100
 H 0.61464500 -1.60795800 3.32713000
 H -0.47426300 0.06365600 5.33762500
 H 1.28465400 -0.01567200 5.01640600
 B 0.51872800 1.49387300 2.71511200
 O 0.50372000 0.15374500 2.24972900
 O 0.27904500 1.52718000 4.08143500
 N 0.67358500 2.58330700 1.86553700
 C 0.47175300 3.89100600 2.48419600
 C 1.77699500 4.56896600 2.87866400
 H 2.45147300 4.66766400 2.01236700
 H 1.58602400 5.57613500 3.29261100
 H 2.30316300 3.98197000 3.65251400
 B 0.93672400 3.09595700 -0.03134600
 O 2.25404100 3.51232000 -0.24344900
 O 0.05106300 4.10173700 -0.41890600
 C 2.22602000 4.73202600 -0.95550200
 C 0.79860400 5.25260200 -0.76085500
 H 2.99301400 5.42125800 -0.56220200
 H 2.44907100 4.54146100 -2.02277300
 H 0.74043100 5.99389000 0.06006100
 H 0.38125900 5.71592900 -1.67059200
 H -0.15258100 3.78737200 3.39128600
 K -0.54275400 -1.85367600 0.33185000
 O -0.98788100 -3.97656600 2.10961200
 O 1.61503300 -3.15364300 1.58584900
 O -1.15631600 -3.49056200 -1.90103100
 O -3.00231000 -1.47083700 -0.94463400
 O 1.48800800 -2.87298600 -1.17850300
 O -2.90139500 -1.96240100 1.84698900
 C 0.11904300 -4.59679800 2.70828000
 C -2.12188800 -3.92176200 2.93123400
 C 1.29761600 -4.50743300 1.77452800
 C 2.76314800 -2.88304400 0.81988900
 C -2.50024300 -3.40751500 -2.30575300
 C -0.22130300 -2.98619600 -2.82623600
 C -3.05938500 -1.99781100 -2.25098500
 C -4.18803900 -1.59202700 -0.20287300
 C 2.67117500 -3.36724700 -0.61190100
 C 1.16025400 -3.43101100 -2.42325900
 C -3.25394500 -3.28298600 2.17111100
 C -3.90727900 -1.19644500 1.22933700
 H -0.09598800 -5.66445300 2.91859200

H -1.90685100 -3.33896300 3.85075400	C 2.74216500 -2.55992900 -1.66368300
H -2.43344000 -4.93995900 3.24192200	C 2.01964400 -0.77006100 -0.41809400
H 1.03565100 -4.99811800 0.81645500	C 3.61791400 -2.38609000 -0.57653100
H 2.15278100 -5.05579700 2.21959000	C 2.93711200 -3.59803400 -2.57438800
H 3.66719100 -3.32225900 1.28887100	C 4.70932100 -3.22356700 -0.36991000
H 2.86784000 -1.78725200 0.83596800	C 4.02950400 -4.44185600 -2.36646300
H -3.06317200 -4.06581100 -1.62204400	H 2.27275400 -3.75333900 -3.42481800
H -2.62203800 -3.80909000 -3.33311100	C 4.90264900 -4.25862700 -1.28544300
H -0.25477500 -1.88111500 -2.87731100	H 5.38701000 -3.06665300 0.47215700
H -0.43263100 -3.37741900 -3.84190600	H 4.20899900 -5.26092700 -3.06868800
H -2.47056600 -1.32408200 -2.89575100	H 5.75210400 -4.93563100 -1.15865400
H -4.09737300 -1.99453600 -2.63412700	N 1.78711800 -1.56810300 -1.53001900
H -4.97173600 -0.91757600 -0.60417500	N 3.14921200 -1.29433700 0.14730500
H -4.58373500 -2.62599100 -0.25556400	N -1.53271600 1.51379700 -1.45666200
H 2.67725100 -4.47534400 -0.65674300	N -1.37662700 2.77057100 0.31403000
H 3.56430100 -3.01214200 -1.16431600	Co 0.86877000 0.74055500 -0.21200200
H 1.18812400 -4.53804100 -2.36147800	H 1.99333200 1.89804300 -0.54220800
H 1.88172700 -3.11296800 -3.20249700	C 1.55516200 2.88445600 -3.77048500
H -4.16507100 -3.29862900 2.80272000	C 2.38972700 1.60222900 -3.95356800
H -3.45940300 -3.88064200 1.26118100	H 2.22602100 3.76694100 -3.79122600
H -3.54146700 -0.15852000 1.24750100	H 1.76675300 0.83072700 -4.44914300
H -4.84964100 -1.24172700 1.81129300	B 1.69962700 1.75031200 -1.79856400
H 0.36413300 -4.10509300 3.67184300	O 1.03206000 2.77277200 -2.45360100
¹²K_{Dipp}	O 2.64529200 1.16611400 -2.62639100
C 0.07548900 -0.07677800 -1.68180100	N 1.29184700 1.12455800 1.60845600
C 0.68215800 -1.17761300 -2.29899100	C 1.63022500 1.44592300 2.66520700
C 0.20495500 -1.70078300 -3.49918000	C 2.06481300 1.84477500 3.98601900
C -0.90928600 -1.08642500 -4.08965100	H 1.23242900 1.76131100 4.70379800
C -1.56318800 -0.00092800 -3.48836000	H 2.89742000 1.19843300 4.30945400
C -1.06910100 0.47273200 -2.27243800	H 2.40798400 2.89216800 3.96731500
H 0.67779100 -2.54947100 -3.99541800	K -2.25189400 -1.78379900 0.10848700
H -1.27755700 -1.46299300 -5.04837300	O -3.12128400 -3.09478500 2.48015700
H -2.41413100 0.46256000 -3.99034600	O -0.51942600 -3.44249500 1.48083400
C -2.60877500 2.37960500 -1.52155400	O -3.95932200 -3.23957300 -1.63085000
C -0.74651400 1.74515800 -0.33530300	O -4.33203200 -0.35137300 -1.09307700
C -2.51283200 3.18553800 -0.37264800	O -1.31435900 -4.01822300 -1.15856000
C -3.66361600 2.54673200 -2.41738300	O -5.19546900 -1.84328200 1.04571700
C -3.45943300 4.16077100 -0.07367600	C -2.04903700 -3.49308400 3.29509700
C -4.60968200 3.53046700 -2.12638600	C -4.24011700 -2.60355900 3.16904700
H -3.75935300 1.93411900 -3.31394700	C -1.07069600 -4.27936300 2.46192700
C -4.51333000 4.32350100 -0.97379400	C 0.32476500 -4.07695000 0.54964900
H -3.37093300 4.77341400 0.82669800	C -5.06886800 -2.47750300 -2.04272100
H -5.44429400 3.68548700 -2.81615800	C -3.11708900 -3.67538200 -2.66776300
H -5.27271200 5.08625900 -0.77945500	C -4.73359000 -1.01541500 -2.27057500

C -5.37262600 0.11028300 -0.26217400
C -0.42035300 -4.87205800 -0.49948600
C -2.12121200 -4.65752600 -2.11047300
C -5.41910300 -2.57259800 2.22015400
C -5.23615600 -0.44700200 1.13701500
H -2.40847900 -4.14321400 4.11802000
H -4.03148400 -1.60082800 3.59636300
H -4.50143500 -3.26810400 4.01790200
H -1.60523200 -5.13539900 2.00635600
H -0.27521900 -4.68450200 3.11992600
H 1.05380700 -4.73743000 1.05856500
H 0.88236300 -3.26862800 0.05491000
H -5.81699300 -2.56954400 -1.23989900
H -5.50292800 -2.89932500 -2.97250500
H -2.57593000 -2.82961900 -3.13649500
H -3.70505800 -4.18589600 -3.45785100
H -3.89024100 -0.92451100 -2.97323700
H -5.60194900 -0.50247400 -2.72918900
H -5.34523800 1.21575800 -0.22160100
H -6.35424500 -0.18942600 -0.67139000
H -0.96848300 -5.72536800 -0.04953600
H 0.32231200 -5.29677100 -1.20630400
H -2.65942900 -5.50785600 -1.64412600
H -1.50513800 -5.05512300 -2.94276800
H -6.30816400 -2.19062800 2.76234900
H -5.63255500 -3.60298000 1.89154700
H -4.32259100 -0.04485600 1.61851100
H -6.10114900 -0.10608000 1.74281400
H -1.55014100 -2.61269100 3.74855800
C 3.87432700 -0.75909700 1.25518900
C 3.66916900 -1.30240700 2.53586800
C 4.83547900 0.23904300 1.00753000
C 4.46866700 -0.82897300 3.58194800
C 5.59889100 0.69006300 2.08970000
C 5.42672400 0.15650000 3.36298700
H 4.34236200 -1.24519500 4.58616400
H 6.35572200 1.46260300 1.92736300
H 6.04659900 0.51077700 4.19244500
C -0.93683000 3.38611900 1.52179500
C -0.00182100 4.43107300 1.45115000
C -1.49323300 2.94843600 2.73772700
C 0.38095000 5.03975000 2.65272700
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H 1.10350800 5.86054700 2.63274400
H -1.49126800 3.27224800 4.87390100
H 0.15544800 5.11737100 4.79556700
C -2.47167600 1.79026100 2.76863000
C -3.54016100 1.92761600 3.84841800
C -1.72125600 0.46172800 2.89500000
H -2.98859600 1.78001500 1.79398300
H -4.05783900 2.90060000 3.78604400
H -4.30047500 1.13424100 3.73507300
H -3.12109500 1.82961400 4.86516900
H -1.00343800 0.32592400 2.06824800
H -1.15873600 0.41495800 3.84509500
H -2.42890200 -0.38593000 2.89501400
C 0.55271300 4.91143200 0.12684100
C 2.07121000 5.06111800 0.15667500
C -0.12650000 6.21345900 -0.30301100
H 0.32574600 4.15116200 -0.63485700
H 2.55286800 4.13774400 0.51964500
H 2.45139300 5.25837700 -0.86063700
H 2.39840000 5.89766200 0.80039200
H -1.22054000 6.09052700 -0.38304700
H 0.07270300 7.02875100 0.41673100
H 0.24871800 6.53386600 -1.29150300
C 2.63629100 -2.37950200 2.80006300
C 1.60781900 -1.93941600 3.84136100
C 3.30088000 -3.69771200 3.19983500
H 2.08831100 -2.54821800 1.86233500
H 1.03364600 -1.06866400 3.48402000
H 0.89173000 -2.75523600 4.03869000
H 2.08179600 -1.67858600 4.80480600
H 4.01487200 -4.03880600 2.43077500
H 3.85169800 -3.60149700 4.15292700
H 2.54319200 -4.49110300 3.33318900
C 5.08342900 0.78431000 -0.38406100
C 6.36494300 0.19491000 -0.97755900
C 5.11679600 2.30983100 -0.41169200
H 4.24790300 0.47696900 -1.02906800
H 6.32752000 -0.90761800 -1.00905100
H 6.50703700 0.55618800 -2.01186200
H 7.25368300 0.48888800 -0.38939800
H 4.20323800 2.73455400 0.03624100
H 5.98973200 2.72041100 0.12725000
H 5.17380900 2.66485900 -1.45502100
C 3.67872200 1.78129000 -4.71845700

H 4.32060300 2.53640100 -4.23119400
H 4.23542300 0.82965500 -4.76299800
H 3.47643100 2.10899600 -5.75331600
C 0.44607700 3.06921300 -4.77824100
H 0.85830700 3.16815900 -5.79802500
H -0.24006900 2.20489300 -4.75663200
H -0.13297900 3.98087000 -4.55189200
¹TS2
C 0.00574700 -1.30842200 -0.36772700
C -1.19013800 -1.99607100 -0.17052100
C -1.21663500 -3.34843400 0.17030200
C 0.00953400 -4.00680500 0.33148900
C 1.23371500 -3.34298700 0.17782900
C 1.20344800 -1.99084600 -0.16376400
H -2.14774500 -3.89727400 0.32172700
H 0.01109700 -5.06828400 0.59619100
H 2.16624700 -3.88768400 0.33527100
C 3.65278300 -1.21156000 -0.26637300
C 1.89858200 0.20616600 -0.60315700
C 4.15188700 0.07904500 -0.53245100
C 4.52304900 -2.27443000 -0.02302800
C 5.51776400 0.34775000 -0.55359000
C 5.89083800 -2.00484900 -0.04661200
H 4.16008900 -3.28248000 0.17846400
C 6.38256700 -0.71705900 -0.30540000
H 5.89700000 1.35310600 -0.75092700
H 6.59543300 -2.81980500 0.14276800
H 7.46256400 -0.54407000 -0.31127900
C -3.64141400 -1.22373100 -0.27801800
C -1.89051000 0.19843900 -0.61254100
C -4.14336600 0.06614600 -0.54233700
C -4.50919800 -2.28861000 -0.03489900
C -5.50979300 0.33202800 -0.56203400
C -5.87759200 -2.02182500 -0.05686200
H -4.14383300 -3.29599000 0.16564100
C -6.37218700 -0.73482200 -0.31400300
H -5.89123800 1.33684600 -0.75788200
H -6.58032500 -2.83835200 0.13268300
H -7.45254100 -0.56401400 -0.31853100
N -2.26694000 -1.09932300 -0.33966100
N -3.04646100 0.88669300 -0.75230400
N 2.27794700 -1.09013200 -0.32790400
N 3.05301900 0.89682800 -0.74360500
C 3.14977100 2.30223100 -1.04381900

H 3.93710200 2.46626300 -1.79800700
H 2.18169700 2.63662600 -1.43895000
H 3.38811700 2.88070200 -0.13446500
C -3.14589200 2.29343100 -1.04435100
H -2.17689900 2.63288800 -1.43303900
H -3.93065600 2.46042900 -1.80059600
H -3.38944000 2.86527000 -0.13213600
Co 0.00186800 0.53847300 -0.62665600
H 0.01819300 3.67526400 1.04024700
C 0.71974200 1.28053700 3.32017000
C -0.79343200 1.52816800 3.25990200
H 0.96263000 0.33937400 3.84860000
H 1.27020500 2.10104700 3.81218300
H -1.35390800 0.93720100 4.00464200
H -1.04520300 2.59548800 3.41091000
B -0.01742900 0.99591200 1.18800300
O 1.11584500 1.17375400 1.96681500
O -1.16525300 1.13890000 1.95213900
N 0.00173900 2.36417300 -0.57481500
C 0.00667900 3.51276500 -0.06560300
C 0.00282000 4.79080800 -0.86227200
H -0.88253000 5.40694600 -0.61196200
H 0.89264200 5.40500200 -0.62331200
H -0.00443300 4.57586600 -1.94413200
¹³W_{Co}
C 0.00676800 0.18039600 -0.63741600
C 1.22270600 -0.37910000 -1.08135800
C 1.24715100 -1.43223800 -2.03056800
C -0.00636800 -1.94048200 -2.46942200
C -1.25513800 -1.40890000 -2.03884500
C -1.21763500 -0.36148600 -1.08617400
H 2.17071900 -1.86002400 -2.41680400
H -0.01148600 -2.76839900 -3.18154800
H -2.18373000 -1.81817500 -2.43307100
C -3.64986800 0.26166000 -0.53224400
C -1.85338600 1.40433900 0.29954400
C -4.10623900 1.31095600 0.28892900
C -4.54535600 -0.61495600 -1.13895700
C -5.46189200 1.52543100 0.51459500
C -5.90490700 -0.40027600 -0.91068400
H -4.21021500 -1.44770200 -1.75841200
C -6.35695600 0.65166700 -0.10254400
H -5.80990000 2.33947900 1.15461100
H -6.63252400 -1.07523400 -1.36993200

H -7.43093600 0.78574100 0.05448900
C 3.66337000 0.21503900 -0.53124200
C 1.88178700 1.38103400 0.29967000
C 4.13350000 1.26249600 0.28460800
C 4.54805800 -0.67220900 -1.13851800
C 5.49205200 1.46416100 0.50471200
C 5.91050000 -0.47006100 -0.91631000
H 4.20263300 -1.50319000 -1.75468100
C 6.37612000 0.57981000 -0.11312600
H 5.85036000 2.27693800 1.14067700
H 6.62966200 -1.15323600 -1.37672400
H 7.45198300 0.70396400 0.03908100
N 2.28226500 0.33362500 -0.51010200
N 3.01717500 1.93888900 0.76225200
N -2.26751800 0.36555800 -0.51501500
N -2.98129900 1.97308600 0.76655800
C -3.01144200 3.10246500 1.66251600
H -3.56683000 3.93839700 1.20448900
H -3.49108200 2.82148800 2.61529200
H -1.97293700 3.40485000 1.85678100
C 3.06204700 3.07086300 1.65422200
H 3.53322000 2.78625700 2.61015900
H 3.63307400 3.89587300 1.19549600
H 2.02789000 3.39111000 1.84331500
Co 0.01504800 1.58382300 0.52754800
H 0.01980500 2.36353600 4.27611400
C 0.11300400 4.68898200 -2.15559000
C -0.06602900 3.54577100 -3.16280900
H -0.63655100 5.48947300 -2.27540400
H 1.11744200 5.14733400 -2.22021300
H -1.06597300 3.55830400 -3.63461900
H 0.69102000 3.55598300 -3.96493900
B 0.01453900 2.70041600 -1.05330700
O -0.03853400 4.07215100 -0.88611000
O 0.06810800 2.36463600 -2.38943000
N 0.01735800 1.82772900 2.29333700
C 0.02034400 1.54795300 3.51365400
C 0.02197500 0.15010600 4.07013000
H 0.06767700 -0.58124000 3.24693200
H 0.88605400 -0.00532600 4.74330500
H -0.89152700 -0.03640300 4.66610900
W -0.02001700 -2.21783100 -0.12640800
C -0.09809500 -4.18209800 -0.25785600
O -0.14617400 -5.33448000 -0.38314200

C 1.35865400 -2.42308700 1.26698900
O 2.19593800 -2.49043200 2.06665600
C -1.36452700 -2.32735500 1.31065700
O -2.18091900 -2.33851200 2.13425900
¹⁶W_{Co}
C 0.08323600 -0.31547700 -0.80476400
C -1.10047700 -0.97024600 -1.18192800
C -1.08164300 -2.21412700 -1.86835900
C 0.18879000 -2.79806400 -2.11684000
C 1.41521400 -2.16032800 -1.76592500
C 1.32585700 -0.92672100 -1.07966700
H -1.98360500 -2.72947100 -2.19228600
H 0.22962600 -3.76370300 -2.62488600
H 2.36154300 -2.63366900 -2.02070300
C 3.73730000 -0.18370800 -0.64003100
C 1.93273200 1.14007000 -0.15007400
C 4.18678500 1.03956100 -0.11256100
C 4.63879700 -1.18698600 -0.99002500
C 5.54034500 1.31131400 0.05937600
C 5.99540700 -0.91664100 -0.81360000
H 4.31199700 -2.15449800 -1.37161700
C 6.44083400 0.31122400 -0.30369100
H 5.88179700 2.26615600 0.46514700
H 6.72711300 -1.68591700 -1.07581100
H 7.51362300 0.48501500 -0.18132300
C -3.57103200 -0.37079800 -0.92899400
C -1.89376700 1.04298600 -0.26506700
C -4.13811300 0.79491300 -0.38713300
C -4.37879400 -1.41096200 -1.38585700
C -5.51529700 0.97205800 -0.29848500
C -5.75885000 -1.23592700 -1.29564300
H -3.96482600 -2.33434200 -1.79056700
C -6.32014800 -0.06526400 -0.76567300
H -5.94655200 1.88328800 0.12197500
H -6.41760000 -2.03619900 -1.64432200
H -7.40797100 0.03345900 -0.71265800
N -2.20298300 -0.17556900 -0.84187500
N -3.08412200 1.61168200 0.00559700
N 2.35608700 -0.07487400 -0.66175700
N 3.05775100 1.79858400 0.17189100
C 3.10686100 3.12869100 0.72807000
H 2.07673200 3.39726200 1.00489500
H 3.75069500 3.13260300 1.62301400
H 3.50496600 3.83810800 -0.01642500

C -3.27916000 2.89912600 0.62767400
H -2.29471200 3.26630500 0.94191200
H -3.74250100 3.60207900 -0.08475300
H -3.92950900 2.79223400 1.51129700
Co 0.01703300 1.36864600 -0.02340600
H 0.71615800 4.74120600 -0.16707900
C -0.68667500 0.57763100 3.22775800
C -0.79038800 1.75931400 4.19662500
H -1.68498000 0.23150500 2.90112900
H -0.13569500 -0.28259300 3.63962800
H -1.70902300 1.72950000 4.80684100
H 0.07950300 1.79322600 4.88066800
B -0.26151400 2.54228900 2.13948500
O 0.01537800 1.13857200 2.13850800
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N -0.05309300 3.13475600 0.91967400
C -0.16361200 4.48108900 0.45707800
C -0.30711700 5.52036000 1.56114900
H 0.55643700 5.48745700 2.24947900
H -0.36798500 6.53944300 1.13714200
H -1.21204300 5.34363300 2.16802000
B 0.07988100 2.08693500 -1.78316600
O 1.03493900 3.00033300 -2.19340600
O -0.80736800 1.81530200 -2.81104600
C 0.67571600 3.48225400 -3.47664800
C -0.35679500 2.47130200 -3.98353700
H 0.24781500 4.49757300 -3.37708000
H 1.56982400 3.54665900 -4.11916800
H -1.20750900 2.94448100 -4.50202000
H 0.09251700 1.72631100 -4.66695200
H -1.02659500 4.58633900 -0.23973600
W 0.08698000 -2.52740400 0.21954100
C -1.42503700 -2.52515600 1.48319400
O -2.34534500 -2.48721000 2.18868200
C 1.28834400 -2.19303900 1.74935000
O 2.02061400 -1.95611600 2.61577700
C 0.29623500 -4.45552000 0.57879200
O 0.42559800 -5.59535400 0.74860900
'TSIK
C -0.04545300 -1.08058000 -1.00950700
C -1.23474800 -0.83081900 -1.69050900
C -1.23571700 -0.43635800 -3.02931300
C -0.00033000 -0.33510400 -3.68228100
C 1.21166700 -0.61648100 -3.03644800

C 1.16519000 -0.98551500 -1.69164700
H -2.15441400 -0.21791300 -3.57560900
H 0.01740300 -0.04445400 -4.73667500
H 2.14721600 -0.56093800 -3.59496700
C 3.59088900 -1.33970700 -0.93518300
C 1.81051600 -1.73915500 0.43092400
C 4.06551900 -1.78137500 0.31400100
C 4.47890800 -0.98471700 -1.94945300
C 5.42649700 -1.88190900 0.58867300
C 5.84241500 -1.08510000 -1.67518400
H 4.13358200 -0.63559100 -2.92277500
C 6.31085400 -1.52647000 -0.42892300
H 5.78936700 -2.21936300 1.56229700
H 6.56206500 -0.81377200 -2.45268600
H 7.38781700 -1.59211000 -0.25081900
C -3.69381900 -1.03629700 -0.97900300
C -1.96560200 -1.48212300 0.44325500
C -4.21594800 -1.44244700 0.26290000
C -4.54151400 -0.70077800 -2.03436300
C -5.58625500 -1.51201600 0.49467600
C -5.91483500 -0.77549400 -1.80359500
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H 3.22342900 -1.78220700 3.18091300
H 2.04397800 -3.04177800 2.66071600
C -3.24920300 -2.24910900 2.41526100
H -3.45226400 -1.45175900 3.15157000
H -4.06792300 -2.98556100 2.44435700
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Co -0.07921300 -1.65345800 0.76755300
H -0.13741100 -2.52946600 2.02895400
C 0.37033100 -5.45102200 -0.83967700
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O 0.85236700 -4.22357000 -0.31836500
O -1.41438700 -4.03248500 -0.33943200
N 0.09899800 -0.03260200 2.05897200
C -0.00733900 -1.03397900 2.72624800
C -0.05778000 -1.44588600 4.14919000
H 0.06332900 -0.56407800 4.80029600
H -1.02073700 -1.93183300 4.37738900
H 0.73726200 -2.17570400 4.37371800
K 0.03187900 1.96769000 0.13267100
O -0.59517400 3.25090200 2.53019800
O -2.65280100 2.21014100 0.85207000
O 1.02226700 3.86636300 -1.70893500
O 2.69780400 1.71218600 -0.66445700
O -1.71791400 3.16955700 -1.65066200
O 2.13733500 3.21639200 1.62526000
C -1.82030600 2.76465000 3.00732500
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H 0.61334700 -4.41559900 -3.30962300
H 0.28637600 -2.82919400 -4.06968800
H -0.28004300 -2.33324700 0.14440000
¹TS1_{Dipp}
C 0.01682800 -1.74534800 -1.41990400
C -1.17839500 -2.40908700 -1.69538500
C -1.18925800 -3.67229600 -2.28679500
C 0.04364100 -4.26536500 -2.58966100
C 1.26367200 -3.63878700 -2.30216200
C 1.22595600 -2.37708500 -1.70866500
H -2.11393600 -4.20511500 -2.51409300
H 0.05420400 -5.25357200 -3.05864200
H 2.19978300 -4.14587400 -2.54113400
C 3.66196500 -1.69640500 -1.27414500
C 1.89167800 -0.39270900 -0.65183300
C 4.15444100 -0.53192500 -0.65902300
C 4.53779400 -2.67879600 -1.73676700
C 5.51574200 -0.31425000 -0.47392500
C 5.90319800 -2.46206300 -1.55411900
H 4.18138100 -3.58631500 -2.22442200
C 6.38666200 -1.30216300 -0.93135000
H 5.87978500 0.59516000 0.00934600

H 6.61177000	-3.21762400	-1.90533900	C 3.45245700	2.86745800	2.26224000
H 7.46460400	-1.16890000	-0.80289400	C 3.40806300	3.90410600	0.08448100
C -3.62734800	-1.78819400	-1.24565000	C 3.52236800	4.00674000	1.46845300
C -1.88584400	-0.44041000	-0.63743500	H 3.54148600	2.95853200	3.34890700
C -4.14439100	-0.63368700	-0.63204100	H 3.45770100	4.80903800	-0.52630600
C -4.48141300	-2.79256600	-1.70153900	H 3.66341900	4.98801500	1.93210900
C -5.50990700	-0.44679700	-0.44360900	C 3.14215500	2.56222600	-2.04828800
C -5.85080500	-2.60728200	-1.51442800	C 4.53989800	2.46895100	-2.66760700
H -4.10545000	-3.69315500	-2.18727200	C 2.35591100	3.70693700	-2.68203900
C -6.35902500	-1.45662100	-0.89414500	H 2.59869100	1.63374700	-2.28321200
H -5.89354000	0.45606400	0.03675500	H 5.10637000	1.60539400	-2.28202500
H -6.54284500	-3.38050300	-1.86014600	H 4.46611400	2.35933500	-3.76442700
H -7.43933500	-1.34804900	-0.76239300	H 5.12592700	3.38228800	-2.45604400
N -2.25392700	-1.62033300	-1.24744000	H 1.36146000	3.81438600	-2.21998300
N -3.05385500	0.16507800	-0.29905100	H 2.89099700	4.67102100	-2.61045600
N 2.28475200	-1.56150000	-1.26826300	H 2.19918600	3.49893000	-3.75471900
N 3.04691300	0.23934000	-0.31816300	C 3.21665800	0.37017800	2.57067100
Co -0.00113800	-0.14033100	-0.47200400	C 2.06450900	0.45545000	3.56946100
H -0.01266300	0.76512400	0.76796200	C 4.55136000	0.12749700	3.27590800
C 0.81435100	-2.99921400	2.43942100	H 3.00756800	-0.49756500	1.92867800
C -0.68855900	-3.22597500	2.19561600	H 1.10360900	0.58051800	3.04460100
H 0.96590100	-2.57976300	3.45423600	H 2.00451400	-0.47275300	4.16464100
H -0.82323000	-4.09919500	1.52615900	H 2.18685700	1.29693700	4.27582700
B 0.02178700	-1.44895700	0.94498200	H 5.37837900	0.02921900	2.55148500
O 1.16936500	-1.99933800	1.49567400	H 4.80300400	0.95112100	3.96890800
O -1.09926600	-2.07023700	1.47940400	H 4.50898100	-0.80589600	3.86566200
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C -0.03371500	1.91196300	-0.35496900	C -2.48891600	3.56573400	-2.75433600
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H -0.07304300	4.01216900	-0.00323800	H -2.72373900	1.50091200	-2.30772300
H -0.94109200	3.01737800	1.21839300	H -1.48357500	3.66998900	-2.31591400
H 0.84225800	3.05209900	1.21194200	H -2.35804300	3.34384200	-3.82784800
C -3.20474700	1.46253700	0.27955200	H -3.01630300	4.53394800	-2.68228300
C -3.33867800	2.57227700	-0.57963000	H -5.23130900	1.46763400	-2.27843100
C -3.28381100	1.57708600	1.67790900	H -5.25655700	3.23960300	-2.49817400
C -3.57023600	3.81947100	0.00802900	H -4.60776900	2.18464700	-3.78627400
C -3.52394000	2.84769000	2.21466900	C -3.11807700	0.38248700	2.59489600
C -3.67117800	3.95702400	1.38966200	C -4.44042500	0.00793200	3.26495600
H -3.67595900	4.70155300	-0.62871900	C -2.02056300	0.62965900	3.62783000
H -3.59506800	2.96826500	3.29954100	H -2.79227700	-0.47440800	1.98676700
H -3.85873400	4.94245100	1.82727800	H -5.22080500	-0.21741900	2.51770000
C 3.16328200	1.52584200	0.29177800	H -4.31089100	-0.89016300	3.89554900
C 3.27428000	1.60198900	1.69073000	H -4.81405100	0.82333700	3.91141100
C 3.22880800	2.66471400	-0.53695500	H -1.07153400	0.89710800	3.13439700

H -2.28467600 1.44108000 4.32982100
H -1.84381300 -0.28141500 4.22499800
C -1.51589800 -3.42305800 3.44316400
H -1.39527100 -2.56975300 4.13296700
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H -1.21063500 -4.34405600 3.97077100
C 1.67750000 -4.22686600 2.26766400
H 1.39877100 -5.00670600 2.99872200
H 1.56271400 -4.64045500 1.25036500
H 2.74133900 -3.97650800 2.42088700
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C 0.92778300 0.06563500 -0.74212500
C 0.54039600 -1.18550900 -1.22737400
C -0.52361100 -1.33039500 -2.11976800
C -1.21837500 -0.17086100 -2.50480700
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C 0.16690100 1.18503000 -1.08748900
H -0.81144300 -2.29736400 -2.53598700
H -2.03603800 -0.25851000 -3.22806300
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C 1.85299600 2.05044800 0.29279000
C 1.30836100 4.23892100 0.47205800
C -0.75691700 4.37029900 -0.81695400
C 1.25462800 5.59035400 0.79998500
C -0.80923400 5.72601200 -0.48750200
H -1.55146300 3.90907700 -1.40398100
C 0.17942900 6.32801900 0.30316000
H 2.02153400 6.05552500 1.42371400
H -1.64395600 6.33054300 -0.85416600
H 0.10598800 7.39354000 0.53875800
C 1.43279200 -3.53940800 -0.72183400
C 2.44580900 -1.64139500 0.05985400
C 2.56672900 -3.90057100 0.03216800
C 0.60006000 -4.51292200 -1.27045500
C 2.90904500 -5.23261600 0.24587800
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H -0.29090200 -4.25057200 -1.84111400
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H 0.30783900 -6.63514300 -1.47316300
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N 1.40485800 -2.15730700 -0.69652200
N 3.15397500 -2.72222200 0.46609500

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H 3.09974900 3.79615900 2.63505700
H 3.94773300 2.54011000 1.68624200
C 4.35000500 -2.67669200 1.26500400
H 4.18231200 -3.16253200 2.23983500
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H 4.60830300 -1.62438300 1.43595400
Co 2.48990100 0.25389600 0.25797700
H 5.62064800 0.61744400 0.07405800
C 2.13041400 1.52297200 -4.09403200
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O -3.88162600 2.32115500 -0.61249500
O -4.90692900 -2.46577700 -0.46760600
O -2.71547300 1.55859100 1.72696700

C -0.95721700 -2.13380800 2.16825300	H -0.25705100 -5.05557500 -0.14365100
C -1.00835300 0.15371900 2.62003300	H -2.38772200 -3.79892700 -0.18614400
C -1.78177100 -3.28269900 1.65711700	C -3.83453100 -1.05411600 0.17966600
C -3.08699300 -3.95743600 -0.20196000	C -2.05133900 0.36545400 -0.02820700
C -6.01923500 1.41022800 -1.40550900	C -4.31725900 0.26898900 0.08213900
C -6.57109800 -0.83902500 -0.95879600	C -4.71743600 -2.12124200 0.33934200
C -4.80926000 2.28888200 -1.66370700	C -5.67858600 0.55665400 0.11957400
C -4.34819200 2.85147000 0.60142900	C -6.08336900 -1.83102800 0.37852600
C -4.53395400 -3.67769800 0.13835700	H -4.36240800 -3.14776600 0.43992000
C -6.16492100 -1.98895700 -0.07283500	C -6.55840400 -0.51817300 0.26565400
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C -3.21647900 2.86280800 1.59754400	H -6.79665100 -2.65118700 0.50251600
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H -0.43262800 -0.01500900 3.54819900	C 1.75312600 0.28560800 0.24198400
H -2.64552000 -3.44318300 2.33312100	C 3.98520300 0.07766800 0.60582400
H -1.16100200 -4.20064600 1.66882000	C 4.24916600 -2.33458800 0.83466300
H -2.81513900 -4.97919500 0.12614500	C 5.34602300 0.29941500 0.79783600
H -2.96638700 -3.91173600 -1.29796300	C 5.61424100 -2.11035600 1.03031700
H -6.72134800 1.88167700 -0.68789800	H 3.84100600 -3.34560100 0.86596700
H -6.56406300 1.29367600 -2.36389500	C 6.15614200 -0.81896400 1.00744200
H -6.70086500 -1.19029800 -2.00228900	H 5.76320900 1.30932200 0.78716500
H -7.54801800 -0.45635700 -0.60207300	H 6.27251400 -2.96603400 1.20710800
H -4.25296900 1.89916100 -2.53244200	H 7.23070300 -0.68231400 1.16031800
H -5.16242700 3.30996400 -1.91742600	N 2.08385700 -1.05683800 0.38894800
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H -5.16825500 -4.50953100 -0.23169400	C -3.25889200 2.51281000 -0.20324200
H -6.13830000 -1.66151800 0.98845300	H -3.92487500 2.78494300 -1.04049500
H -6.93554900 -2.78175200 -0.15902100	H -3.62105800 3.00498800 0.71726700
H -1.23692300 2.21643200 3.02674500	H -2.24086600 2.86437400 -0.42682700
H -2.52887400 1.19949700 3.74960200	C 3.07339200 2.37637300 0.28802200
H -2.41284800 3.54946600 1.26706100	H 3.41882400 2.80126900 1.24757200
H -3.61202900 3.23400900 2.56421000	H 3.78572500 2.64512800 -0.50946200
H -0.11596700 -1.92946500 1.47941900	H 2.08885800 2.79456800 0.03836300
³²	Co -0.14516900 0.67124100 0.20980400
C -0.20831500 -1.22548900 0.50836200	H 0.59049300 3.36811200 -2.31387100
C 0.98295300 -1.94563200 0.38472800	C 0.59397500 0.20949100 -3.59021400
C 0.99243800 -3.32514800 0.16859400	C 2.07632700 0.44137800 -3.23338300
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C -1.45485200 -3.26914700 0.02292400	H 0.44315400 -0.04410300 -4.65302200
C -1.40733600 -1.89113200 0.24092600	H 2.44209700 -0.27585900 -2.48015400
H 1.91741500 -3.89907200 0.07170800	H 2.74048700 0.39488100 -4.11382900

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 O -0.05143900 1.44721200 -3.30970300
 O 2.12529300 1.75530200 -2.68915800
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 C -0.28292300 2.95668900 2.31351000
 C -0.35271400 4.03132600 3.28232700
 H 0.43203000 3.90603000 4.04804800
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¹TS2W_{PMc}
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 C -1.53741200 -0.42478700 -2.50252300
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 C 0.95295000 4.39702300 -0.11396600
 C -1.02254100 4.32980600 -1.54187300
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 H -1.82372800 6.26455100 -2.02730400
 H -0.11946100 7.53538500 -0.75376900
 C 1.55756800 -3.43697100 -0.75603500
 C 2.12666600 -1.53032900 0.34817500
 C 2.67756600 -3.70084800 0.05879100
 C 1.04828200 -4.42570000 -1.60088200
 C 3.29418500 -4.94917300 0.07758100
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 H 4.16522900 -5.14301800 0.70799400
 H 1.28987700 -6.46341600 -2.23925100
 H 3.23073600 -6.92860400 -0.76922800
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 C -4.17918400 2.41490700 0.04263000
 C -5.50444800 0.00958100 0.58453500

H -4.87299800 -0.43511400 -2.38265900	C -1.99304700 0.62201000 -0.28675700
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H -4.11141500 1.13671700 -2.74672900	C -4.21203700 -2.01778000 -1.55430600
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H -5.16849300 2.81983400 -0.24147200	C -5.60494500 -1.96317300 -1.51907700
H -4.03385700 2.57751800 1.12379800	H -3.70748600 -2.88639700 -1.97723800
H -5.31237700 0.03064600 1.66948600	C -6.28591600 -0.86169000 -0.98199800
H -6.39290500 0.63206900 0.37016400	H -6.11686100 1.08887300 -0.03792400
H -5.73150100 -1.02998000 0.29545700	H -6.17734000 -2.80418200 -1.92039200
P -2.73219900 -2.46908800 0.48990500	H -7.37949600 -0.85743300 -0.97277700
C -3.85595400 -3.28047000 -0.73772000	N -2.17443800 -0.61122200 -0.89002800
C -3.72043500 -2.78484400 2.02715600	N -3.24309400 1.07309500 -0.05254800
C -1.51753400 -3.84161000 0.73140900	N 2.35242000 0.02441800 -0.81892700
H -3.36407100 -3.28354600 -1.72509100	N 2.87197300 1.93553500 0.05324500
H -4.10968200 -4.31929000 -0.45454500	C 2.81130100 3.24663300 0.64847000
H -4.79001600 -2.70101700 -0.83315000	H 1.75291200 3.47651000 0.82701700
H -4.57212200 -2.09216500 2.10333900	H 3.37165700 3.25420200 1.59873000
H -4.10375600 -3.82175800 2.04128600	H 3.24080100 3.99202700 -0.04084400
H -3.07391500 -2.64538300 2.91038200	C -3.59168300 2.34530500 0.52637200
H -0.72326600 -3.51035400 1.42092400	H -2.66683300 2.86140800 0.79429600
H -1.99731100 -4.75028300 1.13936400	H -4.14813900 2.95111800 -0.20703800
H -1.04290300 -4.10329500 -0.22522700	H -4.20748300 2.19564700 1.42865900
l¹TS4W_{CO}	Co -0.12307000 1.14342800 -0.05253200
C 0.11058100 -0.44163800 -0.94389800	H -0.33364500 4.91782000 -0.47140900
C -0.99029400 -1.27018700 -1.23815400	C -0.61093100 0.73319000 3.29314400
C -0.83459900 -2.54991800 -1.83593100	C -1.11536800 1.98297500 4.01923500
C 0.48890400 -2.99795500 -2.07936500	H -1.43700400 0.06596900 2.98981500
C 1.63410900 -2.19649000 -1.80050900	H 0.11665100 0.14631600 3.87474600
C 1.41240100 -0.93617800 -1.20066800	H -2.07459800 1.81868700 4.53723000
H -1.67494300 -3.19615500 -2.08015900	H -0.37864900 2.35089300 4.75773000
H 0.63583300 -3.98801300 -2.51554500	B -0.54483900 2.53710400 1.89628900
H 2.62730300 -2.57851000 -2.02761200	O 0.01712000 1.26659800 2.13965600
C 3.73618300 0.07401800 -0.86049200	O -1.28107500 2.95053600 2.99488400
C 1.81183500 1.16436500 -0.24993400	N -0.38110900 3.15012100 0.64717400
C 4.06566900 1.32111200 -0.30231500	C -0.76127600 4.54715600 0.47490600
C 4.73049700 -0.79613400 -1.30360500	C -0.26385400 5.46777500 1.58139500
C 5.38492600 1.74471200 -0.17734800	H 0.83639800 5.42415900 1.66869600
C 6.05350200 -0.37366400 -1.17523500	H -0.54240300 6.51223000 1.35127900
H 4.50303200 -1.77346300 -1.72954100	H -0.69679200 5.20541200 2.55957100
C 6.37760500 0.87424000 -0.62476200	B -0.30012500 2.62557500 -1.20658000
H 5.63140700 2.71646800 0.25642200	O 0.76746200 3.28598300 -1.82987700
H 6.85583300 -1.03653600 -1.51124600	O -1.49701600 2.95357300 -1.85847100
H 7.42755300 1.16869200 -0.54125700	C 0.29673700 3.89037600 -3.01239300
C -3.51508600 -0.92968600 -1.03052800	C -1.23018500 3.91103600 -2.85739300

H 0.72970400 4.90025200 -3.12445800
 H 0.60858200 3.28833400 -3.88819800
 H -1.60017100 4.90474800 -2.53704700
 H -1.75571200 3.64199800 -3.79053400
 H -1.86049200 4.66966700 0.37581600
 W 0.38997500 -2.56724500 0.24493000
 C -1.09819500 -2.63849300 1.53150400
 O -2.01162000 -2.63901800 2.24831700
 C 1.53940100 -1.95605300 1.72717200
 O 2.23330100 -1.55404500 2.56454300
 C 0.84400900 -4.41721800 0.75540500
 O 1.11644500 -5.51451600 1.01386800
¹⁵W_{PMc}
 C 0.55986000 -0.20866800 -0.48043400
 C -0.44014800 -1.04476800 -1.02616300
 C -1.27006500 -0.63454800 -2.11147400
 C -1.16290200 0.74042100 -2.51227400
 C -0.20252700 1.64705500 -1.94945300
 C 0.63358400 1.12730300 -0.91707500
 H -1.96438400 -1.30305300 -2.62006200
 H -1.78524600 1.09756800 -3.33800800
 H -0.12006400 2.66294900 -2.33259700
 C 2.46088400 2.90152800 -0.56766900
 C 2.54495800 0.84667400 0.42467200
 C 3.65910400 2.80035500 0.16866800
 C 2.17523800 4.05516500 -1.29756100
 C 4.58738400 3.83677400 0.20702900
 C 3.10942100 5.09097200 -1.26576600
 H 1.25045800 4.15958000 -1.86514600
 C 4.29516300 4.98807900 -0.52515200
 H 5.51038900 3.74984900 0.78544300
 H 2.90634600 6.00579200 -1.83024400
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 C -0.90073600 -3.54769500 -0.68975300
 C 0.82284400 -2.47352300 0.35486700
 C -0.22128700 -4.47107200 0.13230800
 C -1.99813500 -3.95070300 -1.45023700
 C -0.61847300 -5.80171500 0.22545800
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 C -1.71984700 -6.19745500 -0.53470600
 H -0.08885800 -6.50797600 0.86948600
 H -3.25344100 -5.62553900 -1.94476100
 H -2.06080900 -7.23573400 -0.48698600
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 H 4.50195000 0.00470000 1.83152300
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 H 1.22315200 -4.76798900 2.54173900
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 H 4.71864000 -2.46669000 0.36327300
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 C 1.56943900 -1.34250900 -4.01641200
 H 1.52846000 0.85689900 -3.82522900
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 H 0.47161300 -1.25436000 -4.04711900
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 C 1.87710500 0.02667200 4.60514400
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 H 1.43719200 0.93598400 5.05310900
 H 1.05877700 -1.87780000 5.37234900
 H -0.15818600 -0.80217000 4.62661300
 H 2.86170500 -1.45801200 1.77071000
 W -1.63161400 0.79595000 -0.33274700
 P -1.41607300 2.50667500 1.38851300
 C -0.54444300 1.98202400 2.92225100
 C -2.85498300 3.41959900 2.12398300
 C -0.40671100 3.99983700 0.98359300

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 H -3.61315400 2.72367700 2.51210600
 H -2.52576700 4.08146700 2.94642400
 H -3.32272400 4.04513400 1.34386500
 H -0.76798900 4.45264600 0.04462400
 H -0.45476500 4.75466100 1.78988800
 H 0.64451600 3.70979200 0.84668700
 P -3.73550200 1.68562400 -1.11116600
 C -4.56198200 0.71827900 -2.46193800
 C -3.59656700 3.33016000 -1.95152000
 C -5.26661500 2.01854300 -0.11478000
 H -4.84485100 -0.27749900 -2.08016700
 H -5.46858000 1.22924700 -2.83553200
 H -3.87102400 0.57035600 -3.30772200
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 H -3.27877400 4.08833400 -1.21530400
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 H -5.65914200 1.07347500 0.29545300
 P -2.86139500 -0.60568200 1.23392000
 C -4.18931200 -1.67203400 0.50649000
 C -3.85922900 0.08050600 2.63902000
 C -1.95054000 -1.91291200 2.17631600
 H -3.77142700 -2.24787100 -0.33418300
 H -4.60330900 -2.37657700 1.25191000
 H -5.00776300 -1.04308200 0.11909400
 H -4.56591700 0.83548100 2.26346600
 H -4.42835900 -0.71957000 3.14686900
 H -3.19808800 0.55926100 3.37993800
 H -0.94166200 -1.57468500 2.45859100
 H -2.50996900 -2.21656500 3.08012000
 H -1.83481600 -2.80595300 1.54227800
¹³Dipp
 C 0.00154000 -1.85843900 -1.27490800
 C -1.19578500 -2.48186300 -1.62758800
 C -1.20756600 -3.72510300 -2.25798400
 C 0.02560900 -4.33452900 -2.52764800
 C 1.24682100 -3.73564600 -2.18960500
 C 1.21087400 -2.49073400 -1.56222700
 H -2.13203000 -4.22437000 -2.55189900
 H 0.03543100 -5.30910700 -3.02433900
 H 2.18139300 -4.24396500 -2.43092700
 C 3.64179200 -1.83616700 -1.09225900
 C 1.88468700 -0.46772900 -0.56870300
 C 4.14357700 -0.65471200 -0.52048600
 C 4.50781500 -2.85278500 -1.49633300
 C 5.50736100 -0.43625800 -0.35269000
 C 5.87451500 -2.64169000 -1.31814700
 H 4.14376900 -3.78246000 -1.93391600
 C 6.36871900 -1.45345400 -0.75995900
 H 5.87815300 0.49247700 0.08676000
 H 6.57599200 -3.42300600 -1.62434200
 H 7.44800000 -1.32308900 -0.63991900
 C -3.64169400 -1.83806700 -1.22164400
 C -1.90463100 -0.46014100 -0.66052900
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 C -4.49350600 -2.86036100 -1.64032200
 C -5.52753600 -0.47301800 -0.46409300
 C -5.86329300 -2.66992700 -1.46012500
 H -4.11641100 -3.77931700 -2.08952400
 C -6.37438300 -1.49732100 -0.88453300
 H -5.91063100 0.44501900 -0.01246300
 H -6.55386900 -3.45673900 -1.77701200
 H -7.45536400 -1.38494300 -0.76149400
 N -2.26964200 -1.66216200 -1.23702400
 N -3.07447500 0.14039400 -0.32640500
 N 2.26847600 -1.67412500 -1.12276600
 N 3.04474500 0.14544800 -0.21921100
 Co -0.01633800 -0.18077600 -0.45636500
 H -0.06476800 2.80140500 1.51110900
 C 0.67331800 -2.94763400 2.54511500
 C -0.80926300 -3.22691000 2.23546900
 H 0.76092600 -2.45082200 3.53209400
 H -0.88685800 -4.15006100 1.62645700
 B -0.06469500 -1.52878600 0.90235600
 O 1.06334700 -2.01293700 1.54943400
 O -1.20261900 -2.13658200 1.41502600
 N -0.01265200 1.55531900 -0.11670100
 C -0.01941200 2.69367900 0.40052800
 C 0.02846000 4.01041300 -0.32657900
 H 0.08017800 3.86752000 -1.41567300
 H -0.86783100 4.61050200 -0.08423000
 H 0.91079300 4.58966500 0.00145200
 C -3.22628000 1.45811800 0.20180300
 C -3.49797200 2.50273500 -0.70078600

C -3.15033600	1.65463800	1.58811700	H 4.68444100	0.49850700	3.50499800
C -3.66542200	3.78571800	-0.17354100	H 3.62820500	-0.92893400	3.71697400
C -3.32082500	2.95830900	2.06670900	C -2.87380700	0.51735300	2.54854600
C -3.57366200	4.01376000	1.19708600	C -3.99362200	0.35687200	3.57616700
H -3.86584800	4.62356000	-0.84721900	C -1.51246500	0.70081700	3.21664100
H -3.25512000	3.14811300	3.14222000	H -2.81452800	-0.41510800	1.96791800
H -3.70281700	5.02674300	1.59088900	H -4.97310000	0.21216600	3.08675900
C 3.19713200	1.49087400	0.24061500	H -3.80265000	-0.52526100	4.21359200
C 3.06554500	1.77813800	1.61067600	H -4.07400600	1.23628500	4.24071600
C 3.52523100	2.46894900	-0.71417800	H -0.71692100	0.73158000	2.45444200
C 3.28084500	3.09994400	2.01174900	H -1.47158700	1.63316700	3.80885100
C 3.73248100	3.77582700	-0.26076000	H -1.30027500	-0.13917100	3.90079200
C 3.61594700	4.08760700	1.08879200	C -1.70410000	-3.35317800	3.44517700
H 3.18070000	3.36758300	3.06611500	H -2.75412800	-3.49031700	3.13519400
H 3.97948200	4.56370100	-0.97776300	H -1.41041700	-4.22500600	4.05631600
H 3.77889600	5.11551700	1.42759900	H -1.64324900	-2.44892400	4.07503100
C -3.57123500	2.26195600	-2.19682100	C 1.56739100	-4.16453500	2.50966700
C -2.26421200	2.67687400	-2.87475500	H 1.26386100	-4.89644400	3.27932000
C -4.77810300	2.93811200	-2.84371400	H 1.51447800	-4.65037500	1.51947400
H -3.68730100	1.17848900	-2.35475400	H 2.61626900	-3.87889400	2.69941600
H -1.40280400	2.16794300	-2.41076700	¹²W_{PMc}		
H -2.28773400	2.41937100	-3.94930000	C -0.63707600	0.28037900	-0.44146200
H -2.10349500	3.76690900	-2.78941100	C 0.37195200	1.08156100	-1.02657600
H -5.72079200	2.64595100	-2.34823400	C 1.16306000	0.64621700	-2.12729100
H -4.70396100	4.03977300	-2.81143800	C 0.99020800	-0.71295200	-2.54400500
H -4.85058600	2.64714400	-3.90666200	C -0.01278300	-1.56791300	-1.98649900
C 3.60381800	2.14759900	-2.19510300	C -0.81015700	-1.02518100	-0.93742600
C 4.85152900	2.72474500	-2.85993500	H 1.87698200	1.29276200	-2.63705600
C 2.32619000	2.59713900	-2.90681700	H 1.58330100	-1.08930900	-3.38198400
H 3.66238600	1.05374200	-2.30119500	H -0.15936600	-2.56928700	-2.38834100
H 5.77218600	2.40548400	-2.34049300	C -2.77648200	-2.66725100	-0.69307100
H 4.91724800	2.37842100	-3.90658600	C -2.71352000	-0.65696000	0.38357200
H 4.83817200	3.82901700	-2.88174000	C -3.98028800	-2.49377800	0.02077300
H 1.43647600	2.14809800	-2.43406300	C -2.57564400	-3.80679000	-1.47213500
H 2.21652300	3.69625200	-2.86893200	C -5.00095200	-3.43908800	-0.01854000
H 2.34914600	2.29375600	-3.96933500	C -3.59978600	-4.75354000	-1.51292500
C 2.70022900	0.69527600	2.60685000	H -1.65352600	-3.96500700	-2.03142800
C 1.99717600	1.23378300	3.84884500	C -4.79248200	-4.57729500	-0.79799100
C 3.92339800	-0.13265800	3.00995000	H -5.93231800	-3.29063000	0.53344300
H 2.00123400	0.01097300	2.10131500	H -3.46490500	-5.65370300	-2.11968000
H 1.16343200	1.90604500	3.58709600	H -5.57417800	-5.34032300	-0.85580400
H 1.58130000	0.39617900	4.43558200	C 0.87873600	3.59254900	-0.76703800
H 2.68782200	1.78392700	4.51382400	C -0.87577400	2.57711700	0.27804600
H 4.39733300	-0.62093300	2.14306700	C 0.17589900	4.55761700	-0.01526100

C 1.99714900 3.95564800 -1.51674200
C 0.56387500 5.89374900 0.00943500
C 2.38733800 5.29538200 -1.48947500
H 2.55319400 3.22645200 -2.10662600
C 1.68556700 6.24999800 -0.74025500
H 0.00960000 6.63493200 0.59050700
H 3.26175900 5.60487200 -2.06931200
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H -4.58609800 0.26341500 1.84855900
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H -2.53122100 3.75098200 1.81240700
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H -2.09894200 1.05232000 5.69585300
W 1.48297700 -0.83456000 -0.35601800
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C 3.74799900 -0.25630700 2.62073500
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H 4.70294200 0.16972000 -2.09399300
H 5.31289500 -1.34197100 -2.85308300
H 3.73054600 -0.65622400 -3.33816200
C 5.06652700 -2.15867600 -0.14590900
H 5.49221600 -1.22201300 0.25120600
H 4.81578100 -2.80994800 0.70566000
H 5.83946700 -2.65720100 -0.75975800
C 3.37199900 -3.40944100 -2.00593200
H 2.57953300 -3.32896300 -2.76974900
H 4.30818700 -3.74916400 -2.48803600
H 3.05038900 -4.16958600 -1.27305400
C 2.51671600 -3.57057800 2.07060300
H 2.11027500 -4.28645200 2.80889500
H 3.04864300 -4.14143200 1.28986100
H 3.24265500 -2.91644800 2.57575200
C 0.12635000 -4.02658000 0.75707400
H 0.55000100 -4.47342300 -0.15838800
H 0.07198200 -4.80120100 1.54404700
H -0.89549000 -3.68881100 0.53279000
C 0.21229600 -2.08606900 2.78488800
H -0.07257800 -2.94744900 3.41825200
H 0.81575500 -1.38154900 3.38176600
H -0.68892600 -1.55278400 2.44038200
¹H_{Dipp}
C -0.09984000 -0.06638000 -1.51616400
C 0.61266300 -0.99917100 -2.27907700
C 0.23088900 -1.32537600 -3.58016900
C -0.86909900 -0.65489500 -4.13452700
C -1.56671800 0.33669900 -3.42918500
C -1.16635600 0.61205100 -2.12170100
H 0.77829600 -2.04756900 -4.18802800
H -1.16731900 -0.88579000 -5.16131400
H -2.36241300 0.89724400 -3.92438100
C -2.67199800 2.51297300 -1.24952400

C -0.80011300 1.81124900 -0.15427300	C 0.38523300 -4.30826900 0.03330800
C -2.53069200 3.26943700 -0.06944700	C -5.07431700 -2.19084500 -2.00240800
C -3.75943700 2.71465100 -2.09812200	C -3.18854400 -3.32099600 -2.91230700
C -3.47462800 4.21776700 0.31206800	C -4.70035800 -0.72152700 -2.06600200
C -4.69590200 3.67896100 -1.72713100	C -5.09938800 0.19817800 0.10970800
H -3.88772200 2.13356400 -3.01180500	C -0.43579600 -4.90586900 -1.08840000
C -4.56127300 4.41468800 -0.53975800	C -2.20039400 -4.40239400 -2.56169200
H -3.36474100 4.77907900 1.24244300	C -5.14738700 -2.70413200 2.32503400
H -5.55825500 3.86077600 -2.37489400	C -4.86482900 -0.49966000 1.43017900
H -5.32058300 5.15670300 -0.27749500	H -2.16007300 -4.82277000 3.70765200
C 2.80026200 -2.27498300 -1.83869700	H -3.52162300 -2.03351700 3.61601900
C 1.97351200 -0.71851800 -0.38290700	H -4.15518700 -3.66682500 3.95206800
C 3.69102500 -2.15143500 -0.75631500	H -1.53045700 -5.50804000 1.41426200
C 3.06270100 -3.17107700 -2.87633300	H -0.12125600 -5.29220100 2.49992700
C 4.86624000 -2.89297300 -0.68266700	H 1.10392200 -5.06567300 0.39944000
C 4.23840500 -3.91668200 -2.80147800	H 0.96093600 -3.45426000 -0.35340500
H 2.38441500 -3.29095800 -3.72135500	H -5.76429100 -2.36519600 -1.16154000
C 5.12836700 -3.77920700 -1.72595900	H -5.59330400 -2.47322200 -2.94141600
H 5.55000200 -2.78079600 0.16155400	H -2.64273100 -2.42479800 -3.26913700
H 4.47264900 -4.62102300 -3.60464600	H -3.82631800 -3.68613200 -3.74300700
H 6.04450100 -4.37592000 -1.70559600	H -3.92151900 -0.55958500 -2.82864300
N 1.75953500 -1.40433100 -1.56333300	H -5.58591500 -0.12942300 -2.36766500
N 3.14177900 -1.21054200 0.11136100	H -5.00248000 1.29214900 0.24688800
N -1.60936600 1.62894300 -1.25329100	H -6.13062700 -0.01276800 -0.22545300
N -1.36740500 2.82208000 0.55280500	H -0.98961300 -5.80554000 -0.74965500
Co 0.71532600 0.68638500 -0.03366100	H 0.25837400 -5.23240900 -1.89052600
H 1.88089000 1.89119600 0.18291800	H -2.74528600 -5.30103800 -2.20707000
C 1.70278200 3.43856100 -2.88789600	H -1.63323800 -4.68042100 -3.47336800
C 2.53707300 2.19305700 -3.23944200	H -5.93039600 -2.28780500 2.99031200
H 2.38273800 4.29275900 -2.69194800	H -5.51075700 -3.66502800 1.92513800
H 1.94211200 1.53474700 -3.90485500	H -3.87466100 -0.21212700 1.84219800
B 1.67581000 1.95277000 -1.14554100	H -5.62943300 -0.16050700 2.15844000
O 1.06848700 3.09564600 -1.66758100	H -1.25546000 -3.28848200 3.51088900
O 2.69673400 1.52802700 -1.99787100	C 3.78886500 -0.78807400 1.31929900
K -2.19021200 -1.95519300 0.07539700	C 3.48259800 -1.44631900 2.52904900
O -2.91831700 -3.51233600 2.29438000	C 4.75753500 0.23129000 1.24744800
O -0.39271600 -3.79743400 1.09106000	C 4.17657000 -1.05186100 3.67685400
O -3.97105700 -3.03610400 -1.77943700	C 5.42489300 0.58267000 2.42630500
O -4.16759000 -0.23736100 -0.85343800	C 5.14100200 -0.05017600 3.62886300
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O -4.94787600 -1.88052600 1.20810100	H 6.18322600 1.37000900 2.39672800
C -1.82054100 -4.07171400 2.96623600	H 5.67407800 0.23862400 4.53979500
C -3.89631000 -2.96174600 3.13577200	C -0.82079600 3.36753000 1.75369700
C -0.93039300 -4.75700200 1.96335300	C -0.18958300 4.62431700 1.71482700

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 C -0.40596600 3.16827800 4.11412000
 C 0.19599900 4.42309900 4.10701900
 H 0.79459500 6.11487600 2.92298400
 H -0.47022800 2.60843800 5.05069000
 H 0.59446800 4.84263300 5.03556100
 C -1.54081500 1.23438200 2.94141500
 C -2.41114000 0.95988200 4.16484600
 C -0.44372600 0.17836100 2.80794600
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 H -3.18666000 1.73497900 4.29045100
 H -2.91859200 -0.01526100 4.06040000
 H -1.81935700 0.91669600 5.09534300
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 H 1.91573200 6.36158600 0.92937500
 H -1.87424500 6.52290800 0.55539500
 H -0.46413400 7.38474400 1.22976000
 H -0.65875900 7.23388900 -0.53652800
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 C 1.75402000 -2.65261700 3.94667900
 C 3.14949600 -3.92751100 2.31815200
 H 1.71312700 -2.41234600 1.82639600
 H 1.31459900 -1.68378000 4.23535900
 H 0.94095000 -3.39529400 3.89230500
 H 2.42608600 -2.97620600 4.76071200
 H 3.58283000 -3.97282200 1.30661700
 H 3.96142500 -4.11654500 3.04345700
 H 2.41859700 -4.75076100 2.40996900
 C 5.11030900 0.93498800 -0.04625400
 C 6.48480200 0.49799300 -0.55706200
 C 5.04359900 2.45503400 0.10013500
 H 4.36341700 0.65962700 -0.80335800
 H 6.53123800 -0.59180100 -0.72263400
 H 6.70814000 0.99218200 -1.51974900
 H 7.28655700 0.76804200 0.15451800
 H 4.06667400 2.77616400 0.49920800
 H 5.83273900 2.84401100 0.76863800
 H 5.17764400 2.93370200 -0.88475200
 C 3.87366400 2.47777000 -3.88164600
 H 4.48559500 3.13636600 -3.24089700
 H 4.42996600 1.53906900 -4.04624200
 H 3.73771600 2.97082400 -4.86027400
 C 0.68470200 3.83340600 -3.93171700
 H 1.18173600 4.10311900 -4.88036000
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¹H_{Dipp}
 C -0.08047900 1.69909400 1.40801000
 C -1.27083200 2.41462500 1.56941900
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 C 1.15975400 3.64551500 2.19815800
 C 1.12437800 2.34809800 1.68757800
 H -2.21348200 4.27995000 2.20151600
 H -0.05156400 5.32395800 2.80293600
 H 2.09537800 4.16004800 2.42542400
 C 3.57315100 1.61257400 1.37709100
 C 1.80776500 0.34494500 0.68227200
 C 4.06996500 0.42519400 0.80508500
 C 4.44743200 2.57106100 1.89134500
 C 5.43255600 0.15256400 0.74107500
 C 5.81401500 2.30463900 1.81526400
 H 4.08634700 3.49519300 2.34336600
 C 6.30110700 1.11579100 1.25257800
 H 5.79883100 -0.78362200 0.31414800
 H 6.52079000 3.04035000 2.20972600
 H 7.37982300 0.93875100 1.21710000
 C -3.72133700 1.73662900 1.11237800
 C -1.94299100 0.43692900 0.52761200
 C -4.20532100 0.53131100 0.56282800
 C -4.60697300 2.71596300 1.56186600
 C -5.56564800 0.26145800 0.46196200
 C -5.97194700 2.45199900 1.44745900
 H -4.25469500 3.65392700 1.99271700
 C -6.44575800 1.24642100 0.90999100
 H -5.92265600 -0.68563200 0.05089900
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 H -7.52367200 1.07379600 0.84230200
 N -2.34252200 1.62802500 1.08961500

N -3.08813300 -0.22576700 0.22658800	H 2.83851200 -1.34437900 -4.34097800
N 2.19636800 1.51394200 1.29901000	H 5.66444900 -0.18508700 -2.05604600
N 2.96273300 -0.31711600 0.40540800	H 5.31406700 -1.12981700 -3.53018900
Co -0.07030500 0.15546300 0.39954300	H 5.06464800 0.63709900 -3.51839100
H 0.00072600 -0.33629300 -1.21050500	C 2.49508200 -2.63614000 2.06911100
C 0.84284600 2.67527800 -2.65436900	C 3.73949100 -2.38161000 2.92441300
C -0.68141900 2.83087100 -2.49225200	C 1.73663800 -3.84926700 2.60054600
H 1.06508700 2.31966700 -3.68241300	H 1.83062000 -1.76157500 2.17663200
H -0.88605300 3.64036200 -1.76125300	H 4.27014600 -1.46314100 2.62649400
B 0.01797800 1.00896600 -1.30903800	H 3.46019200 -2.27727600 3.98818600
O 1.18717900 1.64804900 -1.74632100	H 4.44824200 -3.22543000 2.83905700
O -1.09408600 1.60460300 -1.92364000	H 0.88772500 -4.12052700 1.95033500
C 3.05130300 -1.60691800 -0.20454400	H 2.39116100 -4.73416200 2.69562400
C 3.37234100 -1.69369000 -1.57075700	H 1.33903500 -3.63082500 3.60661700
C 2.85064300 -2.75083600 0.59667400	C -3.02353800 -2.21077400 2.26708800
C 3.53144800 -2.97037400 -2.12289500	C -1.56326800 -2.14207200 2.72091300
C 3.00884000 -4.00061200 -0.00777300	C -3.82852600 -3.14120400 3.17081800
C 3.35679900 -4.11164500 -1.35155800	H -3.45266200 -1.20188200 2.38045300
H 3.78690100 -3.06819100 -3.18203300	H -0.99064000 -1.39630100 2.13664200
H 2.85762200 -4.90860700 0.58003500	H -1.49762700 -1.84488300 3.78295700
H 3.48139400 -5.10133700 -1.80175900	H -1.07329400 -3.12358600 2.60656100
C -3.11898700 -1.58800600 -0.20033400	H -4.87312200 -3.23790100 2.82649700
C -3.10776900 -2.58167500 0.79788500	H -3.39006400 -4.15349600 3.22353600
C -3.15778400 -1.88936900 -1.57129500	H -3.84672300 -2.74222700 4.20012900
C -3.13211000 -3.91628600 0.38510200	C -3.17532400 -0.80298000 -2.62633200
C -3.18955300 -3.24127000 -1.93272600	C -4.57559900 -0.63970000 -3.22052900
C -3.17426500 -4.24272900 -0.96828100	C -2.13848900 -1.04653600 -3.72082800
H -3.12015200 -4.71559900 1.13061700	H -2.89691000 0.14245500 -2.13761100
H -3.22080800 -3.51419600 -2.99138000	H -5.32113900 -0.39930000 -2.44302800
H -3.19455500 -5.29349900 -1.27367800	H -4.58582400 0.18148500 -3.95991400
C 1.63887000 3.93015900 -2.37818200	H -4.90591800 -1.56182200 -3.73358900
H 2.72003000 3.73136900 -2.47737600	H -1.13174300 -1.18337100 -3.29105500
H 1.37012500 4.73035700 -3.09086900	H -2.37807600 -1.93393400 -4.33461600
H 1.44662900 4.29194200 -1.35300200	H -2.09818800 -0.17628300 -4.39846300
C -1.43002500 3.11455800 -3.77369800	¹⁴K
H -2.51627900 3.16239100 -3.58435900	C -0.31402800 -1.85454200 -0.88752900
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H -1.24191600 2.32045900 -4.51765100	C 0.96039400 -2.60232300 -2.83728100
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C 1.49007100 -1.84359900 0.74705700
C 3.75579500 -2.06798000 0.70121800
C 4.18167900 -2.55623400 -1.64671200
C 5.11358600 -2.11246400 1.01060600
C 5.54171800 -2.58982200 -1.33819500
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H 5.47492100 -1.95820300 2.03004600
H 6.26204600 -2.79760900 -2.13455300
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C 2.90086700 0.59734700 -2.69781700
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H 1.93686900 5.74454000 0.43597200
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H -2.65287100 4.81160100 0.17729400
H -3.92507000 2.64600600 0.21475000
H -2.90467500 1.18876200 0.41737600
H 2.74604300 2.71168800 -3.12548500
H 2.30981100 1.64177700 -4.48598200
H 0.13138300 0.00567000 -3.11872700
H 0.14448300 0.92579800 -4.65238600
H 2.35550700 -0.33572200 -2.91625200
H 3.92949200 0.47432500 -3.08638200
H 4.90980700 0.55963000 -0.80330200
H 4.40512900 2.18495100 -1.34668100
H -3.10970400 2.96716500 -2.09023800
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H -2.11702300 0.77591200 -3.82029700
 H 3.88916300 4.30521800 0.72446000
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 H 3.58071400 0.77028400 1.25529300
 H 4.78103100 2.09004900 1.10381600
 H -0.70199100 4.89710100 1.73521900
¹⁵K_{Dipp}
 C -0.29258000 -0.47018600 -1.13214300
 C 0.77521900 0.29445500 -1.59648000
 C 1.74511900 -0.24648100 -2.44289100
 C 1.60123700 -1.58652200 -2.83438800
 C 0.53185300 -2.37776000 -2.39636000
 C -0.40224900 -1.79813000 -1.53279700
 H 2.59618500 0.33165100 -2.80701000
 H 2.35053700 -2.02237000 -3.49980200
 H 0.45139200 -3.40908500 -2.74186600
 C -2.02480300 -3.67098700 -0.90703000
 C -2.30232900 -1.51870900 -0.17575800
 C -3.16446100 -3.61591600 -0.09009700
 C -1.60743700 -4.88175000 -1.46260200
 C -3.91417200 -4.74865400 0.21070400
 C -2.35986300 -6.01773200 -1.16735200
 H -0.72816800 -4.95532700 -2.10209100
 C -3.49266300 -5.95600300 -0.34265900
 H -4.79279400 -4.68614800 0.85623600
 H -2.05546100 -6.98001000 -1.58873700
 H -4.05423900 -6.86982300 -0.12953700
 C 1.37693400 2.76528300 -1.32928900
 C -0.36997900 1.80519400 -0.20504600
 C 0.76863900 3.73901900 -0.52309900
 C 2.44531000 3.09844300 -2.16041400
 C 1.25211700 5.04200000 -0.44962400
 C 2.91515400 4.40983400 -2.11198100
 H 2.90242300 2.37026000 -2.82828100
 C 2.34311300 5.36293000 -1.25543400
 H 0.78428100 5.77891400 0.20624000
 H 3.74863700 4.70094500 -2.75806300
 H 2.74556700 6.37960700 -1.23365100
 N 0.67813000 1.59632100 -1.07745800
 N -0.30279800 3.12288400 0.11970900
 N -1.54233300 -2.37409000 -0.94730600
 N -3.31271300 -2.29125700 0.31348100
 Co -1.54754000 0.28028700 0.04225500
 H -4.12581500 0.15404200 -0.16523400
 C -2.93913000 -0.25581000 -4.08584600
 C -1.65393300 0.58700300 -4.21372500
 H -3.74390800 0.20726200 -4.69235900
 H -0.77505500 -0.07372600 -4.06831200
 B -2.58400700 0.93328400 -2.18322500
 O -3.29830300 -0.12951200 -2.71814000
 O -1.71690000 1.48149400 -3.11610800
 N -2.81476100 1.57985900 -0.92715200
 C -3.52424000 1.04628400 0.05009900
 C -4.02751000 1.82933300 1.22398300
 H -4.97482900 2.33376200 0.94478900
 H -4.25661200 1.15774700 2.06810600
 H -3.31659600 2.59947600 1.55049800
 B -0.35001100 -0.50476100 1.37810600
 O -0.40355000 -1.84420200 1.76576400
 O 0.88552700 0.03364200 1.76274400
 C 0.86490300 -2.25594600 2.22989100
 C 1.58515000 -0.92731300 2.53668400
 H 0.72290600 -2.84927200 3.15098300
 H 2.63162900 -0.95366900 2.19144100
 H -1.50032300 0.24086500 1.63228200
 K 4.16929100 -0.94263800 -0.00625800
 O 4.43600600 0.66324200 2.36758700
 O 5.07785300 -3.55420100 0.34074000
 O 4.44501100 1.70973300 -0.27384000
 C 5.19255400 0.09537300 3.40955600
 C 4.67418900 2.02919900 2.12788800
 C 5.25523300 -4.38682600 -0.77523500
 C 5.92564100 -3.85891500 1.41688700
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 C 3.97035200 2.41625400 0.84808200
 C 6.45945900 -0.55081800 2.88354700
 H 4.55155500 -0.65647500 3.90221500
 H 5.44793300 0.85226300 4.17557300
 H 4.27129800 2.64519000 2.95663100
 H 5.76109800 2.23500800 2.06158900
 C 4.47406600 -3.82030300 -1.94221600
 H 6.33384500 -4.46597400 -1.01911400
 H 4.89326600 -5.41520000 -0.57045100
 C 5.79500300 -2.79828900 2.47814400
 H 6.97816900 -3.89886100 1.07126400
 H 5.67068200 -4.84503700 1.85509500
 C 5.92641900 1.41977600 -2.09967900
 H 5.65851600 3.22770100 -0.98981500

H 6.50734700	1.92621100	-0.09632500	H -3.68607700	6.11884500	2.87489900
H 2.90176600	2.16265300	0.93747000	C -4.46522000	-1.88821900	1.06980100
H 4.05430400	3.50812600	0.68715300	C -5.65975800	-1.61039600	0.36931900
O 6.20341400	-1.56578500	1.94244700	C -4.40084400	-1.87120500	2.47326700
H 7.07850000	0.19840500	2.36151500	C -6.78838600	-1.27347000	1.12106400
H 7.05664400	-0.94618600	3.73021400	C -5.55915400	-1.52041500	3.17693300
O 4.76167600	-2.47218500	-2.21290500	C -6.74058400	-1.22021300	2.51097000
H 4.65465700	-4.45211100	-2.83554900	H -7.72609300	-1.04630800	0.60668400
H 3.39476900	-3.85114500	-1.71810000	H -5.53409000	-1.49509400	4.27021600
H 4.74775000	-2.75655400	2.84286100	H -7.63641300	-0.95015700	3.07839200
H 6.43475200	-3.08312600	3.33730800	C -3.15140300	-2.26390900	3.23014000
O 5.95156900	0.03467000	-1.87546800	C -3.35446500	-3.58992300	3.96555900
H 5.13135000	1.67342400	-2.82909200	C -2.69091100	-1.16559900	4.18683700
H 6.89204900	1.76884000	-2.51902000	H -2.34488300	-2.40676100	2.49913400
C 6.05063600	-2.19093700	-2.69552500	H -3.64210700	-4.39694100	3.26927000
C 6.12378100	-0.72672400	-3.04230800	H -2.41941800	-3.89763500	4.46814500
H 6.82648500	-2.42199800	-1.93928400	H -4.14142500	-3.51355600	4.73794500
H 6.26745400	-2.78745100	-3.60462400	H -2.52308100	-0.21726700	3.64924600
H 7.10837400	-0.51569200	-3.50699800	H -3.42426900	-0.97963600	4.99245000
H 5.33693100	-0.47939700	-3.78393400	H -1.73984500	-1.45499800	4.66839600
C 1.57875600	-0.54894200	4.00208300	C -5.75189900	-1.67183700	-1.14513700
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H 0.54578100	-0.51287400	4.38910900	H -4.72763600	-1.68811500	-1.54711200
C 1.55863100	-3.10163900	1.17954500	H -5.97238000	0.49512300	-1.38999900
H 1.66403900	-2.53259900	0.23820800	H -6.34608500	-0.46156100	-2.84133100
H 2.55604700	-3.43334600	1.51850800	H -7.51221000	-0.40720800	-1.49747700
H 0.96024600	-3.99986700	0.95058000	H -5.95501300	-3.85569800	-1.24301900
C -2.78552400	-1.70510100	-4.48118600	H -7.50744600	-2.97335400	-1.24013800
H -3.72722700	-2.25667800	-4.31782700	H -6.49051500	-2.99284400	-2.70758800
H -2.52307800	-1.78820100	-5.55082000	C -2.27142900	4.71380300	-1.35155900
H -1.98993900	-2.18595600	-3.88708400	C -1.73523500	6.02412900	-1.93371200
C -1.51168900	1.33843800	-5.51503300	C -3.70610900	4.48711700	-1.83087700
H -0.58317100	1.93473900	-5.51545200	H -1.66989600	3.88040800	-1.74210700
H -1.47171700	0.63906400	-6.36872100	H -0.67659500	6.19241300	-1.67928800
H -2.36351800	2.02559600	-5.66207600	H -1.81466500	6.00876800	-3.03551300
C -1.25061800	3.88974200	0.86893300	H -2.31551800	6.89105100	-1.56796800
C -1.18360700	3.87263100	2.27444200	H -4.14496400	3.59577000	-1.35781000
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C -2.07918100	4.68425800	2.97768900	H -3.71209000	4.32817900	-2.92368600
C -3.03645800	5.48982400	0.91792500	C -0.16097500	3.02709700	3.00740900
C -2.99424400	5.48938300	2.30692000	C -0.67357200	2.49946700	4.34375400
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H -3.76811100	6.11887600	0.40334400	H 0.06497200	2.15058500	2.38168400

H -1.63380400 1.96809200 4.22581000
H 0.05385200 1.78996700 4.77145600
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H 1.56463000 4.13929500 2.23384800
H 0.98672900 4.69828400 3.82613100
H 1.89980000 3.16728400 3.69655900
¹²
C 0.00114000 1.18642300 -0.03249800
C 1.19981300 1.86368800 0.18742300
C 1.22847600 3.20490300 0.57113900
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C -1.19669000 1.86647100 0.18378700
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C -5.88115700 1.77683100 0.50624600
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H -5.83764700 -1.57335900 -0.23532300
H -6.59399500 2.57065500 0.74775300
H -7.42632500 0.27734700 0.31774100
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C 1.86831900 -0.32389600 -0.30789600
C 4.11841200 -0.26233500 -0.10414700
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C 5.47451700 -0.56901400 -0.04744200
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H 7.42705000 0.26417300 0.32120800
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N 3.01241500 -1.04585400 -0.38786000
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C -3.07485400 -2.45197600 -0.65630700
H -3.41297800 -3.00051200 0.23870600

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H 3.75802900 -2.65260600 -1.50647300
H 3.41379300 -3.00958700 0.22646000
H 2.06101400 -2.79445800 -0.92558200
Co -0.00091500 -0.61571300 -0.51214400
H -0.00443700 -2.19583600 -0.21428500
C -0.75681200 -2.61449300 3.06208000
C 0.74180500 -2.32548400 3.16902500
H -1.33229800 -2.22955200 3.92255500
H -0.95563500 -3.70273400 2.97872000
H 0.93916500 -1.44707800 3.81565400
H 1.31886900 -3.17849100 3.56863400
B -0.00821100 -1.67789700 1.10977000
O -1.15205200 -1.96425000 1.87775500
O 1.13381500 -2.04452200 1.84756500
N 0.00376200 -0.71029800 -2.43631700
C 0.00826300 -0.72784700 -3.59260700
C 0.01477500 -0.73570400 -5.04217000
H 0.91123600 -0.21591700 -5.42099200
H 0.01860400 -1.77096900 -5.42344300
H -0.88024500 -0.21953900 -5.42922100
¹⁴Dipp
C -0.07822700 2.84354300 -0.10897900
C 1.11953400 3.54935600 -0.13793600
C 1.15602300 4.92900000 -0.34560500
C -0.06186200 5.59168400 -0.54774200
C -1.28687900 4.91163800 -0.55749000
C -1.26608600 3.53461300 -0.33437100
H 2.08682700 5.49803100 -0.36974500
H -0.05459900 6.67262100 -0.71580600
H -2.20893700 5.46419900 -0.74698100
C -3.72561200 2.77677000 -0.24377000
C -1.98242000 1.30749700 -0.12690600
C -4.23709500 1.48942300 0.00482700
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C -5.59602400 1.26046600 0.19463400
C -5.94605300 3.64208000 -0.17535700
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H -5.97063300 0.26077100 0.42399200
H -6.64029700 4.48416400 -0.24826000
H -7.52264200 2.21992700 0.23393600

C 3.57419500	2.81316400	0.05430600	H -2.85647300	-2.55646800	3.33369300
C 1.84647200	1.31493500	0.07324200	H -4.30474600	-3.79167300	-0.51608400
C 4.10522500	1.51517000	0.14216300	H -3.74894000	-4.31594600	1.83957400
C 4.41727500	3.92643300	0.04575800	C 3.22702600	-0.78305900	0.16369500
C 5.47420700	1.28195900	0.23738600	C 3.60903800	-1.42480600	-1.02875600
C 5.78845400	3.69429600	0.13025000	C 3.15150400	-1.46610800	1.39269400
H 4.03079100	4.94367800	-0.01551300	C 3.93792800	-2.78297400	-0.96244700
C 6.31114100	2.39545000	0.22770700	C 3.49803900	-2.81908900	1.40435500
H 5.86645600	0.26650200	0.32449900	C 3.89644600	-3.47226100	0.24216300
H 6.47198400	4.54818200	0.12668100	H 4.22955300	-3.30764900	-1.87657900
H 7.39323100	2.25455200	0.30057400	H 3.45086400	-3.37789700	2.34113500
N 2.20177500	2.64571900	0.01294100	H 4.16284900	-4.53314000	0.27598400
N 3.02270500	0.63664500	0.14271000	C -4.05643700	-1.43249300	-1.83161400
N -2.35138300	2.62174500	-0.30385000	C -5.53448600	-1.63832300	-2.16366100
N -3.14293700	0.62731300	0.05399700	C -3.16905700	-2.28070500	-2.74494500
Co -0.07220500	0.97360500	-0.04080500	H -3.81748200	-0.37426800	-2.02286500
C -0.27898900	-4.12773100	0.34785400	H -6.18699800	-0.99270400	-1.55204800
C 0.33756600	-4.34999500	-1.04547100	H -5.72476500	-1.39863100	-3.22512800
H -1.36435500	-4.34922500	0.28975500	H -5.84285100	-2.68654800	-1.99857100
H 1.41343300	-4.59818500	-0.93023900	H -2.10507900	-2.19548400	-2.47171100
B 0.03335900	-2.12867100	-0.66540100	H -3.44657300	-3.34914000	-2.68921900
O -0.12251600	-2.74467500	0.58096500	H -3.28474900	-1.96289900	-3.79668300
O 0.23358300	-3.08665400	-1.66949100	C 3.66749200	-0.71542500	-2.36802100
N -0.04091700	-0.77558700	-0.88077800	C 2.83384000	-1.45012700	-3.42181500
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H -1.90447200	0.35175500	-2.53919200	H 1.84345000	-1.73889500	-3.03342900
H -0.75259000	1.52028800	-3.26080100	H 2.69508800	-0.81055900	-4.31167000
H -0.70709200	-0.19730400	-3.74273900	H 3.33996500	-2.37341200	-3.75754700
H 1.16329200	0.38537700	-2.16202600	H 5.70702600	0.06597000	-2.14942700
C 0.33126600	-4.95111500	1.45745400	H 5.60761900	-1.50846600	-2.98758500
H -0.15093600	-4.71573100	2.42202300	H 5.11727500	-0.01353100	-3.82975200
H 0.19515100	-6.03016100	1.26310700	C -2.36977200	0.08140700	2.73681000
H 1.41065400	-4.74264500	1.54798500	C -0.84214300	0.07710300	2.66606300
C -0.33947800	-5.42046700	-1.87000200	C -2.84267600	-0.00902100	4.18481700
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H -0.25651900	-6.40726500	-1.38024000	H -0.48545400	-0.03959800	1.61679500
H -1.40951100	-5.18310500	-2.00606000	H -0.41723800	0.99327600	3.10962700
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C -3.92354600	-3.00251000	0.13871000	C 2.72445500	-0.76417800	2.66833500
C -3.60958300	-3.29902200	1.46008900	C 3.89528600	-0.02853100	3.32607400

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H 1.97096000 -0.01206900 2.38182600
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H 4.69062700 -0.74025500 3.61333600
H 1.27246100 -2.30803000 3.18701200
H 2.79346300 -2.39997600 4.12751300
H 1.61099500 -1.12855200 4.49060600

¹TS1

C 0.00158100 1.14354800 -0.39632600
C 1.20424100 1.83915100 -0.35010500
C 1.23464600 3.23284700 -0.28613600
C 0.01024600 3.91368600 -0.26226500
C -1.21860100 3.24117400 -0.28887600
C -1.19658900 1.84734300 -0.35245100
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C -5.87785500 1.86189000 -0.04783000
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H -5.86049500 -1.56953600 -0.02933000
H -6.58559300 2.69433800 0.00332600
H -7.43521900 0.36942900 0.09192800
C 3.64415500 1.03303400 -0.22841400
C 1.88254100 -0.40476100 -0.39134200
C 4.12899700 -0.28915900 -0.20140000
C 4.52141900 2.11311800 -0.14051500
C 5.48663100 -0.57211200 -0.08930400
C 5.88248300 1.82969900 -0.02569000
H 4.16910800 3.14482300 -0.16037000
C 6.35983500 0.51173700 -0.00036700
H 5.85389300 -1.60103000 -0.07366300
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N 2.27121700 0.91607400 -0.35042100
N 3.02447500 -1.12157300 -0.30193300
N -2.26908400 0.93036600 -0.34682100
N -3.02934100 -1.10387000 -0.26271800

C -3.10121000 -2.53569500 -0.15153500
H -3.69258900 -2.81263400 0.73700100
H -3.56197800 -2.98163100 -1.05031400
H -2.07963200 -2.91775800 -0.02718400
C 3.09591000 -2.55574000 -0.22729300
H 3.57183800 -2.97697500 -1.12998100
H 3.67261000 -2.85722600 0.66316700
H 2.07315500 -2.94338400 -0.13348200
Co -0.00439000 -0.71506300 -0.49663000
H -0.00697100 -2.26913900 -0.40162500
C -0.71786100 -1.29955700 3.55863400
C 0.75491700 -0.87774600 3.58205800
H -1.34987800 -0.69368700 4.23026300
H -0.84978700 -2.36374700 3.83340300
H 0.88869100 0.13735300 4.00094500
H 1.39313800 -1.57088500 4.15681000
B 0.00618100 -0.91430800 1.42199300
O -1.11874600 -1.10961300 2.21501600
O 1.14240600 -0.87639900 2.22140500
N -0.01896800 -1.10300900 -2.53119400
C -0.02179800 -2.17754500 -1.98443900
C -0.03737000 -3.62807000 -2.29037100
H -0.02213400 -3.77783300 -3.38255600
H 0.83701800 -4.12909900 -1.84120700
H -0.94256700 -4.10092200 -1.87232200

HBpin

C -0.68321700 -0.36713700 -0.36607700
C 0.68319400 -0.36716600 0.36606800
H -0.55832700 -0.74334000 -1.39884600
H 0.55826600 -0.74339900 1.39881900
B 0.00006800 1.75285600 -0.00008800
H 0.00000000 2.96152100 0.00010700
O 1.04393200 1.01352900 0.45919400
O -1.04392800 1.01356700 -0.45913200
C 1.76487400 -1.15694700 -0.33207000
H 2.71772900 -1.08326300 0.21878500
H 1.48369200 -2.22316200 -0.39370500
H 1.92410600 -0.77701800 -1.35666900
C -1.76489100 -1.15691900 0.33206400
H -2.71772300 -1.08324300 -0.21883000
H -1.48370600 -2.22313300 0.39370900
H -1.92416900 -0.77699100 1.35665800

¹2K

C -0.17278400 -1.43775800 -0.64953000

C -1.36794000 -1.48187000 -1.37638100
C -1.39393000 -1.79142900 -2.73588800
C -0.17825900 -2.09224400 -3.36624200
C 1.03887100 -2.08460100 -2.66962200
C 1.01831100 -1.74859200 -1.31536600
H -2.32195400 -1.82186600 -3.30958500
H -0.18068900 -2.35334300 -4.42843600
H 1.95952600 -2.35941600 -3.18819800
C 3.44473300 -1.83215100 -0.48722600
C 1.68130300 -1.41175500 0.89810000
C 3.93074100 -1.64962100 0.82249200
C 4.32278000 -2.06192500 -1.54454500
C 5.29059000 -1.69859000 1.11454000
C 5.68728900 -2.10676700 -1.25352000
H 3.96895600 -2.20111300 -2.56652100
C 6.16550600 -1.93080400 0.05236100
H 5.66012900 -1.56054400 2.13354500
H 6.39803500 -2.28815200 -2.06479600
H 7.24130600 -1.97839100 0.24336500
C -3.81016700 -1.19631600 -0.63541000
C -2.05069400 -1.02026900 0.81169300
C -4.30795000 -0.96417200 0.66271100
C -4.67896900 -1.31656200 -1.71908500
C -5.67123200 -0.84342700 0.91480400
C -6.04629800 -1.20124400 -1.46516600
H -4.31608400 -1.49606900 -2.73148400
C -6.53621500 -0.96902000 -0.17219200
H -6.04819400 -0.65941400 1.92369100
H -6.75087900 -1.29658200 -2.29624700
H -7.61489100 -0.88579700 -0.01210000
N -2.43327600 -1.20994400 -0.50300200
N -3.20862200 -0.86615600 1.50066200
N 2.07472600 -1.68668400 -0.39486700
N 2.82789500 -1.40769500 1.62749100
C 2.89196100 -1.27606700 3.05864400
H 3.50141900 -2.09099100 3.48348100
H 3.33581100 -0.30829100 3.35551600
H 1.87254200 -1.35402800 3.45893700
C -3.29372600 -0.65922900 2.92128300
H -3.52757400 0.39525200 3.15392800
H -4.07676900 -1.30684600 3.34813200
H -2.32788900 -0.93018800 3.36864700
Co -0.19091800 -1.20488600 1.20119500
C 0.14206000 -5.28403400 0.51591900

C -1.33231500 -4.99468200 0.20535300
H 0.70564300 -5.61663200 -0.37266600
H 0.25732700 -6.05245100 1.30417800
H -1.49464200 -4.81940600 -0.87529400
H -2.00866900 -5.80442600 0.52862500
B -0.40667400 -3.18372900 1.20546700
O 0.65645100 -4.05339200 0.98219500
O -1.61775500 -3.81068100 0.92048900
N -0.05375100 0.16255400 2.53343000
C 0.03751600 0.87890400 3.44134800
C 0.15949100 1.67848300 4.64482400
H 1.19385800 2.04284100 4.76361900
H -0.52000900 2.54628600 4.61159000
H -0.09784000 1.06724200 5.52836700
K 0.19999300 1.79345500 -0.31138600
O -0.02194800 4.10514400 1.25984400
O -2.34680500 2.69977400 0.54353200
O 0.89386000 2.49953300 -2.93964100
O 2.77348900 1.12428800 -1.18899700
O -1.77716600 2.03951000 -2.15510400
O 2.52430400 3.48335100 0.23925700
C -1.24490100 4.26961500 1.92509800
C 1.12016700 4.34426400 2.03669000
C -2.36610800 4.04197000 0.94657100
C -3.33419200 2.33684900 -0.39114300
C 2.26120700 2.33048200 -3.22558300
C 0.01408600 1.69295200 -3.68514700
C 2.85396800 1.08402600 -2.59462500
C 3.86639300 1.71382900 -0.53200100
C -2.97975400 2.67864700 -1.82109400
C -1.39206900 2.20044600 -3.49507000
C 2.29363800 4.56003100 1.10658800
C 3.37655200 2.46025300 0.68389000
H -1.32908000 5.29530400 2.33838100
H 1.30601000 3.49531700 2.72715400
H 0.99336300 5.25543000 2.65661000
H -2.23853900 4.72829500 0.08604200
H -3.32934000 4.28718300 1.43919400
H -4.30809400 2.79812400 -0.13492600
H -3.44552000 1.24714700 -0.30769100
H 2.76543900 3.22876900 -2.83171700
H 2.42646200 2.30131500 -4.32248600
H 0.07289000 0.62889000 -3.37993800
H 0.26070500 1.74778000 -4.76497300

H 2.29557800 0.18973000 -2.91608700
H 3.90123700 0.95506200 -2.92922900
H 4.59759800 0.93810100 -0.23041000
H 4.38105000 2.43594700 -1.19303300
H -2.88349800 3.77478000 -1.96867200
H -3.80832300 2.32973600 -2.47167500
H -1.43596100 3.27117700 -3.78020000
H -2.07240100 1.63631200 -4.16513900
H 3.19850700 4.79209900 1.70248200
H 2.07324500 5.43052600 0.46597300
H 2.85517800 1.76204800 1.37355300
H 4.24960800 2.87799100 1.22436800
H -1.33905100 3.55144200 2.76537600
H -0.36944800 -2.40176300 2.30643500

³TS4

C 0.25318300 -1.78516700 -0.26057800
C 1.49815200 -2.37062600 -0.03426900
C 1.65265900 -3.71605400 0.30483600
C 0.49724400 -4.48381900 0.48487500
C -0.77384900 -3.90327400 0.42379300
C -0.85862500 -2.55182800 0.08356700
H 2.63259200 -4.16387900 0.48428600
H 0.59200100 -5.54083400 0.75089500
H -1.65264300 -4.49365900 0.69298100
C -3.36368100 -2.01825900 0.14839500
C -1.77967000 -0.38948700 0.31209900
C -4.00339000 -0.76791300 0.22434000
C -4.10535100 -3.19200500 0.00985000
C -5.39065700 -0.64810300 0.19365000
C -5.49387700 -3.07235200 -0.02432900
H -3.62762600 -4.16815400 -0.08144100
C -6.12821900 -1.82442400 0.07217300
H -5.87962500 0.32642900 0.26224100
H -6.10164800 -3.97552100 -0.13103300
H -7.22052700 -1.77319700 0.04702500
C 3.89126700 -1.47104500 -0.20671500
C 2.10224600 -0.08986100 0.07310600
C 4.34039600 -0.13755800 -0.21416900
C 4.78673400 -2.52623100 -0.38731000
C 5.68700700 0.18367200 -0.37019900
C 6.13352300 -2.20435600 -0.54677000
H 4.45579800 -3.56486300 -0.41594700
C 6.57950200 -0.87394600 -0.53217400
H 6.02978300 1.22082800 -0.36360700

H 6.85864800 -3.01101500 -0.68812700
H 7.64575000 -0.66272700 -0.65420000
N 2.52057500 -1.39281900 -0.03839400
N 3.21894000 0.66069000 -0.05789700
N -2.00997100 -1.73785900 0.19924700
N -3.00311700 0.18715800 0.31201900
C -3.27152300 1.60169600 0.37186300
H -3.91477300 1.89174600 -0.47637100
H -3.77386400 1.86047500 1.31854900
H -2.31530000 2.13165900 0.31209600
C 3.26118900 2.10098100 -0.05849900
H 3.61686300 2.48446400 0.91108900
H 3.93141600 2.44389500 -0.86377300
H 2.24339900 2.46030000 -0.24784700
Co 0.10659200 0.22557300 -0.08345400
H 0.95381900 3.72673500 0.85643200
C -1.53728900 1.03567300 -3.36662300
C -1.37479100 2.50980400 -3.75991900
H -1.18065200 0.33708000 -4.14131800
H -2.59085100 0.78600700 -3.13291800
H -0.56267300 2.64162000 -4.50088600
H -2.29780400 2.94303400 -4.18213100
B -0.58941400 2.20567700 -1.65934200
O -0.75058500 0.91869300 -2.20141500
O -1.03324400 3.16868100 -2.55745500
N -0.06451800 2.36991700 -0.38332600
C 0.19316300 3.72928800 0.05516900
C -1.03439700 4.48479100 0.55524800
H -1.49439100 3.97675400 1.41893300
H -0.76149400 5.51123500 0.86457600
H -1.79319700 4.56317900 -0.24241900
B 0.10303600 1.29951100 1.53801800
O -1.01391800 1.58352300 2.31536900
O 1.25056000 1.76763100 2.16692200
C -0.59739400 2.16204500 3.53442000
C 0.88062500 2.50478500 3.31612400
H -1.21240400 3.04949300 3.76445800
H -0.73624300 1.42942300 4.35177400
H 1.03202300 3.58545400 3.13133900
H 1.51896600 2.21267800 4.16755100
H 0.63765500 4.31856200 -0.77295200

¹TS2W_{Co}

C -0.00227300 -0.07396000 0.49279600
C -1.21659900 -0.63846500 0.93471900

C -1.25651400 -1.73983600 1.82704700
C -0.01103800 -2.29612600 2.22812600
C 1.24195900 -1.74532200 1.83093800
C 1.21021100 -0.65010300 0.93626500
H -2.18481300 -2.17041900 2.19782200
H -0.01445000 -3.16063400 2.89516300
H 2.16676400 -2.17937300 2.20639500
C 3.65206000 -0.06931000 0.42703900
C 1.89967500 1.20614600 -0.31048100
C 4.15009700 1.01029400 -0.32465300
C 4.51166700 -1.02133000 0.97168900
C 5.51455100 1.18833900 -0.53367100
C 5.87808300 -0.84492600 0.75782100
H 4.14565900 -1.88120000 1.53350300
C 6.37307300 0.24212300 0.02346100
H 5.89771300 2.03314000 -1.11045100
H 6.57810700 -1.57653700 1.17095500
H 7.45213100 0.34728400 -0.12011400
C -3.65560400 -0.03919300 0.43044500
C -1.89507000 1.22267800 -0.31026100
C -4.14689500 1.04251000 -0.32284000
C -4.52140300 -0.98463600 0.97683700
C -5.51031500 1.22921500 -0.53139500
C -5.88664600 -0.79957400 0.76340800
H -4.16101000 -1.84643800 1.53925600
C -6.37482100 0.28962800 0.02759900
H -5.88824600 2.07555900 -1.10936700
H -6.59123400 -1.52612400 1.17771200
H -7.45322200 0.40163500 -0.11573200
N -2.27999000 0.11422800 0.42072900
N -3.04288200 1.76606700 -0.75850500
N 2.27741800 0.09348900 0.41851400
N 3.05093900 1.74248600 -0.75809900
C 3.15255600 2.93109400 -1.56782600
H 3.92389800 2.78425300 -2.34050800
H 2.17944000 3.10764900 -2.04430200
H 3.41570300 3.80295200 -0.94466600
C -3.13673500 2.95192800 -1.57342400
H -2.16469000 3.11663100 -2.05605500
H -3.91331700 2.80865900 -2.34148500
H -3.38823400 3.82952500 -0.95361200
Co 0.00506500 1.52462600 -0.44084400
H -0.01208900 5.04284100 -0.20638200
C 0.79069600 4.00684500 2.71110000

C -0.72674200 3.82428800 2.85267100
H 1.33919600 3.77225300 3.63930800
H 1.05861100 5.03613400 2.40638000
H -0.98903200 3.20229000 3.72895800
H -1.26841200 4.78174400 2.93869600
B 0.01882800 2.66953200 1.04216900
O 1.16387700 3.10329600 1.68645100
O -1.11637900 3.15266800 1.66876700
N 0.00974400 3.19827100 -1.17116500
C 0.00370500 4.45458000 -1.15671400
C 0.01128600 5.31085700 -2.39465000
H 0.02299400 4.68448400 -3.30230200
H -0.87932300 5.96809200 -2.42127700
H 0.89538600 5.97726000 -2.40465400
W -0.00952400 -2.43613100 -0.12150600
C 0.08613900 -4.40536400 -0.11314600
O 0.14376400 -5.56288700 -0.06332200
C -1.42717800 -2.57903300 -1.48544800
O -2.28683300 -2.61592600 -2.26223000
C 1.30847400 -2.44391600 -1.59162500
O 2.10824100 -2.39575900 -2.42906000
¹TS1W_{Co}
C 0.00005600 -0.05009300 -0.53170700
C -1.23619700 0.45082700 -0.97892100
C -1.31440500 1.52486700 -1.90201600
C -0.08596300 2.11883300 -2.31011200
C 1.18627800 1.63682900 -1.88888000
C 1.19167800 0.56132000 -0.96466200
H -2.25500000 1.90484300 -2.29631000
H -0.12024900 2.96334100 -3.00167000
H 2.09535000 2.10124500 -2.26661100
C 3.65455400 0.00451700 -0.50919100
C 1.93131600 -1.28582800 0.26717300
C 4.18098400 -1.10483300 0.17749500
C 4.49310000 0.97266800 -1.05669600
C 5.55155400 -1.29076600 0.32616500
C 5.86730100 0.78649800 -0.90674900
H 4.10402900 1.85377100 -1.56825700
C 6.38932000 -0.32555700 -0.23164800
H 5.95444600 -2.15165500 0.86468400
H 6.55147900 1.53267500 -1.32037000
H 7.47296200 -0.43412300 -0.13171600
C -3.64615500 -0.29165300 -0.52361700
C -1.83210900 -1.43133400 0.27872700

C -4.09065000 -1.41411900 0.19799300	O -0.22519900 5.45039000 -0.13648400
C -4.55383700 0.59614300 -1.09652800	³⁵
C -5.44396700 -1.69261800 0.35916200	C 0.20414400 -0.76365100 -0.77002500
C -5.91070100 0.31642300 -0.93649000	C -0.97588000 -0.87832100 -1.52979300
H -4.23103200 1.48685900 -1.63609800	C -0.97145700 -1.20890500 -2.88322000
C -6.35022100 -0.80853300 -0.22527600	C 0.26066400 -1.34383300 -3.53095200
H -5.78423100 -2.56176300 0.92669700	C 1.45267600 -1.01792400 -2.87049800
H -6.64714100 0.99805000 -1.37123900	C 1.39292000 -0.68840700 -1.52122000
H -7.42304800 -0.99187600 -0.11811300	H -1.90497700 -1.30079300 -3.44484800
N -2.26375800 -0.34633300 -0.45849300	H 0.28676200 -1.60463200 -4.59295300
N -2.95516700 -2.07294600 0.65724500	H 2.39302700 -0.95912700 -3.42517000
N 2.27952800 -0.15286900 -0.44460900	C 3.78937900 -0.27487700 -0.75768300
N 3.09871400 -1.85711700 0.61962400	C 2.04740600 0.95492600 0.05003800
C 3.22448900 -3.10493700 1.32710800	C 4.28535000 0.64147800 0.18629400
H 3.93117100 -3.76352000 0.79646900	C 4.63080500 -1.18646600 -1.39096900
H 3.58281300 -2.93793000 2.35754300	C 5.63921200 0.69567700 0.50858600
H 2.23944700 -3.58818800 1.34268400	C 5.98554000 -1.13476200 -1.06603500
C -2.99376100 -3.29145200 1.42365900	H 4.24304600 -1.91864800 -2.10221000
H -3.32983700 -3.09658300 2.45668800	C 6.48299200 -0.20727000 -0.13713700
H -3.68125200 -4.00978800 0.94739600	H 6.02365700 1.40956100 1.24109900
H -1.98304400 -3.72075400 1.43782500	H 6.67552600 -1.83676200 -1.54320900
Co 0.06118200 -1.57113500 0.52675200	H 7.55286000 -0.19746000 0.09048800
H 0.10381900 -2.93302000 1.27253100	C -3.38207800 -0.97659900 -0.70773000
C 0.83753300 -4.36626200 -2.45199600	C -1.89250700 0.53769700 0.12736700
C -0.33742100 -3.59975100 -3.06844200	C -3.98889200 -0.28414100 0.35441200
H 1.71333700 -4.42192400 -3.12058100	C -4.05260900 -1.99035200 -1.38635100
H 0.55788700 -5.39851500 -2.16809500	C -5.29352600 -0.56251800 0.75369500
H -0.02016600 -2.96643700 -3.91801900	C -5.35914800 -2.27048400 -0.98598900
H -1.14796000 -4.26090300 -3.41933200	H -3.57233200 -2.55164300 -2.19033000
B 0.14141700 -2.73687100 -1.00899100	C -5.97155600 -1.56599500 0.06116300
O 1.16585000 -3.63224300 -1.28565500	H -5.76545000 -0.02182400 1.57760300
O -0.80676600 -2.77226100 -2.01950800	H -5.91596100 -3.06057700 -1.49813900
N 0.03486700 -0.82331600 2.45340000	H -6.99857800 -1.81270600 0.34566800
C 0.08859100 -2.01787500 2.58444800	N -2.10836900 -0.44699300 -0.81073300
C 0.15125900 -3.08915600 3.60421400	N -3.04590200 0.61163100 0.83561200
H 0.14803200 -2.63855800 4.61023900	N 2.42727000 -0.04562600 -0.80876200
H -0.71169800 -3.76919300 3.50714000	N 3.19106100 1.35972000 0.64658000
H 1.06621100 -3.69164500 3.47729100	C 3.26503900 2.39366100 1.64560800
W -0.10906400 2.32670900 0.02623300	H 3.65250800 1.98485300 2.59450600
C 1.24150600 2.48158900 1.45840900	H 3.92201100 3.21390200 1.30889400
O 2.06897500 2.52707600 2.26748800	H 2.25128700 2.78518400 1.80942900
C -1.48713400 2.37691800 1.44035200	C -3.24494500 1.41859600 2.01247800
O -2.32482800 2.35876500 2.24020400	H -4.00481200 2.19767200 1.83793200
C -0.18335100 4.29372600 -0.04495200	H -3.56320900 0.77238300 2.84819700

H -2.29479000 1.90031600 2.27068600
Co 0.00817800 1.06593900 0.38550800
H 0.21521400 0.56223900 3.78857000
C 1.18844400 -3.48913200 0.89584100
C -0.30764400 -3.54038400 0.54627000
H 1.81132100 -3.99281400 0.13029000
H 1.39047700 -3.99182500 1.86637700
H -0.44855200 -3.63576200 -0.55256100
H -0.83422100 -4.38717100 1.02444500
B 0.26367000 -1.37191800 0.88880600
O 1.49915900 -2.12902700 0.98303100
O -0.81915600 -2.32655500 1.01367800
N 0.16617200 -0.22444800 1.91164600
C 0.27283100 -0.35304000 3.16590700
C 0.50037200 -1.63523000 3.90894600
H 1.58335600 -1.85691800 3.95504400
H 0.12725400 -1.56270400 4.94512500
H 0.00601400 -2.47583000 3.39782000
B -0.75929600 3.04287400 0.11912600
O -0.29399400 3.38059900 -1.13932800
O -1.99612800 3.60195800 0.38145600
C -1.31267300 4.11870500 -1.79205200
C -2.53112700 4.00761100 -0.86339900
H -0.97496200 5.16471800 -1.91480500
H -1.50129500 3.69676700 -2.79357000
H -3.07394300 4.96068000 -0.74643300
H -3.24742100 3.24298700 -1.22078000
H 0.01044800 2.76865300 1.07203700
¹LCoW(CO)₃
C 0.00011900 0.55418100 -0.80145200
C 1.21795800 -0.08560600 -1.11639100
C 1.25267800 -1.32091800 -1.81073600
C 0.00005000 -1.92842400 -2.11419200
C -1.25256600 -1.32074000 -1.81096300
C -1.21777400 -0.08547900 -1.11655900
H 2.17591900 -1.82077000 -2.09909900
H 0.00002900 -2.89346800 -2.62515000
H -2.17582800 -1.82046400 -2.09948000
C -3.65270500 0.56468400 -0.66528500
C -1.89028300 1.92738800 -0.10032500
C -4.15257500 1.72933400 -0.05094000
C -4.51591600 -0.44799100 -1.07942800
C -5.51486500 1.92514900 0.15319200
C -5.88187800 -0.25260200 -0.87246800

H -4.15239500 -1.36865800 -1.53617300
C -6.37554100 0.91277400 -0.27109300
H -5.89455800 2.83048800 0.63245700
H -6.58140100 -1.03344200 -1.18384300
H -7.45320000 1.02805800 -0.12463700
C 3.65293400 0.56439900 -0.66511300
C 1.89059900 1.92725100 -0.10024600
C 4.15288800 1.72914200 -0.05101200
C 4.51607300 -0.44841400 -1.07906800
C 5.51519600 1.92492500 0.15303200
C 5.88205400 -0.25305400 -0.87220100
H 4.15248400 -1.36916300 -1.53559600
C 6.37580100 0.91241900 -0.27108300
H 5.89495400 2.83033600 0.63210900
H 6.58152300 -1.03399900 -1.18343500
H 7.45347300 1.02767200 -0.12468700
N 2.27996400 0.72955500 -0.69267100
N 3.05558700 2.51561500 0.26748500
N -2.27973000 0.72979100 -0.69290300
N -3.05522700 2.51571600 0.26761200
C -3.14922200 3.78728300 0.93491800
H -3.75760600 4.49299100 0.34353600
H -3.60167000 3.67023600 1.93477600
H -2.13484400 4.19703000 1.04685900
C 3.14966700 3.78724300 0.93466300
H 3.60220000 3.67028100 1.93449300
H 3.75801400 4.49288200 0.34316100
H 2.13530700 4.19702200 1.04665000
Co 0.00014700 2.15938100 0.03605400
W -0.00015600 -1.66655700 0.23219000
C 1.36739100 -1.46944000 1.63772300
O 2.19699700 -1.30534100 2.43190300
C -1.36756100 -1.46825200 1.63767700
O -2.19706900 -1.30340500 2.43180600
C -0.00080000 -3.60416900 0.60252000
O -0.00109300 -4.75079800 0.78189700
¹⁷W_{Co}
C 0.73241200 0.19359100 -1.11566800
C 1.75921600 -0.77289800 -1.31635800
C 3.06867900 -0.40934400 -1.70151100
C 3.35859200 0.97820200 -1.82586000
C 2.36955900 1.98620200 -1.63717200
C 1.07626200 1.57105400 -1.25556800
H 3.85434400 -1.14074400 -1.88495400

H 4.37342400 1.28108400 -2.09053700
H 2.63825700 3.03271200 -1.77203400
C -0.29598100 3.69918300 -0.93775100
C -1.20104600 1.58725100 -0.74294700
C -1.65596700 3.81611900 -0.58757900
C 0.49727600 4.83090900 -1.10531400
C -2.26124800 5.05865800 -0.42071600
C -0.10889000 6.07766500 -0.93001900
H 1.55598500 4.76243800 -1.35655800
C -1.46366800 6.19115100 -0.59817400
H -3.31844200 5.14668400 -0.15960400
H 0.49304800 6.98223400 -1.05433900
H -1.90660400 7.18329600 -0.47193500
C 1.75973400 -3.31214800 -1.04456900
C -0.15106100 -2.03622200 -0.87339700
C 0.67720100 -4.15202400 -0.71538300
C 3.04551200 -3.82792900 -1.18149800
C 0.84402200 -5.52169000 -0.53148800
C 3.21350800 -5.20244000 -0.99436100
H 3.90139200 -3.19295800 -1.41201000
C 2.13389200 -6.03576500 -0.67910700
H 0.00167700 -6.16790600 -0.27312400
H 4.21459500 -5.63186200 -1.09165100
H 2.30355100 -7.10709700 -0.53800400
N 1.21658900 -2.04208200 -1.14303400
N -0.44539900 -3.34763400 -0.61978000
N -0.06056200 2.33797300 -1.03044500
N -2.15381400 2.53013700 -0.46143800
C -3.50046000 2.24097900 -0.05293600
H -3.53617300 1.22740800 0.36328300
H -3.81251100 2.94436700 0.73619200
H -4.21303000 2.31735700 -0.89482700
C -1.74274600 -3.84446000 -0.25379500
H -2.45952400 -3.01795000 -0.31046000
H -2.06304300 -4.64460600 -0.94393200
H -1.73505900 -4.24696600 0.77489900
Co -0.98164700 -0.31611500 -0.69522700
H -6.14362500 -2.01085700 0.92145800
C -0.86088200 -0.89020800 2.33248100
C -1.73639700 -0.94502000 3.58615900
H -0.29892300 -1.82313000 2.16154000
H -0.15360700 -0.04900700 2.31564400
H -1.38891600 -1.69178200 4.31695200
H -1.80048200 0.03594800 4.08888600

B -3.04684300 -1.08722500 1.76536100
O -1.80976200 -0.73216500 1.27239500
O -3.03293000 -1.30400200 3.11146600
N -4.20789400 -1.20688900 0.94790500
C -5.50507700 -1.41993900 1.59731200
C -6.19523900 -0.11474500 1.95281900
H -6.39436500 0.48730100 1.04862200
H -7.16179000 -0.30927600 2.45019300
H -5.57422600 0.48544900 2.64139300
B -4.16916500 -1.04858400 -0.46093000
O -3.00326600 -0.84405800 -1.18436500
O -5.27198500 -1.09175500 -1.26474500
C -3.37444400 -0.57944500 -2.53815400
C -4.82927100 -1.05290300 -2.61520300
H -3.26524300 0.50220300 -2.72327400
H -2.69362100 -1.11981300 -3.21216700
H -5.46845400 -0.36889900 -3.19573100
H -4.91514700 -2.06454000 -3.04994000
H -5.34472000 -2.02055700 2.50643100
W 2.61950000 0.70391800 0.42442500
C 2.62404700 -0.77586500 1.71139700
O 2.59004200 -1.68332100 2.44171200
C 4.35027000 1.26320300 1.16146800
O 5.39028300 1.60157300 1.55549800
C 1.75109100 1.79184400 1.80428100
O 1.17972900 2.43939900 2.58682900
³⁶
C -0.59112400 1.37059300 0.08169400
C -1.91183000 1.79335800 -0.08094500
C -2.27186500 3.14252300 -0.06032500
C -1.26995800 4.09827400 0.13317700
C 0.05772500 3.72085500 0.33027700
C 0.36671100 2.35883300 0.30761400
H -3.30385200 3.47525100 -0.17052000
H -1.54109200 5.15793100 0.15701500
H 0.82673400 4.47053200 0.53536000
C 2.78586500 2.09753500 -0.25104300
C 1.81500200 0.64637400 1.20154900
C 3.66500800 1.01562100 -0.04072300
C 3.09633000 3.10642100 -1.15553300
C 4.89079600 0.93622500 -0.69517200
C 4.32813800 3.02508000 -1.81808700
H 2.40370000 3.92827000 -1.34691400
C 5.21243300 1.96816100 -1.58615700

H 5.56992500 0.09680800 -0.52838600
H 4.60010200 3.80840000 -2.53158200
H 6.16943900 1.93884800 -2.11531000
C -4.16789200 0.68120800 -0.63435000
C -2.33776500 -0.55224900 -0.10277800
C -4.50242100 -0.68546600 -0.71103300
C -5.12760800 1.65077900 -0.93920400
C -5.77585100 -1.12485200 -1.06437300
C -6.40136800 1.21292500 -1.29526000
H -4.90794400 2.71698900 -0.91453100
C -6.72667200 -0.15048600 -1.35411200
H -6.01641000 -2.18952800 -1.11259100
H -7.16623600 1.95666700 -1.53629700
H -7.73989800 -0.45168800 -1.63484500
N -2.83085700 0.71210600 -0.25341900
N -3.35225000 -1.38694600 -0.38917200
N 1.67506300 1.87017500 0.54434500
N 3.06248300 0.16484400 0.85917700
C 3.66782400 -1.04315000 1.34618000
H 3.03863300 -1.46148500 2.14094500
H 3.75732800 -1.78862600 0.53624000
H 4.67219100 -0.82670300 1.75128900
C -3.24567900 -2.82499600 -0.38961300
H -2.18147400 -3.08717000 -0.31630300
H -3.79800500 -3.26172300 0.46025000
H -3.65033300 -3.23141300 -1.33105000
Co -0.22446500 -0.61082000 0.12154200
H -0.48126500 -3.47967100 1.12890600
C 2.66875500 -1.13502700 -2.92180100
C 2.91683600 -2.64863000 -2.99492300
H 2.42531300 -0.69368600 -3.90385300
H 3.54453100 -0.59400100 -2.51473400
H 2.43233400 -3.09895300 -3.88374700
H 3.99076500 -2.90396900 -3.02888800
B 1.46014200 -2.19841900 -1.31922900
O 1.57752700 -1.00413800 -2.04143400
O 2.32923100 -3.16569600 -1.82090100
N 0.57929800 -2.31265200 -0.24634300
C 0.38621500 -3.56582100 0.44410400
C 1.57837600 -4.04410700 1.26437700
H 1.81016700 -3.31738500 2.05923700
H 1.36260400 -5.02030400 1.73868400
H 2.46727800 -4.16750800 0.62209800
B 0.88488100 0.17732700 2.32656200

O 0.91854300 -1.08930200 2.90574200
O 0.05379000 1.03560700 3.02408800
C 0.12704500 -1.03495500 4.07998700
C -0.69918700 0.24475500 3.91985300
H -0.49156400 -1.94469700 4.15583100
H 0.79037200 -0.98886500 4.96437500
H -1.69539300 0.03556600 3.48453600
H -0.84437600 0.78667100 4.86920600
H 0.11994800 -4.37010000 -0.27510100
³⁶K
C -1.75517700 1.61919900 -0.81337800
C -2.60123900 0.80598900 -1.62301000
C -2.76806000 1.03966100 -2.98086200
C -2.00508000 2.04560100 -3.58960100
C -0.99845000 2.71403700 -2.88215700
C -0.84988000 2.45809100 -1.52436900
H -3.42499100 0.41198800 -3.58662000
H -2.13069100 2.24169100 -4.65793500
H -0.30918800 3.37397600 -3.41231900
C 1.06408100 3.92998100 -0.74257800
C 0.48789900 2.00459000 0.36193200
C 1.87742400 3.79528900 0.39534600
C 1.18815600 5.03132800 -1.58788300
C 2.87096700 4.72399800 0.69970600
C 2.17740800 5.96446500 -1.28054100
H 0.53435300 5.17699000 -2.44877000
C 3.01038100 5.81024900 -0.16163900
H 3.50792900 4.60884100 1.57968000
H 2.30155300 6.83931000 -1.92481800
H 3.77669200 6.56291200 0.04412100
C -4.14597200 -1.14076300 -1.07629200
C -2.25815500 -0.70552900 0.14660300
C -4.03808300 -2.08918200 -0.04483600
C -5.22199800 -1.15789800 -1.96190400
C -4.97947800 -3.10361800 0.11651800
C -6.16524800 -2.17097700 -1.79888600
H -5.33590200 -0.40448400 -2.74312000
C -6.04361900 -3.13120200 -0.78211400
H -4.89275000 -3.83935800 0.91925100
H -7.02270600 -2.21379800 -2.47628100
H -6.80537300 -3.91021100 -0.68683200
N -3.04333300 -0.31251700 -0.92133600
N -2.89345000 -1.77715700 0.67155100
N 0.22430200 2.82471200 -0.72202300

N 1.48207300 2.63289400 1.03802100
C 2.03911600 2.18052200 2.28885300
H 1.32945600 1.46440900 2.72331300
H 3.01822500 1.69307800 2.14098500
H 2.15500100 3.04080100 2.96742200
C -2.43832000 -2.52605000 1.81487500
H -1.55938400 -2.00596600 2.22208100
H -3.22744100 -2.55424800 2.58462400
H -2.18086100 -3.55751300 1.52346700
Co -0.98546900 0.70269900 0.88807400
H -2.69047200 0.40282100 3.21454800
C 2.34785800 -1.87523000 3.15471500
C 1.87287900 -1.67724900 4.60024500
H 2.23271600 -2.92071800 2.81705700
H 3.40318100 -1.58366200 3.00977000
H 1.86318200 -2.61978600 5.17528300
H 2.51483600 -0.95644400 5.14420300
B 0.40698200 -0.65595400 3.19097600
O 1.50460500 -1.03720400 2.38698200
O 0.57119800 -1.16000600 4.48279000
N -0.65987300 0.10613500 2.74411900
C -1.69383200 0.45810400 3.69933700
C -1.50887600 1.85807300 4.27215400
H -1.45581100 2.60593900 3.46075900
H -2.33554200 2.13520600 4.95307700
H -0.56524900 1.91811900 4.84373300
B -2.43730600 2.26503800 0.51979900
O -2.09254600 3.52177700 0.97473800
O -3.70044900 1.88979100 0.93133000
C -3.22514200 4.07074500 1.62901200
C -4.17266200 2.88006100 1.83115200
H -2.91893000 4.54098500 2.57773500
H -3.66853700 4.85007200 0.98235200
H -4.12814200 2.48452200 2.86135600
H -5.22239900 3.12168100 1.59681500
H -1.72357500 -0.26229600 4.54065500
K 1.78395700 -1.34454100 -0.26725500
O 4.20336100 -2.83495300 -0.38802900
O 4.33518800 -0.01843700 -0.29686400
O 1.04858100 -1.77161900 -3.01572000
O -0.35475100 -3.16470700 -0.87173700
O 2.37810900 0.58276000 -2.19110400
O 1.89542800 -4.04947400 0.63180200
C 5.39923200 -2.13445600 -0.17251200

C 4.20927900 -4.12648300 0.15628900
C 5.33687300 -0.80855600 -0.88014900
C 4.20047200 1.26932900 -0.84197600
C 0.12611500 -2.81012800 -3.22685200
C 0.58124500 -0.47904200 -3.32087200
C -0.92273900 -2.91103100 -2.13533800
C -0.17100500 -4.52314600 -0.57523400
C 3.59001000 1.28366300 -2.22701300
C 1.76091100 0.44800500 -3.44222200
C 2.86943900 -4.77235300 -0.07378500
C 0.62439300 -4.64016500 0.70554000
H 6.26274000 -2.70652600 -0.56959700
H 4.42144800 -4.08992600 1.24448500
H 4.99434700 -4.74829500 -0.32148300
H 5.13708700 -0.98726100 -1.95491300
H 6.32422100 -0.31027100 -0.79381200
H 5.17763600 1.79281300 -0.87215400
H 3.54402300 1.82033800 -0.15359100
H 0.71921100 -3.73925700 -3.27894700
H -0.38085600 -2.68666700 -4.20595300
H -0.11201500 -0.09955600 -2.54378600
H 0.03385800 -0.48303500 -4.28432000
H -1.46932600 -1.95858600 -2.04739400
H -1.66231500 -3.69189000 -2.40008200
H -1.14931600 -5.02893600 -0.43623900
H 0.34911300 -5.04745000 -1.40169100
H 4.27128600 0.82533600 -2.97291100
H 3.43618400 2.33931600 -2.53256300
H 2.47694800 0.03090800 -4.17944600
H 1.41423700 1.43132300 -3.81691800
H 2.91266700 -5.82088900 0.28406500
H 2.65428200 -4.79123000 -1.16123400
H 0.09433200 -4.11085500 1.51388500
H 0.70354600 -5.70934500 0.98868900
H 5.56701200 -1.97634300 0.91279500
³TSIW_{Co}
C -0.00003100 -0.05012300 -0.53176800
C -1.23624600 0.45097600 -0.97886200
C -1.31438300 1.52504500 -1.90193300
C -0.08589200 2.11883000 -2.31013900
C 1.18631800 1.63663900 -1.88902600
C 1.19163900 0.56112900 -0.96480900
H -2.25495600 1.90516300 -2.29614100
H -0.12012300 2.96334700 -3.00168900

H 2.09542700 2.10092200 -2.26683200
C 3.65446800 0.00411600 -0.50931100
C 1.93111800 -1.28616000 0.26692300
C 4.18080200 -1.10525600 0.17741200
C 4.49309100 0.97224800 -1.05673100
C 5.55135200 -1.29123000 0.32621100
C 5.86727200 0.78604100 -0.90664900
H 4.10409200 1.85336000 -1.56833100
C 6.38919600 -0.32603500 -0.23150800
H 5.95416700 -2.15213900 0.86475500
H 6.55151100 1.53220200 -1.32019700
H 7.47282600 -0.43462800 -0.13147000
C -3.64626400 -0.29123000 -0.52344400
C -1.83231100 -1.43115000 0.27878500
C -4.09085900 -1.41367900 0.19812700
C -4.55387100 0.59668600 -1.09629000
C -5.44419900 -1.69205700 0.35931000
C -5.91075900 0.31709500 -0.93623000
H -4.23099100 1.48739200 -1.63583100
C -6.35037800 -0.80785100 -0.22506200
H -5.78453200 -2.56120500 0.92679900
H -6.64714100 0.99881600 -1.37093200
H -7.42322100 -0.99109400 -0.11788800
N -2.26387200 -0.34606500 -0.45837100
N -2.95543500 -2.07264800 0.65732000
N 2.27943200 -0.15322600 -0.44485400
N 3.09846900 -1.85750500 0.61944900
C 3.22414900 -3.10531000 1.32698000
H 3.93067300 -3.76402600 0.79629300
H 3.58262500 -2.93829200 2.35736100
H 2.23903900 -3.58841800 1.34269700
C -2.99417200 -3.29123000 1.42360100
H -3.33100300 -3.09654200 2.45641700
H -3.68111900 -4.00975300 0.94682500
H -1.98332900 -3.72020500 1.43841300
Co 0.06098000 -1.57118700 0.52670200
H 0.10350600 -2.93304300 1.27242200
C 0.83610900 -4.36719300 -2.45150600
C -0.33741500 -3.59919500 -3.06879300
H 1.71229700 -4.42403500 -3.11948700
H 0.55491900 -5.39906400 -2.16773400
H -0.01870100 -2.96614100 -3.91802000
H -1.14846800 -4.25931600 -3.42043800
B 0.14095800 -2.73699900 -1.00896800

O 1.16456100 -3.63352800 -1.28497800
O -0.80659200 -2.77128500 -2.02011800
N 0.03505500 -0.82301800 2.45325000
C 0.08855200 -2.01754600 2.58449600
C 0.15108100 -3.08877800 3.60430100
H 0.14795600 -2.63812900 4.61030400
H -0.71198400 -3.76868200 3.50728700
H 1.06593600 -3.69141400 3.47737900
W -0.10873900 2.32670100 0.02620400
C -0.18255700 4.29373400 -0.04500500
O -0.22410300 5.45040800 -0.13656400
C -1.48664400 2.37721000 1.44047900
O -2.32422800 2.35923300 2.24045100
C 1.24199300 2.48129200 1.45825700
O 2.06955200 2.52657200 2.26725700

MeCN

N 1.43487300 0.00008800 -0.00008800
C 0.27784400 -0.00018800 0.00017200
C -1.17420400 0.00005600 -0.00003000
H -1.55525100 0.98737900 0.31003400
H -1.55533800 -0.22501400 -1.01011800
H -1.55536400 -0.76218600 0.69984300

¹LCo

C -0.00000300 0.66074800 0.00023800
C -1.20002000 1.36810400 0.00006100
C -1.22726700 2.76303900 -0.00011500
C 0.00000000 3.44174000 -0.00014900
C 1.22726400 2.76303500 0.00002300
C 1.20001500 1.36809900 0.00018200
H -2.15842100 3.33313300 -0.00029800
H 0.00000100 4.53583300 -0.00030400
H 2.15841700 3.33312900 -0.00003600
C 3.64589000 0.57313700 0.00004000
C 1.88180300 -0.88664100 0.00013600
C 4.14881100 -0.74536300 -0.00007500
C 4.51812800 1.66227600 0.00003700
C 5.51457600 -1.01248300 -0.00018800
C 5.88773600 1.39360300 -0.00009700
H 4.15451300 2.69021000 0.00015400
C 6.38083700 0.08171400 -0.00020800
H 5.89336600 -2.03749600 -0.00025800
H 6.59179600 2.23083300 -0.00010300
H 7.46135100 -0.08823700 -0.00030500
C -3.64589000 0.57313800 -0.00004200

C -1.88179000 -0.88663300 -0.00003200
C -4.14880300 -0.74536500 -0.00005000
C -4.51813000 1.66227400 -0.00001600
C -5.51456600 -1.01248900 -0.00003700
C -5.88773800 1.39359700 -0.00001400
H -4.15451400 2.69020800 0.00002600
C -6.38083200 0.08170600 -0.00002900
H -5.89335300 -2.03750400 -0.00003100
H -6.59180100 2.23082500 0.00000800
H -7.46134600 -0.08825000 -0.00002700
N -2.27245300 0.44451400 -0.00002000
N -3.05024000 -1.58686700 -0.00007700
N 2.27245100 0.44450600 0.00018100
N 3.05025200 -1.58686900 -0.00004000
C 3.13978400 -3.02154300 -0.00004400
H 3.67074600 -3.38192800 -0.89850500
H 3.67022200 -3.38199900 0.89870300
H 2.11991400 -3.43362400 -0.00036700
C -3.13976500 -3.02154000 -0.00002800
H -3.67009000 -3.38197100 0.89879500
H -3.67083600 -3.38195800 -0.89841300
H -2.11989300 -3.43361800 -0.00046600
Co -0.00001300 -1.15294400 0.00013200

¹⁷K_{Dipp}

C 0.59238900 0.03410800 1.23796500
C 1.05482400 1.18097000 1.90630400
C 2.06359300 1.12016500 2.86837300
C 2.64405700 -0.12750100 3.14760000
C 2.23527800 -1.29267200 2.47855000
C 1.21616000 -1.18876100 1.53195800
H 2.40304900 2.00357800 3.41028700
H 3.43975000 -0.19442200 3.89455300
H 2.71253000 -2.24221300 2.71809500
C 0.90035700 -3.54557600 0.61545400
C -0.40282400 -1.76560500 -0.06792100
C -0.00184100 -4.00285600 -0.35851600
C 1.80417700 -4.42574300 1.21102500
C -0.00812200 -5.32632700 -0.79294000
C 1.79320200 -5.75506800 0.78627000
H 2.49960000 -4.10020300 1.98271000
C 0.90806000 -6.19907500 -0.20595000
H -0.70936400 -5.66367600 -1.55924200
H 2.49025700 -6.46467600 1.24135200
H 0.92762700 -7.24688200 -0.51842400

C 0.65185400 3.64964000 1.48997000
C -0.64587400 2.00184400 0.50982300
C -0.24068200 4.26025800 0.59317200
C 1.60281500 4.40894600 2.17172400
C -0.20004800 5.62767800 0.33293900
C 1.63831000 5.78274300 1.92051300
H 2.31173400 3.95896500 2.86522800
C 0.75538500 6.38346300 1.01442400
H -0.89614000 6.08610700 -0.37308000
H 2.37445900 6.39972400 2.44399100
H 0.81082500 7.46165800 0.83907600
N 0.36852100 2.29719200 1.42748700
N -1.03696700 3.25468200 0.06105700
N 0.63688700 -2.19616800 0.75455500
N -0.77556800 -2.91247200 -0.73780700
Co -0.88805400 0.10328500 0.15475600
H -4.80658900 1.12632000 3.85619500
C -3.59396900 -0.22519000 -1.39295300
C -4.97678600 0.41730100 -1.25037900
H -3.70772300 -1.30252900 -1.58314600
H -4.91651400 1.48716400 -1.52338800
B -4.07493800 0.10590000 0.81080500
O -3.01474200 -0.08831700 -0.07704500
O -5.24999100 0.33830800 0.14470700
N -4.00052900 0.08546800 2.22259900
C -5.16537600 0.56508300 2.97794000
C -6.08141400 -0.56272300 3.42078900
H -5.54764100 -1.27519700 4.07439100
H -6.94054400 -0.16410000 3.98936400
H -6.47463400 -1.11592200 2.55019600
B -2.99506200 -0.58061500 2.99366500
O -2.14943700 -1.54147200 2.51398100
O -2.87157400 -0.36964300 4.34068000
C -1.31719000 -1.97056100 3.58940300
C -1.91953700 -1.29816100 4.84779300
H -0.30594900 -1.57046700 3.40675100
H -2.47145300 -2.04673900 5.44840500
H -5.72662500 1.26672200 2.34688100
C -2.70038100 0.38930900 -2.42846200
H -1.69555300 -0.06166500 -2.36907000
H -3.10097400 0.19850600 -3.43794000
H -2.61337800 1.47455200 -2.28168000
C -6.05954300 -0.26036300 -2.05292400
H -7.03009800 0.23759500 -1.89024500

H -5.82497000 -0.21302800 -3.13058800	H -5.86032600 4.49613500 0.58646700
H -6.15650300 -1.32058200 -1.76242300	H -2.29786100 5.09538100 1.66110200
C -0.89985400 -0.60128900 5.71665400	H -3.79534000 5.89981700 1.12152700
H -1.38727300 -0.11941200 6.58120900	H -3.77973600 4.94248800 2.62882600
H -0.15963800 -1.32684100 6.09769900	C -0.26754000 -2.30467300 -3.52277000
H -0.36411100 0.17123500 5.13794900	C -0.35887100 -1.35498600 -4.71569300
C -1.26684000 -3.47806300 3.65753800	C 0.64159600 -3.48617400 -3.87580400
H -0.84836800 -3.90403300 2.73060100	H 0.20039900 -1.75176300 -2.68934900
H -0.62656400 -3.79970600 4.49828500	H -1.07306100 -0.53425200 -4.54324900
H -2.27727200 -3.89636100 3.81189800	H 0.62963800 -0.90308500 -4.91104700
C -1.84401200 -3.07849200 -1.66744100	H -0.65859700 -1.88221100 -5.63855000
C -1.61531400 -2.80293600 -3.03018600	H 0.81985000 -4.14598700 -3.01190500
C -3.06694900 -3.60093000 -1.19916800	H 0.19005700 -4.09477600 -4.67977500
C -2.65715600 -3.05300800 -3.92879100	H 1.62046700 -3.12457300 -4.23924600
C -4.06513200 -3.86334000 -2.14420400	C -0.05144400 3.52759100 -2.63638900
C -3.86629000 -3.58844900 -3.49309600	C 0.45979800 4.73197700 -3.42711700
H -2.51885700 -2.83798200 -4.99127000	C 0.21096900 2.21659600 -3.37706500
H -5.02334300 -4.27360400 -1.81411500	H 0.51858300 3.48592900 -1.69595100
H -4.66406900 -3.78991000 -4.21439200	H 0.27363400 5.67643200 -2.88704100
C -1.98762200 3.54834200 -0.96040200	H 1.54790900 4.64893800 -3.59608600
C -3.33913600 3.77377900 -0.61961300	H -0.01759600 4.81000300 -4.41987800
C -1.51671100 3.68754700 -2.27960300	H 0.00618300 1.35089400 -2.72623500
C -4.22359000 4.06894200 -1.66309500	H -0.41427400 2.13232300 -4.28404900
C -2.44401700 3.98099600 -3.28529000	H 1.26868200 2.15964500 -3.68484500
C -3.78713900 4.15935900 -2.98234200	K 3.88287800 0.09698700 0.06484800
H -5.27969300 4.23644700 -1.44469800	O 3.96664300 -2.62860300 -0.35824000
H -2.10677400 4.07036800 -4.32175600	O 3.60352200 1.72334600 -2.19659500
H -4.50338300 4.38558500 -3.77798600	O 5.67249700 -1.55417400 1.61052800
C -3.32878900 -3.84497300 0.27571200	C 3.45131800 -2.95748000 -1.62445000
C -3.22119300 -5.32781400 0.63877000	C 5.13244100 -3.31468800 0.01515100
C -4.68813800 -3.30328200 0.71856200	C 3.91362500 3.08390800 -2.04165000
H -2.56573000 -3.29137100 0.84404000	C 3.94858400 1.20934300 -3.45431300
H -2.21849200 -5.73379400 0.43102900	C 6.96921200 -1.07805000 1.36190800
H -3.42484600 -5.47165500 1.71490500	C 5.47719000 -2.93354300 1.43675100
H -3.95808100 -5.92866700 0.07469100	C 4.27885200 -2.37900100 -2.75553500
H -4.85018700 -2.26424100 0.39167100	H 2.42839700 -2.54657900 -1.65097800
H -5.52463000 -3.91042100 0.32860400	H 3.37230600 -4.05687500 -1.74272900
H -4.75648900 -3.31975000 1.81952600	H 4.97076900 -4.41128600 -0.03284000
C -3.82325200 3.73816100 0.82225900	H 5.97731900 -3.07354500 -0.66073800
C -5.33717200 3.59445800 0.95150300	C 3.46851200 3.53373000 -0.66957500
C -3.38980100 4.98822100 1.59673400	H 5.00121800 3.24713500 -2.18722300
H -3.34892300 2.86517600 1.30609200	H 3.38768100 3.69339500 -2.80399000
H -5.73016200 2.71745000 0.41323800	C 3.57440400 -0.24584200 -3.52897700
H -5.60458000 3.48273900 2.01521400	H 5.03827000 1.31655100 -3.63283600

H 3.41776500 1.75731200 -4.25875200
C 7.06490000 0.33344900 1.87716400
H 7.72011200 -1.69758000 1.89258700
H 7.21554600 -1.10187200 0.27998400
H 4.64150700 -3.21381900 2.09714400
H 6.37096600 -3.50254300 1.76041700
O 4.39383600 -0.97783700 -2.65455900
H 5.30219400 -2.79303400 -2.73993900
H 3.82896800 -2.67275800 -3.72242400
O 4.12813700 2.85173300 0.36938900
H 3.60647100 4.62786400 -0.57471700
H 2.39463200 3.32143000 -0.54926500
H 2.50070700 -0.36751700 -3.27643200
H 3.71976900 -0.58754500 -4.57343300
O 6.23978400 1.17476600 1.11426500
H 6.75325100 0.34632500 2.94084000
H 8.11964700 0.67270000 1.82384000
C 5.39936100 3.35529500 0.68258400
C 6.06688800 2.44848000 1.68075700
H 6.03763500 3.42474200 -0.22029800
H 5.31596200 4.37136700 1.11930300
H 7.04575100 2.89225700 1.95329000
H 5.45642900 2.37813400 2.60428100

MECP

C 0.30404813 -1.58385392 0.12096744
C 1.55374115 -2.19290091 0.04400313
C 1.70633083 -3.57834188 0.01802643
C 0.54478159 -4.36131424 0.07067287
C -0.72703538 -3.78875281 0.14314136
C -0.82467362 -2.38975630 0.15611845
H 2.68282027 -4.06329591 -0.03358116
H 0.64053516 -5.45105352 0.06288802
H -1.61066525 -4.42844750 0.20782110
C -3.14342932 -1.83229472 -0.59930497
C -1.98417982 -0.30702944 0.65688969
C -3.82356508 -0.59252275 -0.64811649
C -3.61394503 -2.92573609 -1.32311359
C -4.99991372 -0.43527680 -1.38142036
C -4.79832145 -2.76743066 -2.05403653
H -3.08194481 -3.87774981 -1.32699548
C -5.48208979 -1.54844083 -2.07834388
H -5.52560594 0.52219651 -1.41097919
H -5.19264799 -3.62054641 -2.61366763

H -6.41016821 -1.45861510 -2.65107704
C 3.92485438 -1.24204200 -0.26413948
C 2.09582901 0.09440585 0.01051782
C 4.31932034 0.10396376 -0.38673121
C 4.86414213 -2.26783741 -0.38371234
C 5.63959456 0.46859745 -0.63389062
C 6.18799619 -1.90294651 -0.62659517
H 4.58838394 -3.31831512 -0.29041062
C 6.57290751 -0.55968663 -0.75143034
H 5.93163418 1.51737661 -0.72740838
H 6.94498869 -2.68724187 -0.71809507
H 7.62194641 -0.31394751 -0.94159390
N 2.56213855 -1.20150315 -0.03251314
N 3.17691732 0.87185843 -0.22024288
N -2.02603905 -1.65111315 0.19213950
N -3.10046962 0.31000213 0.08067847
C -3.43327980 1.69994852 0.20921243
H -2.54596770 2.23989792 0.56508229
H -3.72757737 2.10077499 -0.77659105
H -4.26317486 1.85334536 0.92278296
C 3.16185270 2.30739935 -0.34152456
H 2.11391143 2.62939313 -0.27829187
H 3.74877232 2.77328359 0.46769171
H 3.58948076 2.60424227 -1.31377565
C 0.20922778 0.29538195 0.31968312
H 0.65514793 2.78178246 2.40297908
C -1.03863865 1.78216022 -2.88277584
C -0.72040173 3.28841857 -2.91528155
H -0.51756016 1.22152273 -3.67807728
H -2.12446319 1.58743638 -2.98110555
H 0.22103250 3.48608736 -3.46454623
H -1.52129817 3.88185251 -3.39059385
B -0.37621380 2.51426463 -0.81367395
O -0.59092851 1.36944358 -1.61468005
O -0.56720013 3.67103761 -1.56386280
N -0.00089077 2.27331796 0.49102052
C 0.33912557 3.27268152 1.46220518
C -0.79304929 4.24576971 1.77863819
H -1.67554827 3.71256061 2.17177034
H -0.48016557 4.99676467 2.52842423
H -1.10427453 4.78751882 0.86798615
B -1.46826755 0.15999224 2.03250318
O -2.07728412 1.11932451 2.80452075
O -0.29518398 -0.30853912 2.59338034

C -1.28326606 1.34097553 3.95743219
C -0.08772190 0.37708502 3.82358382
H -0.96919261 2.39747095 3.99145192
H -1.88930850 1.13430504 4.85696838
H 0.88185227 0.89904544 3.78167754
H -0.04998933 -0.36566414 4.63788588
H 1.21980162 3.88214685 1.15443459

37

C -0.26833600 -2.00222700 -0.15341600
C -1.54215400 -2.57671800 -0.25737600
C -1.72427800 -3.95918600 -0.30172400
C -0.58452600 -4.77567200 -0.27956000
C 0.71045200 -4.23806700 -0.25748300
C 0.84583600 -2.85011800 -0.21171300
H -2.71395300 -4.41426000 -0.38569500
H -0.70808600 -5.86236600 -0.31665700
H 1.57255200 -4.90710400 -0.30657200
C 3.34036000 -2.36837400 0.04751900
C 1.82150200 -0.72170100 -0.48325100
C 4.00631100 -1.12254200 0.04525600
C 4.03221600 -3.53919300 0.35399900
C 5.36926500 -1.02050400 0.31236800
C 5.40056600 -3.43451000 0.63083900
H 3.53420600 -4.50876500 0.38343500
C 6.05968200 -2.20185000 0.60514300
H 5.88241100 -0.05590700 0.29447300
H 5.96367900 -4.34146100 0.87017100
H 7.13199300 -2.15767900 0.81765800
C -3.86100600 -1.52221500 -0.06859800
C -1.99163300 -0.29277700 -0.60941400
C -4.21696300 -0.15580400 -0.11758800
C -4.81030700 -2.48893100 0.25917300
C -5.51791000 0.27197400 0.13449600
C -6.11775100 -2.05766100 0.51444700
H -4.55288800 -3.54681600 0.32268400
C -6.46863700 -0.70589800 0.44876300
H -5.78578100 1.33077800 0.09503200
H -6.87966000 -2.79947700 0.77158900
H -7.50103800 -0.40511800 0.65039900
N -2.51367000 -1.56534000 -0.36604900
N -3.07057400 0.54348100 -0.43860400
N 2.02593200 -2.08681100 -0.26769900
N 3.05797500 -0.16448700 -0.25370000

C 3.35128600 1.23666400 -0.34622800
H 2.40939900 1.79435500 -0.28493000
H 3.99130300 1.54812900 0.49650700
H 3.86795500 1.48802000 -1.29161700
C -3.02563000 1.97047600 -0.57907100
H -3.16473000 2.47474300 0.39509500
H -2.04467700 2.24311700 -0.98714100
H -3.81318200 2.31992700 -1.27025400
Co -0.04838800 -0.17704200 -0.56896900
H 0.30096900 5.55890800 -0.03366600
C -0.50923500 0.62871600 2.44937700
C -0.25494300 1.71448900 3.50054200
H -1.58150800 0.39406400 2.33331400
H 0.03337500 -0.30997900 2.63499000
H -1.07871300 1.80932400 4.22593200
H 0.68318400 1.54059800 4.05761100
B 0.06755800 2.57133700 1.44791300
O -0.03774000 1.21558900 1.23952100
O -0.13103200 2.92047000 2.75509400
N 0.35392300 3.51345200 0.41794300
C 0.61434100 4.90502800 0.79571400
C 2.07650400 5.15141900 1.12399500
H 2.71980200 4.93461100 0.25282700
H 2.23930600 6.20493200 1.41277200
H 2.40423500 4.51414400 1.96449300
B 0.45293800 3.14977500 -0.94910000
O 0.22641500 1.87042100 -1.42887400
O 0.77462900 4.02745000 -1.94725700
C 0.56634600 1.86060200 -2.81366400
C 0.63703200 3.34526900 -3.18644000
H 1.53313800 1.34207300 -2.93351000
H -0.20089900 1.30082400 -3.37110800
H 1.49512400 3.57976600 -3.83668200
H -0.28438000 3.69251100 -3.68706500
H -0.01274100 5.15504400 1.66627000

[K]·1THF

K 0.32237200 0.09415800 -0.06170800
O 0.64810400 2.73854400 -0.65109500
O -1.89752600 1.51176900 -0.87860000
O 1.31622400 -2.08715700 -1.45159800
O 2.19956600 -1.35684700 1.23017400
O -1.34014100 -1.14027000 -1.81671900
O 2.89114000 1.17903300 0.17920600

C -0.55845400 3.45789500 -0.67439700
C 1.63171300 3.27563600 0.19835300
C -1.56332100 2.71878600 -1.51935900
C -2.82804400 0.69739000 -1.55257100
C 2.38800600 -2.71386900 -0.78047400
C 0.23925700 -2.92621200 -1.79030800
C 2.24227800 -2.67532100 0.73034100
C 3.45116900 -0.74703600 1.43788500
C -2.19028700 -0.27157300 -2.52360500
C -0.75882400 -2.14659900 -2.60725300
C 2.94156200 2.56568400 -0.06363100
C 3.28700600 0.75186500 1.46016400
H -0.39996900 4.46768700 -1.10395900
H 1.32337300 3.17410100 1.26036400
H 1.77504700 4.35680200 -0.00321000
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H 2.49581900 -3.76458000 -1.11318900
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H 0.59355500 -3.78206400 -2.39892900
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H 3.06902300 -3.24729700 1.19540500
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H 4.16168300 -1.01054100 0.63191700
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H -0.24661600 -1.70131400 -3.48406300
H -1.53588400 -2.84230600 -2.98346300
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H 4.25775800 1.20722000 1.73901400
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[K]·2THF

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O -1.65591800 -0.26347700 2.24871400
C 0.78793200 -3.20344700 0.55318300
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1K-BPh₄

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C -2.33891200 1.93739700 3.00305200
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H -2.58556100 0.96412400 4.91180900
H -1.77931200 2.77215100 3.42905600
C -1.47519400 3.84087100 0.49786500

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C 0.01218700 5.98945500 -0.43619600
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C 4.84921300 2.67074100 -1.76214800
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H 4.60050100 4.12637700 1.29975800
H 4.27434100 4.66326500 -1.11869300

TS1K-BPh₄

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C -4.54949800 -1.31769100 -0.03440200
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H	0.23404700	3.35547100	3.59670600	C	3.86836400	-0.95578600	1.12851700
H	1.16812400	3.91365700	1.46991600	C	5.22514500	0.75352800	2.07956100
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H	1.37084300	-3.47234800	-0.11602400	H	3.62351100	-1.65307400	0.32349000
H	1.57604300	-3.25343400	-1.87389600	C	4.37700500	0.82659900	3.18607400
H	0.42789100	-0.54311000	-2.35303400	H	6.09439100	1.41967500	2.03821000
H	2.09615900	-1.18020100	-2.57880600	C	3.25151700	0.00222900	3.26321800
H	-0.85878200	-2.59447600	-2.04369700	H	2.11302600	-1.53253700	2.24648000
H	-0.62801600	-4.26269900	-1.45940200	H	4.59503700	1.53491300	3.99395800
H	-2.28675500	-4.47488300	0.63044700	H	2.57140200	0.05550900	4.11870600
H	-0.51864500	-4.49491900	0.94038400	C	5.40663400	-0.93494300	-1.55993500
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H	2.21801900	1.20619400	-2.29915700	H	5.37014300	-2.90455600	-0.66855000
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H	-1.88996900	-4.02869200	2.96184700	H	4.38813700	-4.05307700	-2.61537400
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B	6.08176000	-0.22651700	-0.23352900	H	3.88793700	-2.77970100	-4.71170400
C	6.56518200	1.30296200	-0.59657700				
C	7.90242300	1.68795000	-0.78259200				
C	5.60907100	2.32551800	-0.75587200				
C	8.26703200	2.99662400	-1.11392300				
H	8.69268400	0.93983900	-0.65742200				
C	5.95184300	3.63507100	-1.09024700				
H	4.55195000	2.08228100	-0.60202600				
C	7.29266600	3.98075000	-1.27334600				
H	9.32550500	3.24912600	-1.24480900				
H	5.16939900	4.39484500	-1.20458000				
H	7.57361900	5.00743600	-1.53192500				
C	7.37447300	-1.14218500	0.21054300				
C	7.69258700	-1.45857600	1.54124900				
C	8.26473100	-1.63202100	-0.76560900				
C	8.82352800	-2.20524000	1.88447600				
H	7.03086600	-1.11305700	2.34320200				
C	9.39996200	-2.37477400	-0.44141800				
H	8.05599100	-1.42492500	-1.82171900				
C	9.68811600	-2.66730900	0.89340700				
H	9.02855600	-2.42956800	2.93769200				