

# Influence of Intramolecular vs. Intermolecular Phosphonium-Borohydrides in Catalytic Hydrogen, Hydride, and Proton Transfer Reactions

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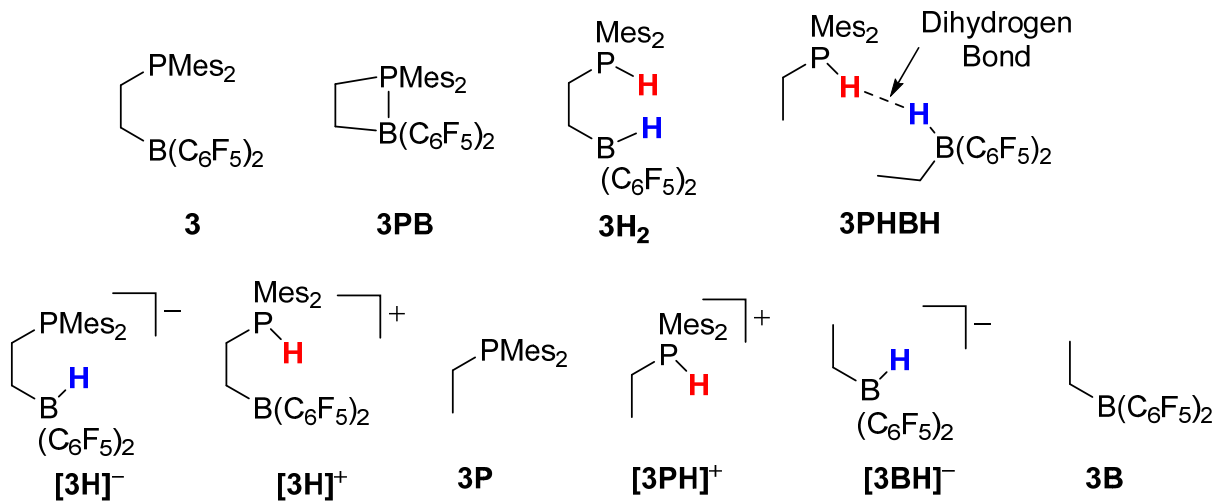
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## *Supporting Information*

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1) Nomenclature for the Intermolecular and Intramolecular Phosphonium-Borohydrides Described Within



**Figure S1.** Representative nomenclature for the respective intramolecular (**3**, **3PB**, and **3H<sub>2</sub>**) and intermolecular phosphonium-borohydrides (**3P**, **[3PH]<sup>+</sup>**, **[3BH]<sup>-</sup>**, and **3B**) for complex **3H<sub>2</sub>** that were investigated in this study.

## 2) Gas Phase Energies of Calculated Intermolecular FLPs

**Table S1.** List of calculated electronic energies, free energy correction, and enthalpy correction for intermolecular FLPs described within. All calculations were implemented using the M06-2X/6-31g(d,p) level of theory at 298K.

Complex	Electronic Energies Gas Phase (Hartrees)	Free Energy Change Gas Phase (Hartrees)	Enthalpy Change Gas Phase (Hartrees)
<b>1P</b>	-1668.560681	0.351227	0.441357
<b>[1PH]<sup>+</sup></b>	-1668.944913	0.361222	0.452670
<b>1B</b>	-2108.316571	0.108593	0.194263
<b>[1BH]<sup>-</sup></b>	-2109.011382	0.113363	0.202592
<b>1PHBH</b>	-3778.076021	0.503944	0.657393
<b>2P</b>	-1285.218856	0.261138	0.329282
<b>[2PH]<sup>+</sup></b>	-1285.597886	0.270925	0.340303
<b>2B</b>	-2108.316571	0.108593	0.194263
<b>[2BH]<sup>-</sup></b>	-2109.011382	0.113363	0.202592
<b>2PHBH</b>	-3394.732688	0.409754	0.545934
<b>3P</b>	-1119.390306	0.367270	0.443977
<b>[3PH]<sup>+</sup></b>	-1119.784295	0.377825	0.455150
<b>3B</b>	-1559.13833	0.121371	0.196600
<b>[3BH]<sup>-</sup></b>	-1559.817006	0.128166	0.204682
<b>3PHBH</b>	-2679.722225	0.529525	0.662215
<b>4P</b>	-1158.685323	0.392464	0.474030
<b>[4PH]<sup>+</sup></b>	-1159.079270	0.403288	0.485262
<b>4B</b>	-1598.432492	0.147063	0.226041
<b>[4BH]<sup>-</sup></b>	-1599.112862	0.153585	0.234547
<b>4PHBH</b>	-2758.316887	0.587503	0.722682
<b>5P</b>	-1197.977151	0.419675	0.503934
<b>[5PH]<sup>+</sup></b>	-1198.374996	0.431354	0.515370
<b>5B</b>	-1637.727583	0.173547	0.256035
<b>[5BH]<sup>-</sup></b>	-1638.407620	0.182112	0.264948
<b>5PHBH</b>	-2836.909846	0.639549	0.782201
<b>6P</b>	-1080.096337	0.337858	0.413399
<b>[6PH]<sup>+</sup></b>	-1080.487770	0.349322	0.424651
<b>6B</b>	-1519.846993	0.093764	0.165678
<b>[6BH]<sup>-</sup></b>	-1520.522560	0.100759	0.174366
<b>6PHBH</b>	-2601.133892	0.475663	0.601067

Complex	Electronic Energies Gas Phase (Hartrees)	Free Energy Change Gas Phase (Hartrees)	Enthalpy Change Gas Phase (Hartrees)
<b>7P</b>	-1158.68188	0.392767	0.473797
<b>[7PH]<sup>+</sup></b>	-1159.080651	0.405549	0.485135
<b>7B</b>	-1598.431549	0.148103	0.226245
<b>[7BH]<sup>-</sup></b>	-1599.113424	0.155586	0.234162
<b>7PHBH</b>	-2758.305470	0.585153	0.721701
<b>8P</b>	-696.7549250	0.248931	0.301089
<b>[8PH]<sup>+</sup></b>	-697.1413471	0.258709	0.312185
<b>8B</b>	-1519.846993	0.093764	0.165678
<b>[8BH]<sup>-</sup></b>	-1520.522560	0.100759	0.174366
<b>8PHBH</b>	-2217.791887	0.383888	0.489235
<b>9P</b>	-696.7549250	0.248928	0.30109
<b>[9PH]<sup>+</sup></b>	-697.1413471	0.258707	0.312186
<b>9B</b>	-527.8599599	0.186042	0.238131
<b>[9BH]<sup>-</sup></b>	-528.4924939	0.191362	0.245266
<b>9PHBH</b>	-1225.771802	0.472925	0.560192
<b>10P</b>	-1313.442026	0.467459	0.549415
<b>[10PH]<sup>+</sup></b>	-1313.834562	0.477872	0.560703
<b>10B</b>	-1753.206131	0.220273	0.301742
<b>[10BH]<sup>-</sup></b>	-1753.889877	0.226809	0.309864
<b>10PHBH</b>	-3067.860723	0.73133	0.872971
<b>11P</b>	-1236.063514	0.430013	0.512128
<b>[11PH]<sup>+</sup></b>	-1236.465266	0.441543	0.523592
<b>11B</b>	-1675.820584	0.183694	0.264647
<b>[11BH]<sup>-</sup></b>	-1676.501498	0.190131	0.272448
<b>11PHBH</b>	-2913.097877	0.658921	0.798239
<b>12P</b>	-1526.740752	0.438502	0.530023
<b>[12PH]<sup>+</sup></b>	-1527.139861	0.448284	0.541223
<b>12B</b>	-1966.492315	0.189872	0.282870
<b>[12BH]<sup>-</sup></b>	-1967.172994	0.195843	0.291146
<b>12PHBH</b>	-3494.424657	0.672645	0.834947
<b>13P</b>	-2076.082851	0.446321	0.556528
<b>[13PH]<sup>+</sup></b>	-2076.47039	0.458355	0.567614
<b>13B</b>	-2515.836664	0.202385	0.309548
<b>[13BH]<sup>-</sup></b>	-2516.527540	0.210898	0.317471
<b>13PHBH</b>	-4593.113963	0.698599	0.887938

Complex	Electronic Energies Gas Phase (Hartrees)	Free Energy Change Gas Phase (Hartrees)	Enthalpy Change Gas Phase (Hartrees)
<b>14P</b>	-1840.299416	0.291302	0.379243
<b>[14PH]<sup>+</sup></b>	-1840.675581	0.300566	0.390591
<b>14B</b>	-2515.836664	0.202385	0.309548
<b>[14BH]<sup>-</sup></b>	-2516.527540	0.210898	0.317471
<b>14PHBH</b>	-4357.319037	0.53753	0.710383
<b>15P</b>	-1727.223973	0.295154	0.383162
<b>[15PH]<sup>+</sup></b>	-1727.599943	0.306679	0.394358
<b>15B</b>	-2402.762759	0.207602	0.313005
<b>[15BH]<sup>-</sup></b>	-2403.449076	0.216424	0.321109
<b>15PHBH</b>	-4131.172729	0.548628	0.718388
<b>16P</b>	-2413.170047	0.378178	0.479046
<b>[16PH]<sup>+</sup></b>	-2413.552747	0.389794	0.490397
<b>16B</b>	-3088.704274	0.285480	0.409330
<b>[16BH]<sup>-</sup></b>	-3089.403805	0.296231	0.417532
<b>16PHBH</b>	-5503.078847	0.712413	0.910290
<b>17P</b>	-1648.634752	0.242505	0.322747
<b>[17PH]<sup>+</sup></b>	-1649.008539	0.252305	0.333892
<b>17B</b>	-2324.171422	0.153933	0.252732
<b>[17BH]<sup>-</sup></b>	-2324.857214	0.162592	0.260841
<b>17PHBH</b>	-3973.994714	0.443397	0.597547
<b>18P</b>	-1278.964289	0.528543	0.611859
<b>[18PH]<sup>+</sup></b>	-1279.360893	0.538780	0.622992
<b>18B</b>	-2102.063789	0.375883	0.476028
<b>[18BH]<sup>-</sup></b>	-2102.748039	0.384699	0.484911
<b>18PHBH</b>	-3382.226527	0.952765	1.110798
<b>19P</b>	-1909.137109	0.616945	0.71945
<b>[19PH]<sup>+</sup></b>	-1909.527313	0.627247	0.730652
<b>19B</b>	-2498.864889	0.339266	0.447345
<b>[19BH]<sup>-</sup></b>	-2499.556477	0.348923	0.456380
<b>19PHBH</b>	-4409.209145	1.005675	1.189918
<b>20P</b>	-1576.735973	0.447032	0.539426
<b>[20PH]<sup>+</sup></b>	-1577.132267	0.455975	0.550632
<b>20B</b>	-2016.488646	0.202541	0.292265
<b>[20BH]<sup>-</sup></b>	-2017.174329	0.209134	0.300561
<b>20PHBH</b>	-3594.428899	0.694784	0.853124

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<b>Complex</b>	<b>Electronic Energies Gas Phase (Hartrees)</b>	<b>Free Energy Change Gas Phase (Hartrees)</b>	<b>Enthalpy Change Gas Phase (Hartrees)</b>
<b>21P</b>	-1694.618639	0.528759	0.628592
<b>[21PH]<sup>+</sup></b>	-1695.019353	0.538061	0.639842
<b>21B</b>	-2134.370621	0.283584	0.381431
<b>[21BH]<sup>-</sup></b>	-2135.054477	0.290551	0.389723
<b>21PHBH</b>	-3830.187216	0.858283	1.032134
<b>22P</b>	-1232.687658	0.383488	0.457493
<b>[22PH]<sup>+</sup></b>	-1233.078840	0.392517	0.468463
<b>22B</b>	-2134.370621	0.283586	0.381432
<b>[22BH]<sup>-</sup></b>	-2135.054477	0.290545	0.389723
<b>22PHBH</b>	-3368.252035	0.710794	0.860812

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### 3) Gas Phase Energies of Calculated Intramolecular Phosphonium-Borohydrides

**Table S2.** List of calculated electronic energies, free energy correction, and enthalpy correction for intramolecular FLPs described within. All calculations were implemented using the M06-2X/6-31g(d,p) level of theory at 298K.

Complex	Electronic Energies Gas Phase (Hartrees)	Free Energy Change Gas Phase (Hartrees)	Enthalpy Change Gas Phase (Hartrees)
1H <sub>2</sub>	-3149.099670	0.440258	0.578193
1	-3147.933589	0.421958	0.557975
[1H] <sup>-</sup>	-3148.632535	0.426764	0.566469
[1H] <sup>+</sup>	-3148.317095	0.432372	0.569322
2H <sub>2</sub>	-2765.756650	0.347038	0.465607
2	-2764.591626	0.332597	0.445853
[2H] <sup>-</sup>	-2765.287884	0.338534	0.454330
[2H] <sup>+</sup>	-2764.970251	0.340346	0.456779
3H <sub>2</sub>	-2599.935517	0.458581	0.580285
3	-2598.764802	0.441879	0.560752
3PB	-2598.771291	0.444495	0.560478
[3H] <sup>-</sup>	-2599.446689	0.449821	0.569002
[3H] <sup>+</sup>	-2599.145728	0.447036	0.571553
4H <sub>2</sub>	-2639.220857	0.488425	0.610615
4	-2638.041299	0.461374	0.589884
4PB	-2638.078393	0.474721	0.591545
[4H] <sup>-</sup>	-2638.726784	0.469586	0.598437
[4H] <sup>+</sup>	-2638.442874	0.474186	0.601512
5H <sub>2</sub>	-2678.486808	0.506039	0.640078
5	-2677.339647	0.486690	0.620080
5PB	-2677.366736	0.503406	0.621951
[5H] <sup>-</sup>	-2678.022676	0.495418	0.628575
[5H] <sup>+</sup>	-2677.733740	0.499386	0.631412
6H <sub>2</sub>	-2560.658760	0.429561	0.550790
6	-2559.472790	0.415599	0.530549
[6H] <sup>-</sup>	-2560.149843	0.420983	0.538550
[6H] <sup>+</sup>	-2559.860458	0.424240	0.541526
7H <sub>2</sub>	-2639.235912	0.488529	0.611412
7	-2638.036536	0.465201	0.589949
[7H] <sup>-</sup>	-2638.713200	0.476667	0.598496
[7H] <sup>+</sup>	-2638.426155	0.477364	0.601495

Complex	Electronic Energies Gas Phase (Hartrees)	Free Energy Change Gas Phase (Hartrees)	Enthalpy Change Gas Phase (Hartrees)
<b>8H<sub>2</sub></b>	-2177.316333	0.337024	0.438150
<b>8</b>	-2176.124580	0.320423	0.417552
<b>[8H]<sup>-</sup></b>	-2176.801223	0.325938	0.426155
<b>[8H]<sup>+</sup></b>	-2176.512436	0.331718	0.428997
<b>9H<sub>2</sub></b>	-1185.304686	0.428862	0.509458
<b>9</b>	-1184.132008	0.411597	0.490101
<b>[9H]<sup>-</sup></b>	-1184.772523	0.415663	0.496812
<b>[9H]<sup>+</sup></b>	-1184.534024	0.422278	0.501194
<b>10H<sub>2</sub></b>	-2794.016662	0.560024	0.686092
<b>10</b>	-2792.823329	0.540349	0.665371
<b>[10H]<sup>-</sup></b>	-2793.510558	0.544384	0.673200
<b>[10H]<sup>+</sup></b>	-2793.222697	0.549506	0.676611
<b>11H<sub>2</sub></b>	-2716.632369	0.525047	0.648873
<b>11</b>	-2715.443406	0.502536	0.628455
<b>[11H]<sup>-</sup></b>	-2716.118297	0.510111	0.636800
<b>[11H]<sup>+</sup></b>	-2715.845750	0.515097	0.640226
<b>12H<sub>2</sub></b>	-3007.310451	0.528511	0.667162
<b>12</b>	-3006.116649	0.510836	0.646564
<b>[12H]<sup>-</sup></b>	-3006.801894	0.516732	0.654654
<b>[12H]<sup>+</sup></b>	-3006.517322	0.524715	0.658127
<b>13H<sub>2</sub></b>	-3556.113736	0.544899	0.693668
<b>13</b>	-3554.948449	0.527385	0.673467
<b>[13H]<sup>-</sup></b>	-3555.624577	0.532462	0.681273
<b>[13H]<sup>+</sup></b>	-3555.318617	0.537398	0.684815
<b>14H<sub>2</sub></b>	-3320.471940	0.381539	0.515619
<b>14</b>	-3319.320696	0.367081	0.495966
<b>[14H]<sup>-</sup></b>	-3319.995309	0.370389	0.504023
<b>[14H]<sup>+</sup></b>	-3319.677353	0.375883	0.506918
<b>15H<sub>2</sub></b>	-3207.387373	0.388891	0.519293
<b>15</b>	-3206.230895	0.368467	0.499105
<b>15PB</b>	-3206.612326	0.369332	0.499317
<b>[15H]<sup>-</sup></b>	-3206.913934	0.377596	0.507720
<b>[15H]<sup>+</sup></b>	-3206.592592	0.381284	0.510575
<b>16H<sub>2</sub></b>	-3893.258372	0.469861	0.615352
<b>16</b>	-3892.113570	0.451878	0.595817
<b>[16H]<sup>-</sup></b>	-3892.778336	0.461093	0.603443
<b>[16H]<sup>+</sup></b>	-3892.467439	0.463043	0.606478



Complex	Electronic Energies Gas Phase (Hartrees)	Free Energy Change Gas Phase (Hartrees)	Enthalpy Change Gas Phase (Hartrees)
17H <sub>2</sub>	-3128.850784	0.335487	0.459082
17	-3127.695871	0.315826	0.438858
[17H] <sup>-</sup>	-3128.376573	0.322884	0.447186
[17H] <sup>+</sup>	-3128.056728	0.327472	0.450160
18H <sub>2</sub>	-2759.498247	0.622553	0.748020
18	-2758.338709	0.600849	0.727492
[18H] <sup>-</sup>	-2759.026103	0.611249	0.736666
[18H] <sup>+</sup>	-2758.734559	0.609554	0.738624
19H <sub>2</sub>	-3389.669572	0.714780	0.856405
19	-3388.505784	0.690849	0.835791
[19H] <sup>-</sup>	-3389.195250	0.698612	0.844341
[19H] <sup>+</sup>	-3388.888251	0.704534	0.847604
20H <sub>2</sub>	-3057.287134	0.540050	0.675833
20	-3056.121890	0.521149	0.656062
[20H] <sup>-</sup>	-3056.805600	0.528669	0.664116
[20H] <sup>+</sup>	-3056.515496	0.532917	0.667401
21H <sub>2</sub>	-3175.184950	0.625110	0.765027
21	-3174.009924	0.604727	0.745155
[21H] <sup>-</sup>	-3174.690574	0.611567	0.753343
[21H] <sup>+</sup>	-3174.404923	0.615245	0.756606
22H <sub>2</sub>	-2713.243981	0.474649	0.593716
22	-2712.070161	0.455753	0.573742
[22H] <sup>-</sup>	-2712.746516	0.462555	0.582173
[22H] <sup>+</sup>	-2712.454201	0.466839	0.585313

## 4) Gas Phase Energies of Calculated Substrates

**Table S3.** List of calculated electronic energies, free energy correction, and enthalpy correction for substrates described within. All calculations were implemented using the M06-2X/6-31g(d,p) level of theory at 298K.

Complex	Electronic Energies Gas Phase (Hartrees)	Free Energy Change Gas Phase (Hartrees)	Enthalpy Change Gas Phase (Hartrees)
Acetone	-193.064159	0.056241	0.090919
Acetonium	-193.3895994	0.069631	0.103636
Isopropoxide	-193.6272234	0.066424	0.099385
Isopropanol	-194.2646994	0.08216	0.115715
Benzaldehyde	-345.4274523	0.080559	0.118281
Benzaldehyde+H+	-345.7617284	0.093755	0.131786
Benzaldehyde+H-	-346.0080492	0.088121	0.126402
Benzyl Alcohol	-346.6261787	0.103356	0.142731
Acetophenone	-384.7325857	0.107201	0.148286
Acetophenone+H+	-385.0751974	0.119708	0.161282
Acetophenone+H-	-385.3106697	0.114879	0.156206
Phenylethanol	-385.9279365	0.129526	0.172098
N-Piperidino-Cyclohex-1-ene	-485.1467583	0.252903	0.300989
N-Piperidino-Cyclohex-1-ene+H+	-485.5485748	0.265364	0.315105
N-Piperidino-Cyclohex-1-ene+H-	-485.6853661	0.258472	0.306772
N-Piperidino-Cyclohexane	-486.3659366	0.275772	0.324557
N-Benzylidene-tert-butylamine	-482.7413479	0.198402	0.249364
N-Benzylidene-tert-butylammonium	-483.1291165	0.211554	0.263597
N-Benzylidene-tert-butylamide	-483.3085612	0.203856	0.256255
N-Benzyl-tert-butyl-amine	-483.9491837	0.222312	0.274272
N-Methylbenzylidene-tert-butylamine	-522.0323116	0.225215	0.279425
N-Methylbenzylidene-tert-butylammonium	-522.4245142	0.238061	0.29276
N-methylbenzyl-tert-butylamide	-522.6085024	0.233266	0.286556
N-methylbenzyl-tert-butylamine	-523.2481333	0.249771	0.303619
N-Benzylidenephénylamine	-556.5194985	0.167038	0.216999
N-Benzylidenephénylammonium	-556.8976654	0.180227	0.230993
N-Benzylanilide	-557.1328906	0.175056	0.225603
N-Benzylaniline	-557.7299899	0.189845	0.241387
N-Methylbenzylidenephénylamine	-595.8177737	0.193038	0.246731
N-Methylbenzylidenephénylammonium	-596.2028096	0.206258	0.260434
N-methylbenzylanilide	-596.4307785	0.20252	0.255311
N-methylbenzylaniline	-597.0273922	0.217402	0.271142

5) **Free Energies of H<sub>2</sub> Transfer from Computed Intramolecular and Intermolecular Phosphonium-Borohydrides**

**Table S4.** List of calculated transfer of H<sub>2</sub> from both intramolecular and intermolecular complexes. All calculations were implemented using the M06-2X/6-31g(d,p)//M06-2X/6-311++g(d,p) level of theory in MeCN at 298K.

Complex	$\Delta G_{H_2}$ Intramolecular (kcal/mol)	$\Delta G_{H_2}$ Intermolecular (kcal/mol)	Difference (Intermolecular – Intramolecular)
8H <sub>2</sub>	15.96	5.13	-10.83
10H <sub>2</sub>	12.45	5.87	-6.58
6H <sub>2</sub>	11.81	-1.44	-13.25
12H <sub>2</sub>	11.70	2.39	-9.31
2H <sub>2</sub>	11.06	7.39	-3.67
7H <sub>2</sub>	11.06	2.29	-8.77
11H <sub>2</sub>	6.90	3.30	-3.6
1H <sub>2</sub>	5.36	2.39	-2.97
13H <sub>2</sub>	3.50	-5.70	-9.2
22H <sub>2</sub>	3.30	4.08	0.78
3H <sub>2</sub>	2.94	0.98	-1.96
18H <sub>2</sub>	2.91	4.08	1.17
15H <sub>2</sub>	2.06	-11.84	-13.9
17H <sub>2</sub>	1.43	-9.99	-11.42
21H <sub>2</sub>	1.42	1.68	0.26
9H <sub>2</sub>	0.24	-15.14	-15.38
20H <sub>2</sub>	-1.99	1.22	3.21
14H <sub>2</sub>	-2.06	-8.98	-6.92
5H <sub>2</sub>	-3.52	0.17	3.69
19H <sub>2</sub>	-3.56	1.67	5.23
16H <sub>2</sub>	-6.88	-5.70	1.18
4H <sub>2</sub>	-12.48	1.14	13.62

**Table S5.** List of calculated transfer of H<sub>2</sub> from both intramolecular and intermolecular complexes. All calculations were implemented using the M06-2X/6-31g(d,p)//M06-2X/6-311++g(d,p) level of theory in toluene at 298K.

<b>Complex</b>	<b><math>\Delta G_{H_2}</math> Intramolecular (kcal/mol)</b>	<b><math>\Delta G_{H_2}</math> Intermolecular (kcal/mol)</b>	<b>Difference (Intermolecular – Intramolecular)</b>
<b>8H<sub>2</sub></b>	12.74	-7.26	-20.00
<b>10H<sub>2</sub></b>	9.92	4.75	-5.17
<b>12H<sub>2</sub></b>	9.72	-7.97	-17.69
<b>6H<sub>2</sub></b>	9.52	-6.45	-15.97
<b>7H<sub>2</sub></b>	9.31	-6.04	-15.35
<b>11H<sub>2</sub></b>	4.72	1.70	-3.02
<b>2H<sub>2</sub></b>	3.69	-2.05	-5.74
<b>13H<sub>2</sub></b>	2.75	-13.58	-16.33
<b>1H<sub>2</sub></b>	-0.32	-5.36	-5.04
<b>15H<sub>2</sub></b>	-0.73	-15.46	-14.73
<b>22H<sub>2</sub></b>	-0.97	-6.01	-5.04
<b>3H<sub>2</sub></b>	-1.08	-2.47	-1.39
<b>17H<sub>2</sub></b>	-1.57	-16.68	-15.11
<b>21H<sub>2</sub></b>	-1.85	-17.19	-15.34
<b>9H<sub>2</sub></b>	-3.59	-24.63	-21.04
<b>14H<sub>2</sub></b>	-4.37	-15.13	-10.76
<b>18H<sub>2</sub></b>	-5.33	-9.23	-3.90
<b>20H<sub>2</sub></b>	-6.40	-0.51	5.89
<b>19H<sub>2</sub></b>	-8.81	-5.16	3.65
<b>16H<sub>2</sub></b>	-9.02	-7.70	1.32
<b>5H<sub>2</sub></b>	-13.27	-2.33	10.94
<b>4H<sub>2</sub></b>	-17.09	-7.40	9.69

6) **Hydride Donor Abilities for Calculated Intramolecular and Intermolecular Phosphonium-Borohydrides**

**Table S6.** List of hydride donor abilities of intramolecular and intermolecular complexes. All calculations were implemented using the M06-2X/6-31g(d,p)//M06-2X/6-311++g(d,p) level of theory in MeCN at 298K. All values reported are in kcal/mol.

Complex	$\Delta G'_{H-}$ (kcal/mol)	$\Delta G''_{H-}$ (kcal/mol)	$\Delta G_{H-}(\text{inter})$ (kcal/mol)
9H <sub>2</sub>	46.85	33.22	32.75
18H <sub>2</sub>	52.37	51.66	53.17
4H <sub>2</sub>	54.13	39.68	55.08
5H <sub>2</sub>	57.64	47.98	52.64
20H <sub>2</sub>	59.43	54.55	58.06
19H <sub>2</sub>	60.08	55.45	57.05
21H <sub>2</sub>	60.26	55.57	56.51
11H <sub>2</sub>	60.88	50.32	53.90
3H <sub>2</sub>	63.51	50.41	54.35
22H <sub>2</sub>	65.33	53.16	56.52
10H <sub>2</sub>	65.41	58.64	55.60
12H <sub>2</sub>	68.55	54.82	54.24
2H <sub>2</sub>	68.72	63.65	64.83
8H <sub>2</sub>	69.15	52.03	53.02
1H <sub>2</sub>	69.44	65.93	64.83
17H <sub>2</sub>	70.48	58.33	53.33
6H <sub>2</sub>	70.43	52.06	53.02
7H <sub>2</sub>	71.35	46.11	54.77
15H <sub>2</sub>	71.83	57.04	53.11
16H <sub>2</sub>	72.11	44.11	58.50
14H <sub>2</sub>	73.54	52.38	55.71
13H <sub>2</sub>	74.81	50.89	55.71

7) **pK<sub>a</sub> Values for Computed Intramolecular and Intermolecular Phosphonium-Borohydrides**

**Table S7.** List of calculated pK<sub>a</sub>'s of intramolecular and intermolecular complexes. All calculations were implemented using the M06-2X/6-31g(d,p)//M06-2X/6-311++g(d,p) level of theory in MeCN at 298K. All values reported are in kcal/mol.

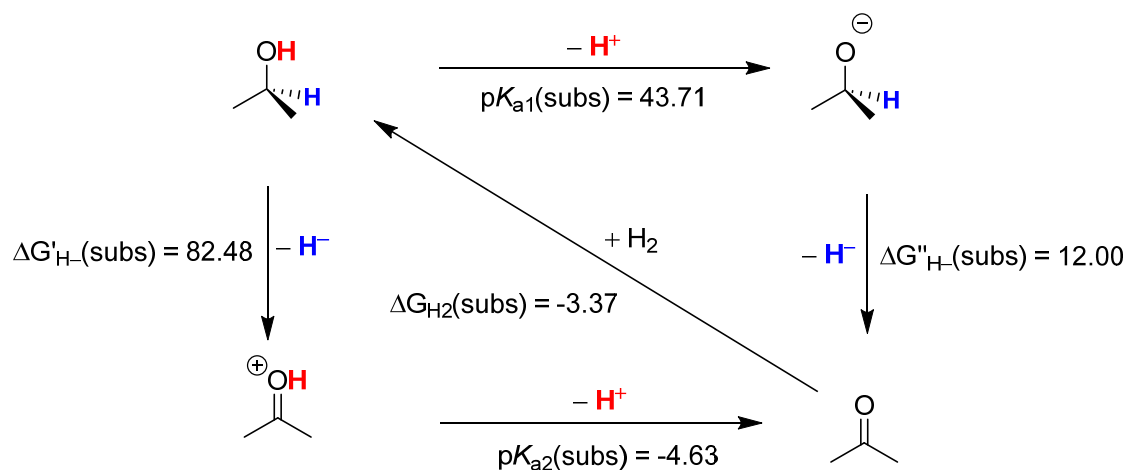
Complex	pK <sub>a</sub> Intramolecular (Neutral)	pK <sub>a</sub> Intramolecular (Cationic)	pK <sub>a</sub> Intermolecular (Neutral)
<b>1H<sub>2</sub></b>	8.96	6.39	7.59
<b>19H<sub>2</sub></b>	10.11	6.71	12.76
<b>17H<sub>2</sub></b>	11.65	2.74	6.94
<b>20H<sub>2</sub></b>	11.91	8.33	11.70
<b>15H<sub>2</sub></b>	13.06	2.21	5.75
<b>14H<sub>2</sub></b>	13.46	-2.06	5.94
<b>21H<sub>2</sub></b>	13.66	10.23	13.17
<b>2H<sub>2</sub></b>	14.81	11.09	11.26
<b>4H<sub>2</sub></b>	15.13	4.53	13.82
<b>5H<sub>2</sub></b>	15.60	8.53	14.90
<b>16H<sub>2</sub></b>	15.98	-4.54	6.30
<b>22H<sub>2</sub></b>	16.81	7.90	14.92
<b>18H<sub>2</sub></b>	17.62	17.10	17.38
<b>3H<sub>2</sub></b>	18.56	8.96	14.23
<b>13H<sub>2</sub></b>	18.62	1.09	8.34
<b>10H<sub>2</sub></b>	19.50	14.54	12.76
<b>11H<sub>2</sub></b>	21.53	13.79	16.27
<b>12H<sub>2</sub></b>	21.75	11.68	15.35
<b>8H<sub>2</sub></b>	23.60	14.36	18.26
<b>6H<sub>2</sub></b>	23.86	10.39	13.44
<b>7H<sub>2</sub></b>	24.35	9.17	14.89
<b>9H<sub>2</sub></b>	25.86	19.19	18.25

## 8) Proton-Hydride Distances for Computed Intramolecular and Intermolecular FLPs

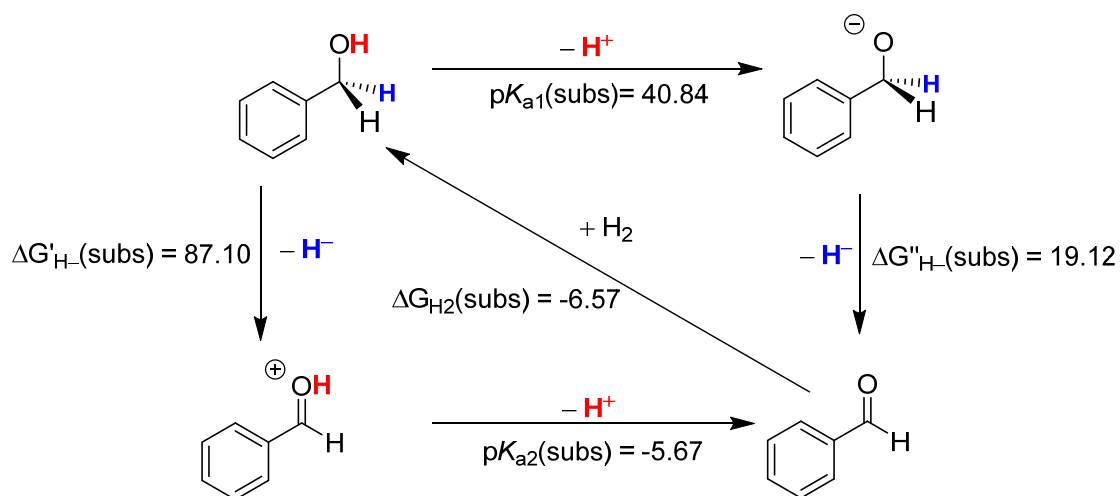
**Table S8.** List of calculated proton-hydride distances for the intramolecular and intermolecular complexes reported within.

Complex	H-H distance Intramolecular (Å)	H-H distance Intermolecular (Å)
1H <sub>2</sub>	7.320	1.593
2H <sub>2</sub>	7.264	1.707
3H <sub>2</sub>	5.092	1.760
4H <sub>2</sub>	6.561	2.248
5H <sub>2</sub>	7.121	1.771
6H <sub>2</sub>	2.729	1.575
7H <sub>2</sub>	3.098	1.657
8H <sub>2</sub>	2.642	2.091
9H <sub>2</sub>	2.575	2.155
10H <sub>2</sub>	4.256	2.091
11H <sub>2</sub>	2.320	1.712
12H <sub>2</sub>	2.438	1.853
13H <sub>2</sub>	2.066	1.909
14H <sub>2</sub>	2.111	1.880
15H <sub>2</sub>	2.089	1.752
16H <sub>2</sub>	2.199	2.151
17H <sub>2</sub>	2.158	1.527
18H <sub>2</sub>	8.384	1.918
19H <sub>2</sub>	7.238	1.871
20H <sub>2</sub>	5.294	1.720
21H <sub>2</sub>	1.806	3.640
22H <sub>2</sub>	1.672	2.010

## 9) Thermodynamic Values for the Reduction of Unsaturated Substrates

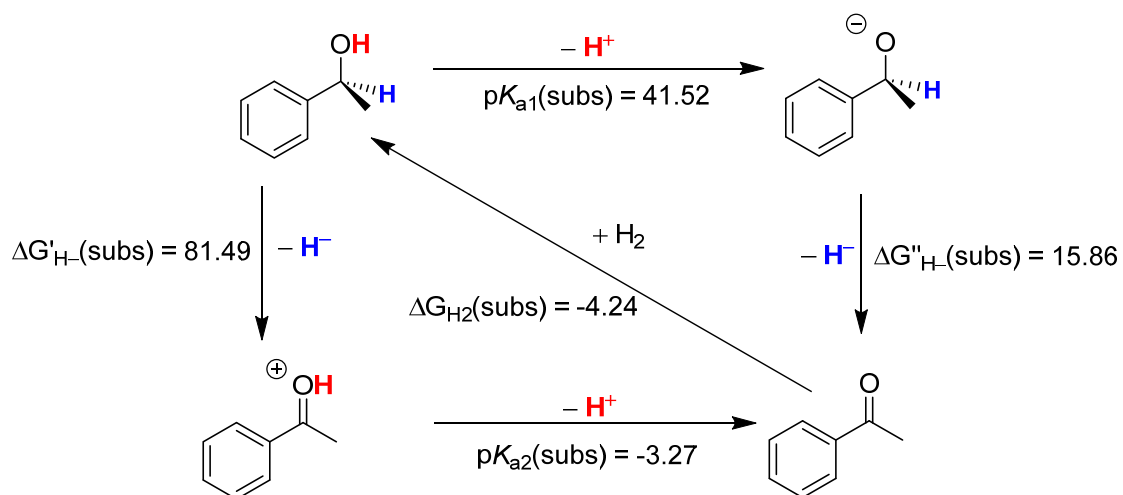


**Figure S2.** Computed thermodynamic values for  $\text{H}_2$ ,  $\text{H}^+$ , and  $\text{H}^-$  addition to acetone.

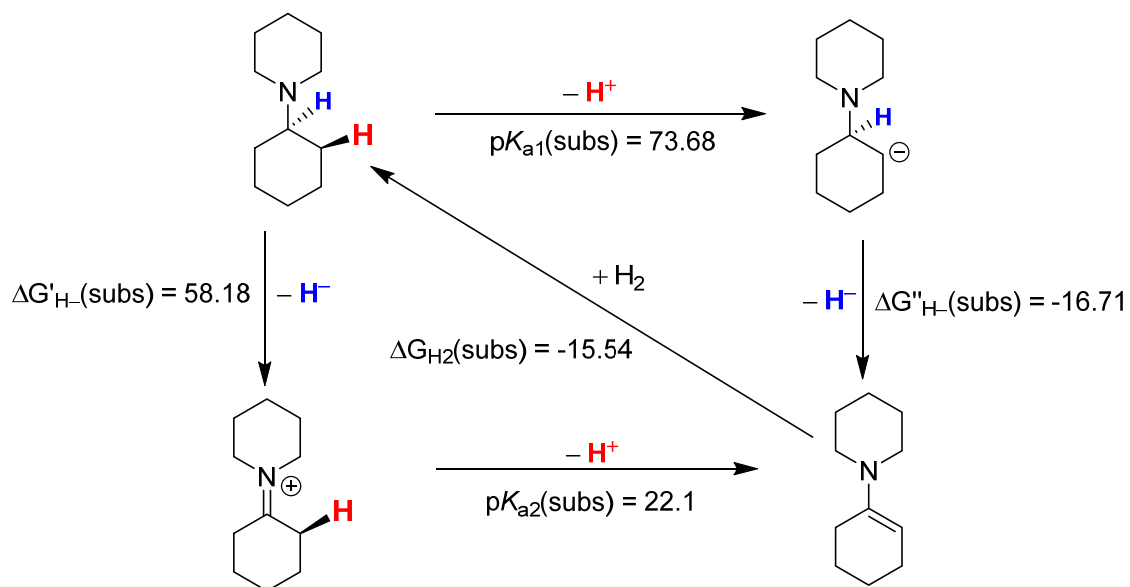


**Figure S3.** Computed thermodynamic values for  $\text{H}_2$ ,  $\text{H}^+$ , and  $\text{H}^-$  addition to benzaldehyde.

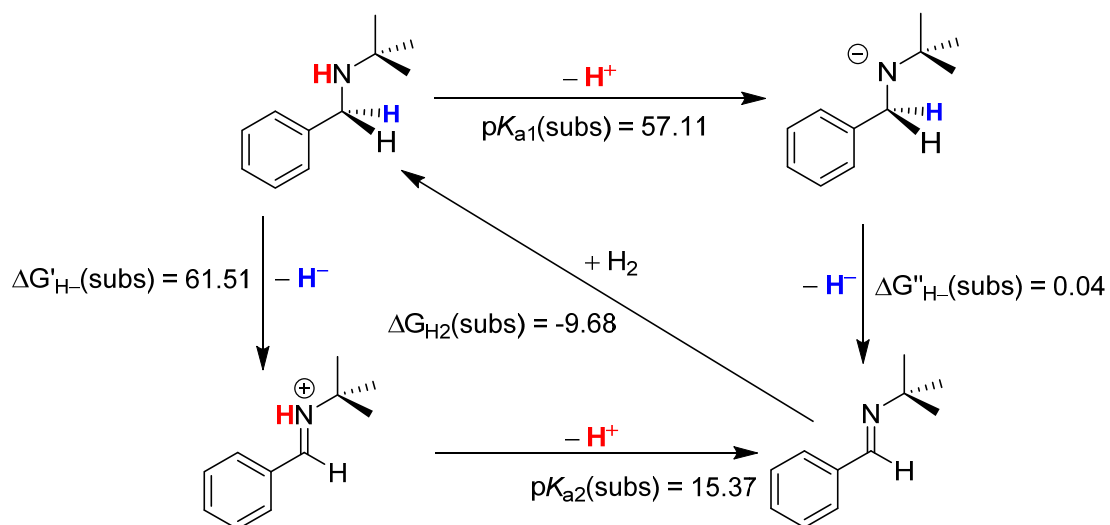




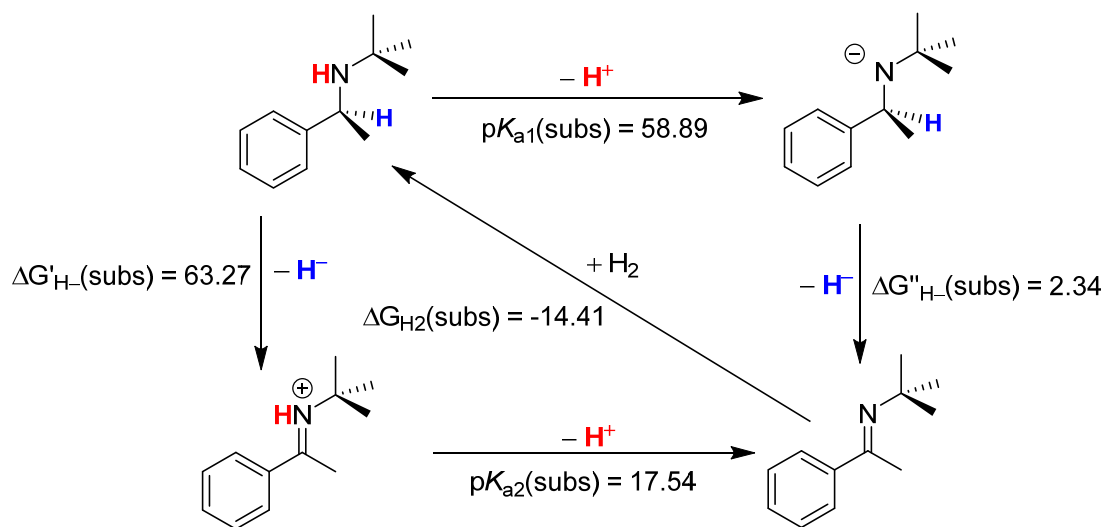
**Figure S4.** Computed thermodynamic values for  $H_2$ ,  $H^+$ , and  $H^-$  addition to acetophenone.



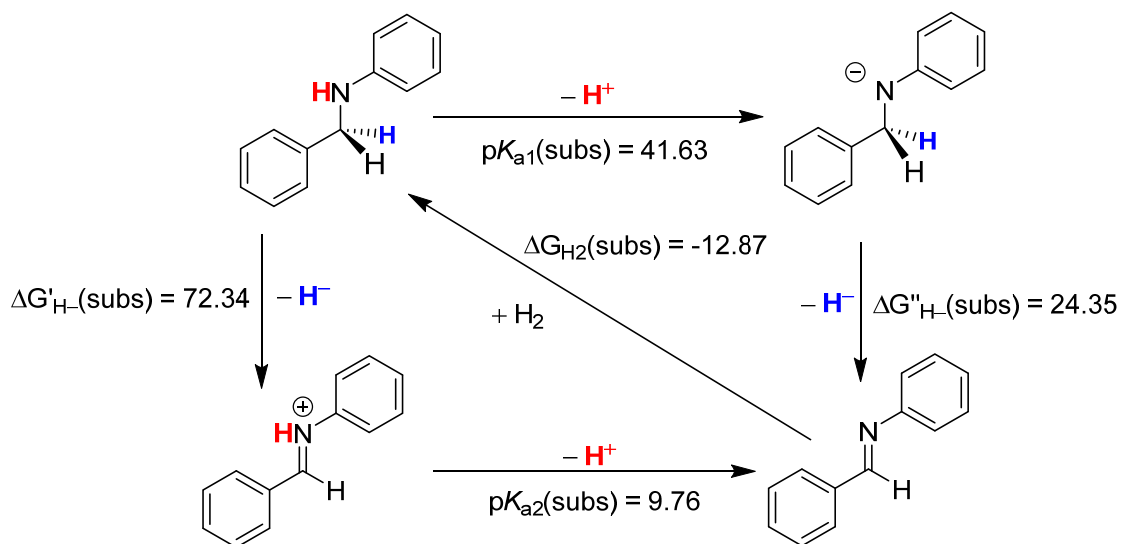
**Figure S5.** Computed thermodynamic values for  $H_2$ ,  $H^+$ , and  $H^-$  addition to N-piperidino-cyclohex-1-ene.



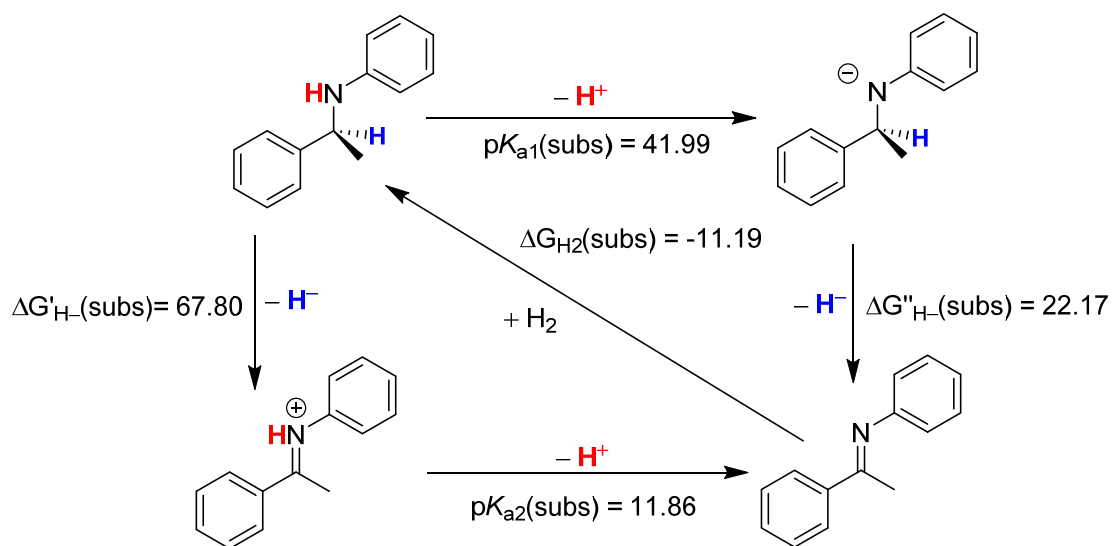
**Figure S6.** Computed thermodynamic values for  $\text{H}_2$ ,  $\text{H}^+$ , and  $\text{H}^-$  addition to N-benzylidene-tert-butylamine.



**Figure S7.** Computed thermodynamic values for  $\text{H}_2$ ,  $\text{H}^+$ , and  $\text{H}^-$  addition to N-methylbenzylidene-tert-butylamine.

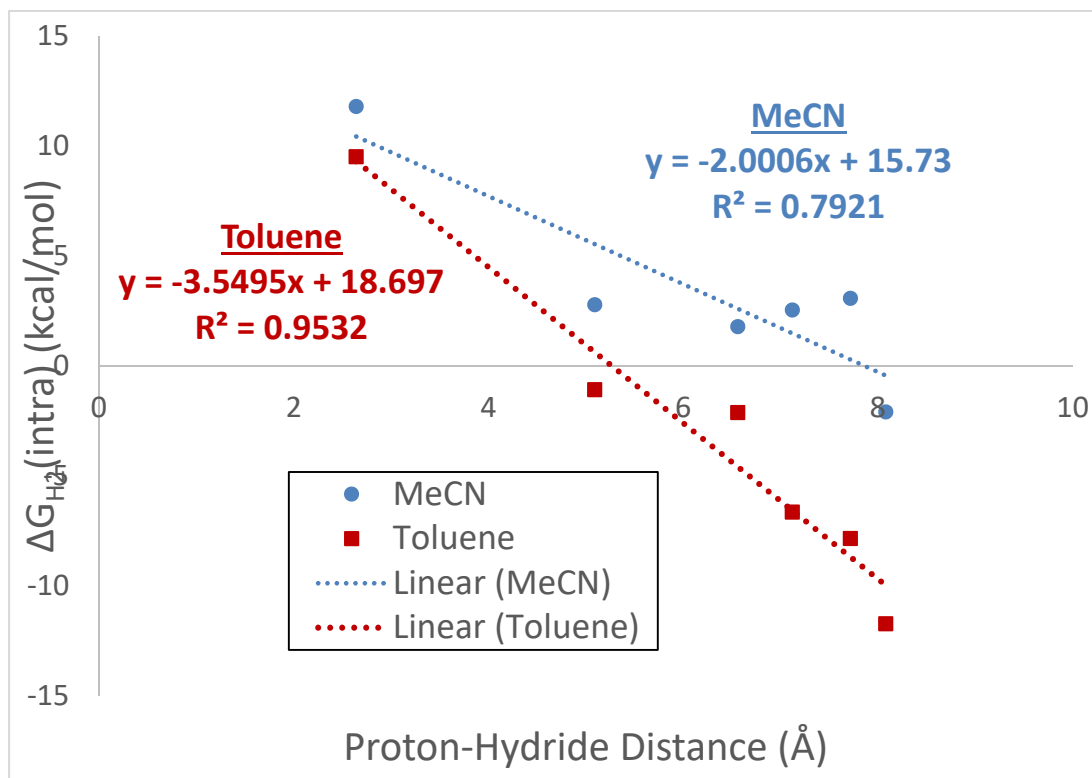


**Figure S8.** Computed thermodynamic values for  $\text{H}_2$ ,  $\text{H}^+$ , and  $\text{H}^-$  addition to N-benzylidene-phenylamine.

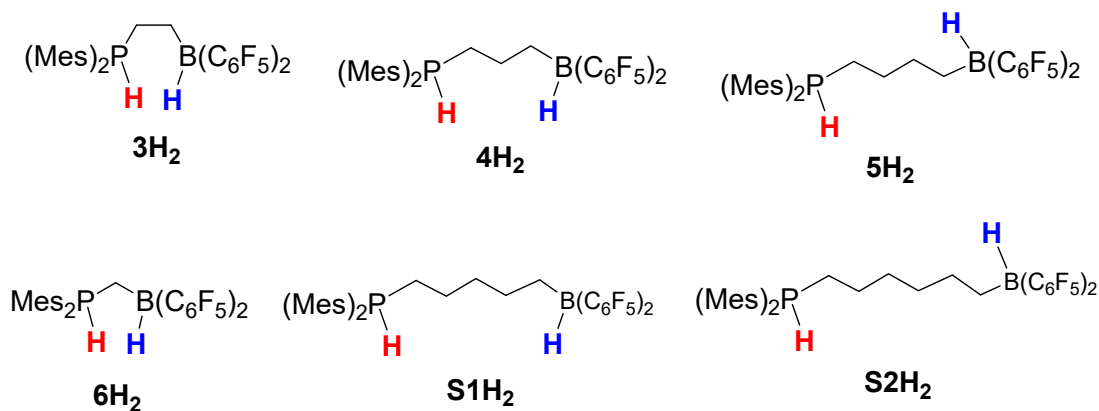


**Figure S9.** Computed thermodynamic values for  $\text{H}_2$ ,  $\text{H}^+$ , and  $\text{H}^-$  addition to N-methylbenzylidene-phenylamine.

10) Plot of Free Energy of H<sub>2</sub> Transfer from Alkyl Linked Phosphonium Borohydrides as a Function of Proton-Hydride Distance

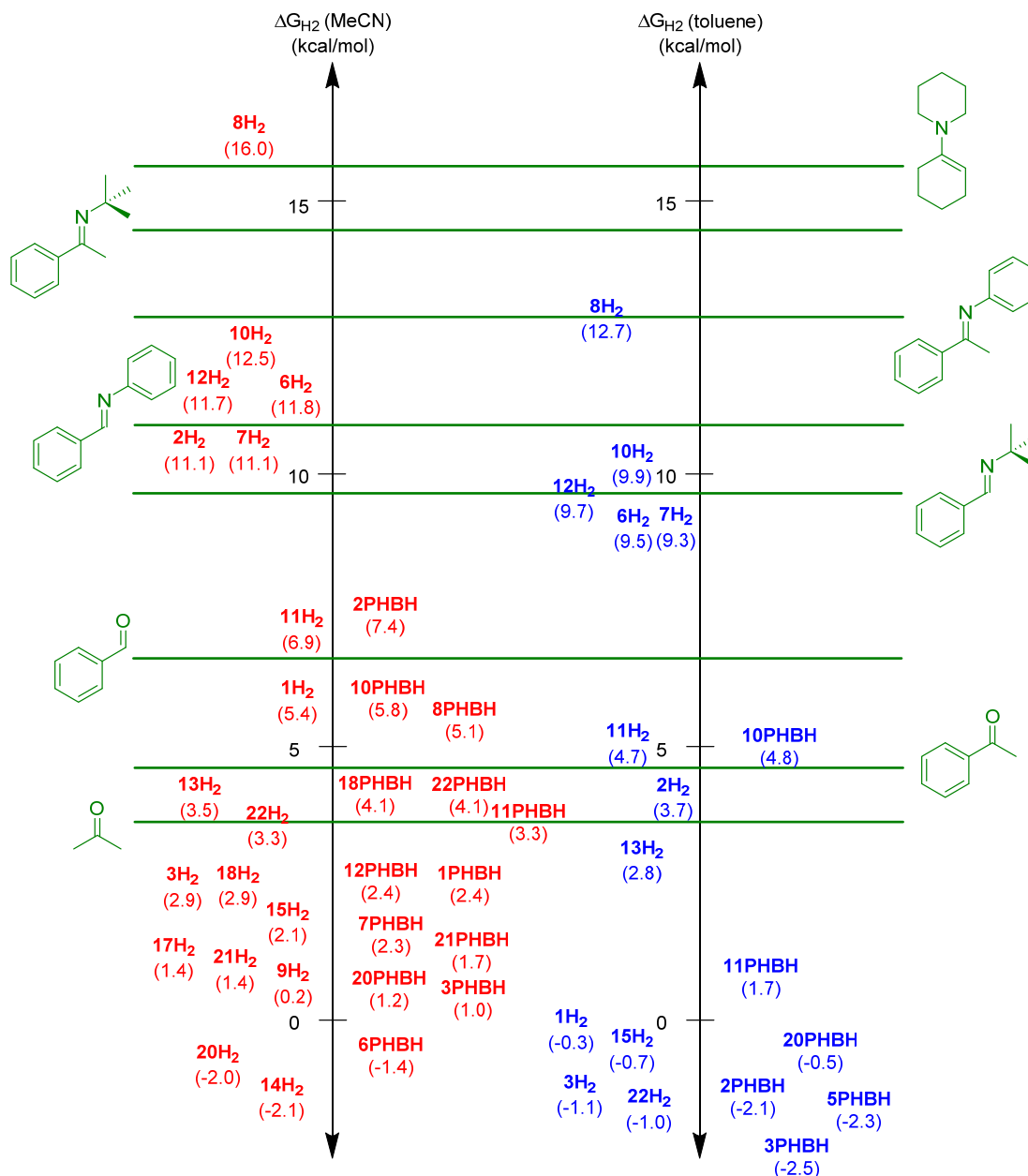


**Figure S10.** Plot of free energy of H<sub>2</sub> transfer from complexes **6H<sub>2</sub>**, **3H<sub>2</sub>**, **4H<sub>2</sub>**, **5H<sub>2</sub>**, **S1H<sub>2</sub>**, and **S2H<sub>2</sub>** (see Figure S11 for the structure of **S1H<sub>2</sub>** and **S2H<sub>2</sub>**) as a function of proton-hydride distance in the respective FLP-H<sub>2</sub> adducts prior to P-B bond formation in toluene and acetonitrile.



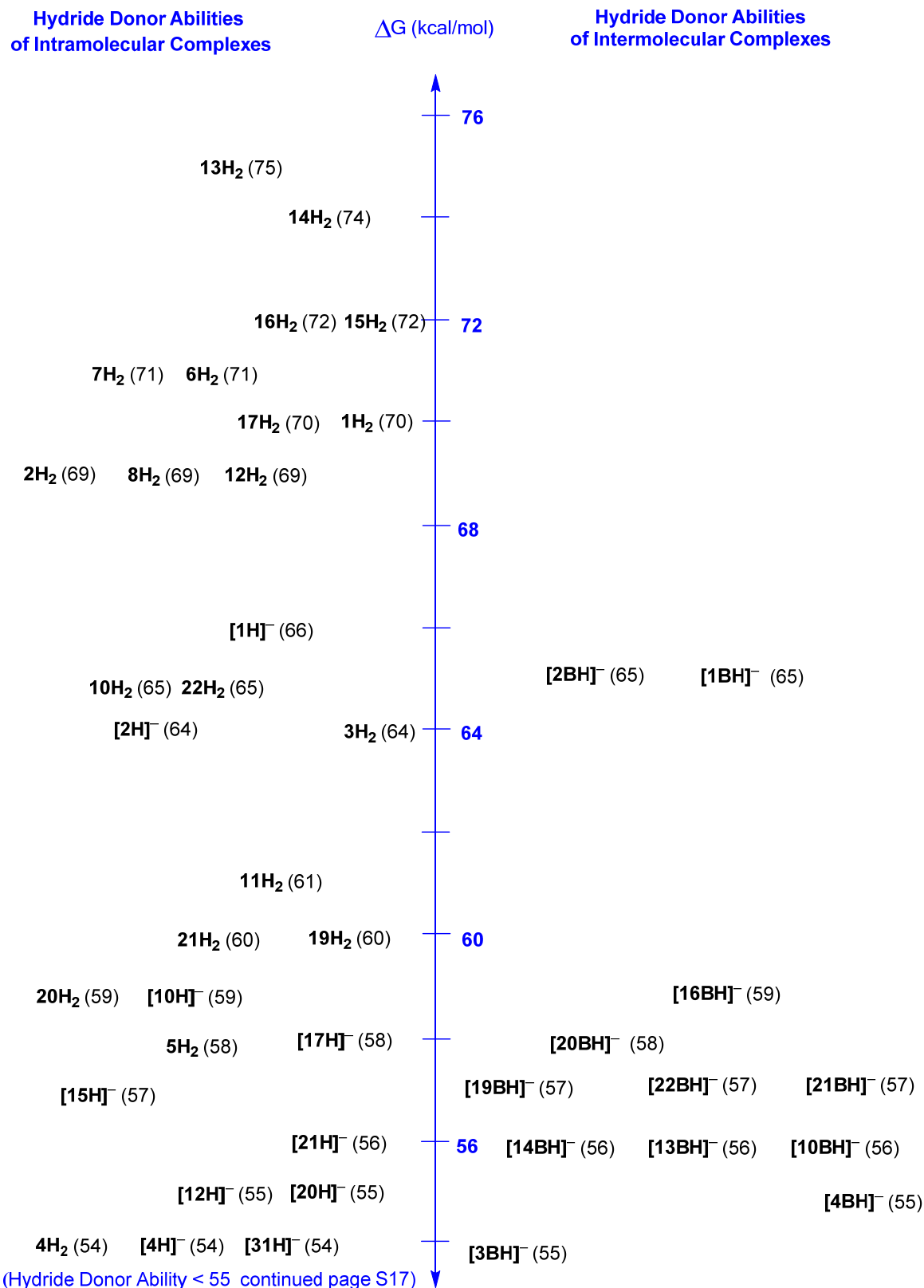
**Figure S11.** Structures of the intramolecular FLP-H<sub>2</sub> adducts described in Figure S10.

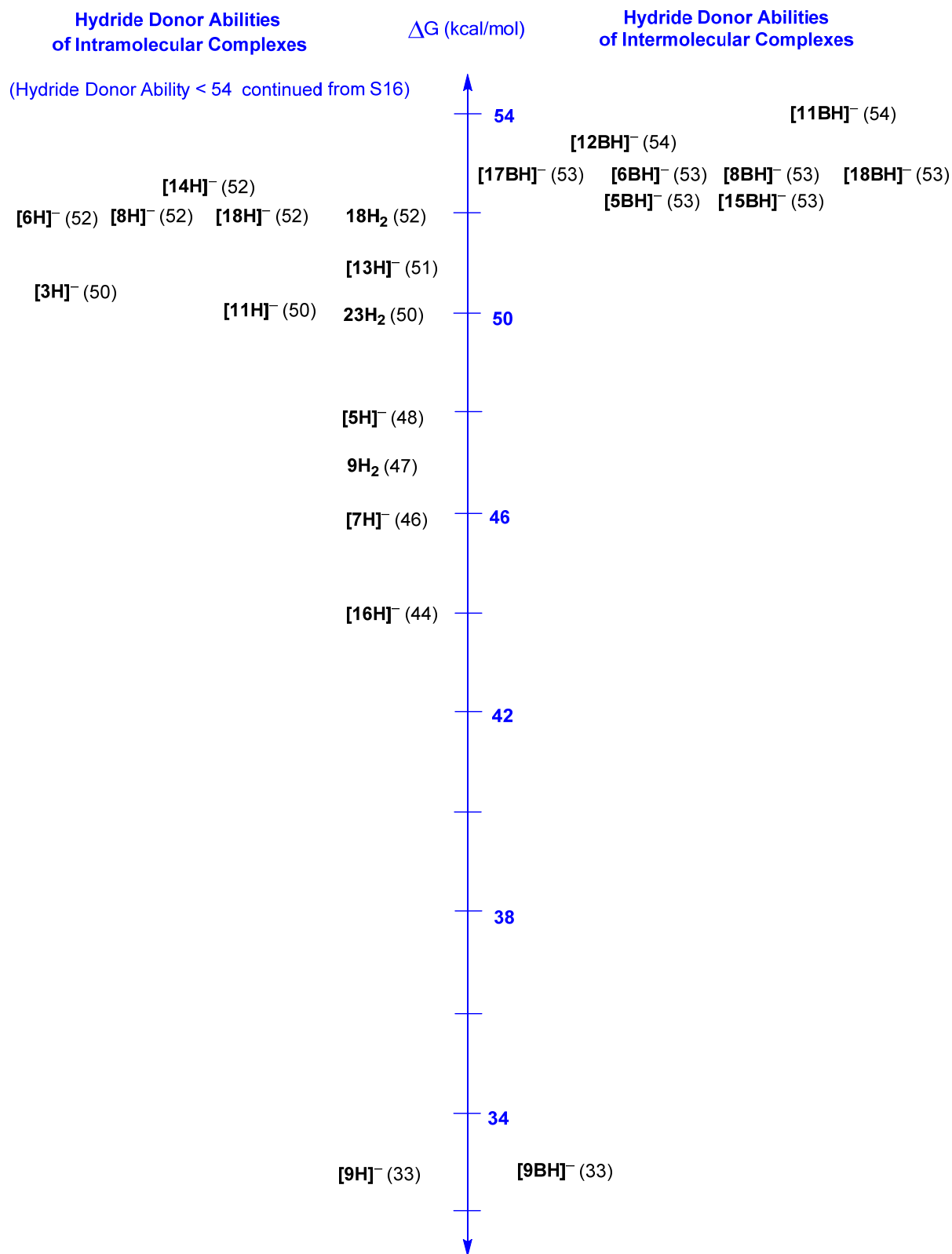
11) **Ladder Diagram of H<sub>2</sub> Transfer from Intramolecular and Intermolecular Phosphonium-borohydrides Compared to the Selected Unsaturated Substrates**



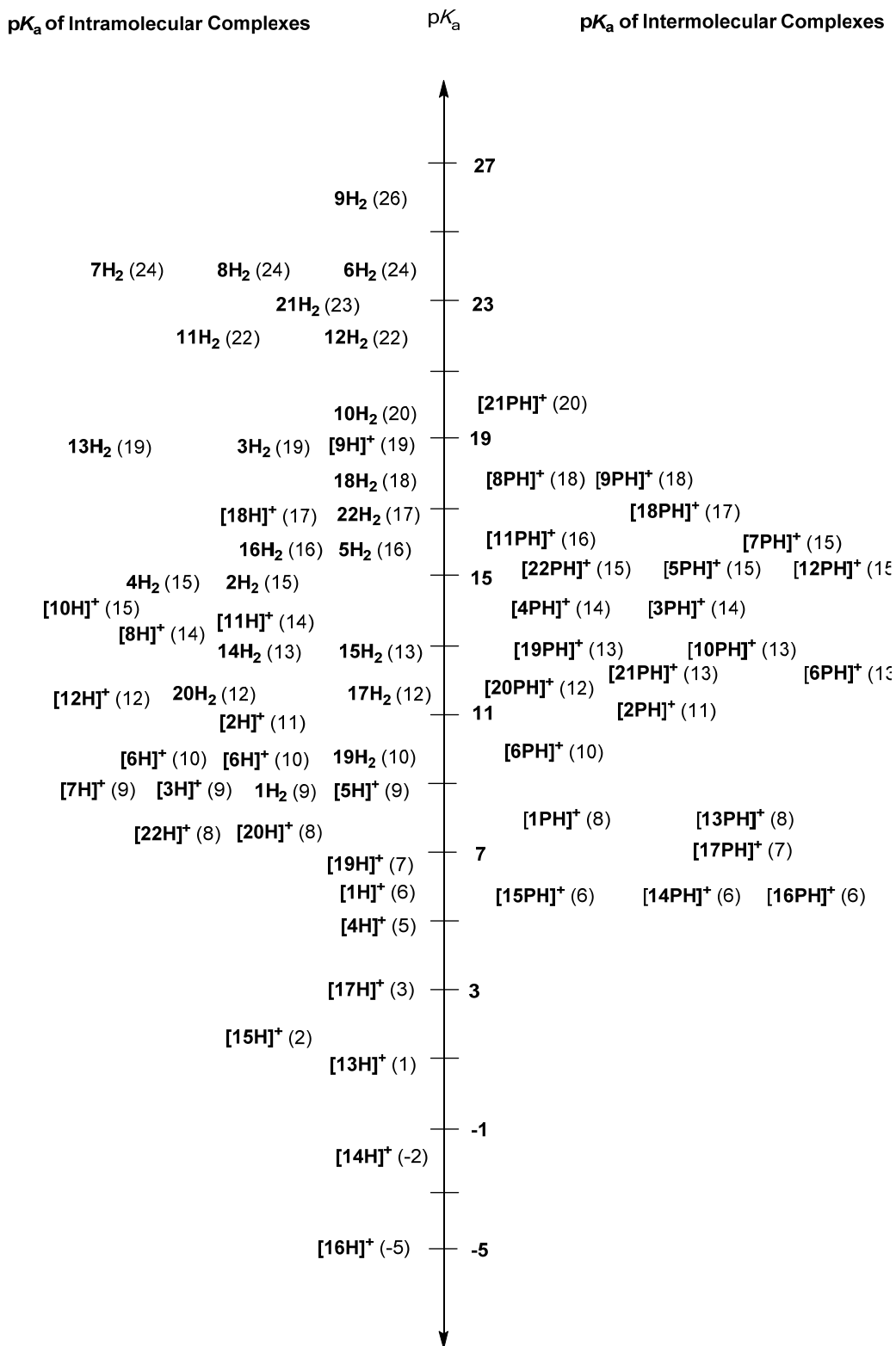
**Figure S12.** Ladder diagram comparing the ability of select intramolecular and intermolecular phosphonium-borohydrides to transfer H<sub>2</sub> to unsaturated substrates. Acetonitrile values are listed in red, toluene values in blue, and substrates in green. H<sub>2</sub> transfer from the phosphonium-borohydrides is thermodynamically favorable for any substrate higher up (above them) in the ladder diagram.

12) Ladder Diagram of Hydride Donor Abilities for Calculated Intramolecular and Intermolecular Phosphonium-Borohydrides





13) Ladder Diagram of  $pK_a$  Values for Calculated Intramolecular and Intermolecular Phosphonium-Borohydrides





## 14) 3D Coordinates of All Computed Structures

The 3D coordinates are organized so that they can be readily visualized in a Mercury. For each complex, the first number is the number of atoms, followed by the complex name, and the 3D coordinates.

76				C	-4.84119	-3.41974	1.33068
1H <sub>2</sub>				H	-4.62176	-4.03524	2.19897
P	-3.21828	-0.24080	-0.69168	C	-3.95184	-2.39796	1.00203
H	-3.13623	-0.44199	-2.06958	C	-5.77168	-1.02566	-2.11750
B	2.80213	-0.20022	1.03435	H	-5.77202	0.05065	-1.91718
H	2.78411	-0.33340	2.23356	H	-6.76810	-1.29513	-2.46913
F	-1.95655	1.01848	1.74181	H	-5.07489	-1.21584	-2.94205
F	0.63304	1.05880	2.38091	C	-6.91155	-4.80884	0.97053
F	1.58864	-1.59112	-1.42788	H	-7.93032	-4.62918	0.62151
F	-0.97812	-1.57390	-2.07050	H	-6.93446	-4.95507	2.05247
F	3.05792	0.85221	-1.64171	H	-6.56352	-5.74280	0.51797
F	3.63054	3.39533	-2.33735	C	-2.73829	-2.20716	1.87982
F	4.09048	5.25828	-0.40580	H	-2.80879	-2.86374	2.74776
F	3.97030	4.55017	2.21715	H	-2.64605	-1.18263	2.24968
F	3.40449	2.03541	2.91657	H	-1.81190	-2.45141	1.35213
F	5.54365	0.02242	-0.27707	C	-1.51770	-0.25975	-0.18994
F	6.99850	-2.02526	-1.12563	C	-1.06116	0.40724	0.94737
F	6.06321	-4.57679	-0.93115	C	0.27738	0.38720	1.28559
F	3.59282	-5.02485	0.13836	C	1.24243	-0.29328	0.53486
F	2.10128	-2.97084	0.98603	C	0.76821	-0.93342	-0.61029
C	-3.94345	1.40292	-0.50466	C	-0.57125	-0.93129	-0.96562
C	-3.60681	2.35250	-1.49604	C	3.23265	1.32549	0.66051
C	-4.15244	3.62899	-1.39697	C	3.29553	1.74444	-0.66383
H	-3.89574	4.36672	-2.15260	C	3.58544	3.04400	-1.04816
C	-5.00548	3.98722	-0.35437	C	3.81792	3.99717	-0.06455
C	-5.30993	3.03024	0.61160	C	3.75601	3.63155	1.27079
H	-5.96390	3.30016	1.43651	C	3.46222	2.31283	1.60935
C	-4.79259	1.73703	0.56916	C	3.74233	-1.37026	0.40880
C	-2.68709	2.04408	-2.65390	C	5.00371	-1.19917	-0.14815
H	-1.74296	1.59565	-2.32894	C	5.79203	-2.25439	-0.60051
H	-2.44310	2.96096	-3.19110	C	5.32192	-3.55320	-0.50289
H	-3.15668	1.36162	-3.37212	C	4.06599	-3.77774	0.04434
C	-5.54918	5.38641	-0.25438	C	3.32125	-2.69495	0.48295
H	-6.47612	5.41203	0.32171				
H	-5.74206	5.80704	-1.24366	75			
H	-4.82621	6.03782	0.24675	[1H] <sup>+</sup>			
C	-5.16150	0.77928	1.67491	P	3.44489	-0.13885	0.67916
H	-5.65561	1.32267	2.48156	B	-2.74699	0.03995	0.09610
H	-4.27699	0.29719	2.09828	F	1.78817	1.39461	-1.36331
H	-5.84103	-0.00496	1.32852	F	-0.86407	1.54202	-1.53429
C	-4.25396	-1.60560	-0.12602	F	-1.25368	-1.44365	2.10371
C	-5.41609	-1.84108	-0.89587	F	1.40014	-1.50893	2.32573
C	-6.26721	-2.87349	-0.51263	F	-1.85845	2.66306	0.96188
H	-7.16574	-3.05539	-1.09626	F	-3.12722	4.95431	0.46389
C	-5.99599	-3.67622	0.59382	F	-5.43447	4.95169	-0.96241

F	-6.46701	2.62387	-1.89225	H	7.04276	-3.36594	0.29676
F	-5.22615	0.31905	-1.40502	H	3.88529	-3.90590	-2.53669
F	-5.43094	-0.38698	1.11844	H	6.14869	-0.16873	1.45290
F	-6.63570	-2.75807	1.32701	H	5.53379	-1.43008	2.54010
F	-5.35627	-5.01086	0.52494	H	7.09547	-1.62131	1.75558
F	-2.84255	-4.87121	-0.48636	H	6.02206	-5.11057	-2.80300
F	-1.60941	-2.51704	-0.69667	H	7.32725	-4.89747	-1.62085
C	4.22807	1.45680	0.40478	H	5.91979	-5.88445	-1.22005
C	4.17227	2.37948	1.47512	H	2.24697	-0.85081	-2.12197
C	4.79769	3.61154	1.31081	H	2.18229	-2.48548	-2.76369
C	5.46856	3.94814	0.13528	H	1.44696	-2.13469	-1.20260
C	5.49192	3.01924	-0.90551	H	3.96290	0.44990	-2.25232
C	4.88322	1.77157	-0.80504	H	5.60899	-0.01406	-1.79944
C	3.47197	2.08935	2.78190	H	5.33278	1.37307	-2.85806
C	6.16313	5.27412	-0.00374	H	7.21443	5.18082	0.28694
C	4.94984	0.83839	-1.98810				
C	4.19061	-1.57318	-0.10680	75			
C	5.43460	-1.96512	0.44290	[1H]			
C	6.08395	-3.06213	-0.11422	P	-3.26299	-0.36805	-1.06419
C	5.53970	-3.77739	-1.18026	B	2.73336	-0.24483	1.01935
C	4.31338	-3.36189	-1.69929	F	-2.04017	0.87840	1.59897
C	3.61471	-2.26912	-1.19214	F	0.49168	0.96577	2.29561
C	6.08099	-1.25085	1.60712	F	1.62927	-1.62843	-1.49580
C	6.24562	-4.97942	-1.74265	F	-0.87862	-1.65408	-2.22933
C	2.30242	-1.90746	-1.84684	F	3.16801	0.89946	-1.60552
C	1.65533	-0.03322	0.50655	F	3.74832	3.46882	-2.18310
C	1.04090	0.74382	-0.47041	F	4.06381	5.27478	-0.16913
C	-0.34070	0.78993	-0.57018	F	3.79508	4.47908	2.41881
C	-1.16864	0.05556	0.27758	F	3.22629	1.93896	3.00337
C	-0.53815	-0.71136	1.25513	F	5.51251	0.05230	-0.25808
C	0.84290	-0.75241	1.37975	F	7.02458	-1.94787	-1.09888
C	-3.49455	1.37399	-0.17478	F	6.15746	-4.52738	-0.92474
C	-2.99424	2.60884	0.25953	F	3.69194	-5.04556	0.12310
C	-3.63282	3.81238	0.01642	F	2.13979	-3.04164	0.96772
C	-4.81736	3.81333	-0.71289	C	-3.85291	1.33882	-0.64027
C	-5.34765	2.61728	-1.18362	C	-3.45853	2.32406	-1.57653
C	-4.68916	1.42953	-0.90694	C	-3.90195	3.63721	-1.43046
C	-3.47226	-1.33489	0.18429	C	-4.74040	4.01548	-0.38643
C	-4.76988	-1.46167	0.69578	C	-5.11344	3.04032	0.53142
C	-5.41299	-2.68327	0.82280	C	-4.67848	1.71480	0.44020
C	-4.75734	-3.84041	0.41770	C	-2.54430	2.00541	-2.73631
C	-3.46740	-3.76685	-0.09779	C	-5.19019	5.44550	-0.23255
C	-2.85075	-2.53149	-0.19296	C	-5.11113	0.77420	1.53865
H	3.57326	-0.38417	2.04622	C	-4.35170	-1.56774	-0.17541
H	4.75508	4.33149	2.12337	C	-5.64218	-1.67771	-0.74741
H	5.99465	3.27792	-1.83342	C	-6.54926	-2.61191	-0.24780
H	3.40907	2.99814	3.38077	C	-6.21765	-3.47060	0.79403
H	2.44943	1.72428	2.64013	C	-4.94412	-3.35787	1.34267
H	4.01825	1.34824	3.37725	C	-4.00523	-2.42822	0.88999
H	6.13585	5.62826	-1.03606	C	-6.10199	-0.77644	-1.86891
H	5.70688	6.03078	0.63692	C	-7.19083	-4.50580	1.29572

C	-2.68736	-2.37620	1.62467	F	-1.77006	2.62888	0.92472
C	-1.57356	-0.37414	-0.36161	F	-2.93050	4.93930	0.28285
C	-1.14373	0.28736	0.78861	F	-5.13862	4.96706	-1.29447
C	0.18665	0.29546	1.17303	F	-6.18466	2.63908	-2.21974
C	1.19660	-0.35232	0.46126	F	-5.05780	0.31325	-1.57557
C	0.76301	-0.98659	-0.69634	F	-5.40577	-0.10252	1.09813
C	-0.56901	-1.00370	-1.09690	F	-6.86435	-2.31169	1.40375
C	3.18223	1.29534	0.71791	F	-5.84173	-4.72983	0.71364
C	3.31948	1.75995	-0.58604	F	-3.32349	-4.91274	-0.28157
C	3.61781	3.07439	-0.90985	F	-1.83451	-2.72371	-0.57591
C	3.77844	3.99829	0.11460	C	4.13567	1.31650	0.63177
C	3.64158	3.58787	1.43008	C	3.99485	2.22179	1.70890
C	3.34476	2.25533	1.70751	C	4.50597	3.51411	1.59587
C	3.72695	-1.38340	0.39809	C	5.17092	3.94113	0.45115
C	4.99114	-1.18115	-0.14246	C	5.29745	3.04015	-0.60231
C	5.81383	-2.21218	-0.59016	C	4.78527	1.74276	-0.54698
C	5.37974	-3.52289	-0.50312	C	3.29196	1.84478	2.99319
C	4.12556	-3.78154	0.03152	C	5.70274	5.34573	0.33737
C	3.34388	-2.72194	0.46508	C	4.94142	0.88532	-1.77848
H	2.69680	-0.42062	2.21416	C	4.33481	-1.57525	-0.13795
H	-3.58230	4.38278	-2.15571	C	5.67229	-1.85440	0.23218
H	-5.75194	3.31911	1.36746	C	6.41201	-2.78331	-0.49822
H	-1.57461	1.63152	-2.39157	C	5.86644	-3.47248	-1.57610
H	-2.36413	2.90096	-3.33493	C	4.54908	-3.18989	-1.92455
H	-2.96997	1.23104	-3.38114	C	3.77086	-2.25547	-1.23885
H	-6.10791	5.51097	0.35727	C	6.35518	-1.14200	1.37616
H	-5.37341	5.90975	-1.20541	C	6.66466	-4.50542	-2.32693
H	-4.42543	6.04168	0.27643	C	2.38159	-2.00384	-1.77546
H	-5.49126	1.35131	2.38514	C	1.72768	-0.26930	0.58932
H	-4.27328	0.16884	1.88673	C	1.13985	0.60673	-0.32108
H	-5.89969	0.08786	1.21462	C	-0.23602	0.70320	-0.45760
H	-7.54080	-2.66872	-0.69273	C	-1.12473	-0.08274	0.28089
H	-4.66696	-4.01044	2.16809	C	-0.52661	-0.96306	1.18498
H	-6.17720	0.26622	-1.54059	C	0.84832	-1.04369	1.34672
H	-7.08368	-1.09054	-2.23038	C	-3.35671	1.35412	-0.29152
H	-5.39819	-0.79413	-2.70743	C	-2.85161	2.58270	0.14686
H	-8.22380	-4.20358	1.10506	C	-3.43832	3.79793	-0.17047
H	-7.07444	-4.66990	2.37028	C	-4.57022	3.81484	-0.97510
H	-7.03045	-5.46814	0.79775	C	-5.10536	2.62209	-1.44425
H	-2.68439	-3.11390	2.42989	C	-4.50172	1.42517	-1.09165
H	-2.52276	-1.39195	2.07187	C	-3.54636	-1.30260	0.24758
H	-1.83383	-2.58333	0.97523	C	-4.85319	-1.26395	0.74348
				C	-5.63164	-2.39803	0.91461
				C	-5.10973	-3.63673	0.56517
74				C	-3.81948	-3.72779	0.05914
1				C	-3.06440	-2.57374	-0.08122
P	3.52111	-0.38623	1.01079	H	4.38522	4.20143	2.43007
B	-2.67680	-0.00810	0.08126	H	5.80072	3.36020	-1.51214
F	1.89160	1.32772	-1.15626	H	2.25290	1.54717	2.81633
F	-0.70120	1.55869	-1.37394	H	3.28091	2.69274	3.68073
F	-1.28085	-1.76090	1.94729	H	3.78389	1.00216	3.48749
F	1.32133	-1.91062	2.24368				

H	6.60888	5.37746	-0.27237
H	5.93453	5.76215	1.32038
H	4.96453	6.00228	-0.13483
H	5.23803	1.50843	-2.62486
H	4.00282	0.39055	-2.03410
H	5.69735	0.10488	-1.65046
H	7.44338	-2.97336	-0.20991
H	4.10863	-3.70554	-2.77491
H	6.44983	-0.06763	1.18274
H	7.35774	-1.54533	1.52969
H	5.79230	-1.25244	2.30864
H	7.73321	-4.28005	-2.29491
H	6.35585	-4.56051	-3.37357
H	6.52286	-5.49861	-1.88828
H	2.23134	-2.57946	-2.69074
H	2.23304	-0.94842	-2.02129
H	1.59722	-2.29410	-1.07098

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**1P**

C	1.707132	-0.782302	0.333165
P	0.137118	-0.076926	0.992969
C	2.849518	-0.275523	0.998066
C	4.114452	-0.759080	0.666036
C	4.293633	-1.752604	-0.290463
C	-1.312211	-0.929759	0.226383
C	-1.916044	-0.608058	-0.988317
C	-3.094577	-1.212502	-1.404711
C	-3.719618	-2.168899	-0.620640
C	-3.134331	-2.506950	0.587030
C	-1.956983	-1.894530	1.002122
F	-1.335114	0.248814	-1.832304
F	-3.613032	-0.871768	-2.586299
F	-3.697504	-3.424755	1.374678
F	-1.447687	-2.262753	2.179100
C	-0.043312	1.647309	0.344227
C	-0.906468	2.456443	1.119287
C	-1.064582	3.803882	0.798364
C	-0.377536	4.390227	-0.259713
C	0.459338	3.579174	-1.020160
C	0.636651	2.220038	-0.752493
C	-1.690219	1.907669	2.289605
C	-0.521720	5.858457	-0.563402
C	1.534710	1.446302	-1.686470
C	3.160429	-2.244706	-0.931225
C	1.874121	-1.782214	-0.648694
C	2.757201	0.817368	2.037050
C	5.662363	-2.295971	-0.605819
C	0.745675	-2.360656	-1.467945
H	4.982057	-0.346610	1.176132
H	-4.636213	-2.643437	-0.947449

H	-1.740456	4.410453	1.396932
H	0.984992	4.012714	-1.868211
H	-1.028517	1.499506	3.058959
H	-2.300705	2.694018	2.737904
H	-2.361603	1.097385	1.985845
H	-1.503777	6.230533	-0.262062
H	0.232279	6.441907	-0.024641
H	-0.391178	6.056625	-1.629940
H	1.727013	2.037994	-2.584074
H	2.498187	1.201752	-1.229372
H	1.071922	0.506546	-1.991746
H	3.278898	-3.011357	-1.693754
H	2.068603	0.545072	2.843428
H	3.739262	1.009989	2.472900
H	2.389949	1.754546	1.604119
H	6.437706	-1.549682	-0.417464
H	5.885708	-3.169242	0.015900
H	5.732949	-2.609074	-1.650351
H	1.145770	-3.055960	-2.208414
H	0.021665	-2.905764	-0.856882
H	0.203016	-1.578556	-2.006585

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**[1PH]<sup>+</sup>**

C	1.756549	-0.657381	0.218909
P	0.141096	0.007807	0.639865
C	2.817808	-0.174530	1.021489
C	4.105900	-0.622629	0.746298
C	4.368372	-1.527534	-0.281759
C	-1.270680	-1.014332	0.171427
C	-1.986811	-0.797327	-1.003091
C	-3.103841	-1.563903	-1.304992
C	-3.531107	-2.557082	-0.434747
C	-2.825614	-2.779446	0.737859
C	-1.704433	-2.014954	1.039456
F	-1.564848	0.119513	-1.873788
F	-3.749133	-1.335250	-2.438629
F	-3.205017	-3.719876	1.589023
F	-1.038528	-2.241844	2.170719
C	-0.162285	1.738599	0.255205
C	-1.001970	2.444414	1.146544
C	-1.231443	3.795720	0.899984
C	-0.659700	4.454726	-0.186459
C	0.156635	3.724258	-1.052592
C	0.423010	2.372532	-0.863532
C	-1.652106	1.808171	2.352743
C	-0.909940	5.916570	-0.432479
C	1.310933	1.665860	-1.857135
C	3.298713	-1.981372	-1.054112
C	1.987448	-1.568435	-0.834046
C	2.613143	0.796229	2.161318

C	5.765405	-2.019702	-0.537198	C	-4.57239	-1.26707	5.34636
C	0.910410	-2.120283	-1.736209	C	-5.02359	1.39565	1.12754
H	0.080264	-0.078559	2.030497	C	-3.44142	3.22679	-2.56420
H	4.928113	-0.252617	1.352577	C	-3.42855	1.94483	-2.01207
H	-4.402967	-3.155760	-0.671922	C	-1.28323	2.64385	1.10767
H	-1.878734	4.347126	1.575972	C	-2.70659	5.64399	-2.64020
H	0.596358	4.224889	-1.911214	C	-4.23440	0.86689	-2.69694
H	-0.917803	1.579816	3.134304	H	-0.93818	0.13862	0.10265
H	-2.380513	2.492581	2.788049	H	-1.53917	4.89346	-0.32111
H	-2.184321	0.883345	2.106953	H	-2.40555	-4.40266	-3.59036
H	-1.636169	6.322925	0.272643	H	-2.52595	-2.42871	3.99843
H	0.019180	6.485119	-0.331990	H	-5.58888	0.52585	3.56622
H	-1.284425	6.079241	-1.446521	H	-0.64387	-1.67648	1.04209
H	1.476127	2.306413	-2.724144	H	-0.87869	-2.72262	2.42751
H	2.287120	1.419901	-1.428928	H	-1.79211	-3.01265	0.94357
H	0.857987	0.738953	-2.217832	H	-4.62709	-2.34478	5.51882
H	3.492703	-2.679933	-1.863321	H	-3.87397	-0.85259	6.07991
H	2.096708	0.321171	3.003670	H	-5.55709	-0.83534	5.53488
H	3.577293	1.143893	2.532767	H	-5.97455	1.59602	1.62363
H	2.040741	1.681289	1.863891	H	-4.47040	2.33753	1.06707
H	6.507745	-1.271326	-0.253736	H	-5.24326	1.07856	0.10458
H	5.959415	-2.920685	0.053523	H	-4.00975	3.39400	-3.47542
H	5.910052	-2.275164	-1.588519	H	-0.40298	2.00122	1.00933
H	1.368110	-2.666953	-2.561252	H	-0.93856	3.61188	1.47456
H	0.256768	-2.817048	-1.202728	H	-1.92219	2.19904	1.87922
H	0.285163	-1.337619	-2.173941	H	-3.04347	6.41897	-1.94625

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**1PHBH**

C	-2.67613	1.74299	-0.84270	H	-3.60794	0.24041	-3.33969
P	-2.32893	0.11946	-0.14641	H	-4.74655	0.21053	-1.98768
C	-2.01389	2.81544	-0.19890	C	2.25267	-1.36590	4.62141
C	-2.06441	4.06804	-0.79432	C	3.31704	-1.46085	3.73824
C	-2.74410	4.28711	-1.99340	C	3.20178	-1.01659	2.42588
C	-2.46127	-1.23079	-1.34152	C	2.03115	-0.45991	1.91850
C	-3.54729	-2.10454	-1.37074	C	0.99804	-0.34613	2.84120
C	-3.52763	-3.23214	-2.17601	C	1.08048	-0.80090	4.14973
C	-2.42287	-3.51532	-2.96937	F	4.47444	-1.99165	4.14781
C	-1.34835	-2.64366	-2.95949	F	4.27824	-1.14704	1.64125
C	-1.37481	-1.49993	-2.16813	F	-0.18302	0.21445	2.47614
F	-4.63633	-1.83661	-0.64603	F	0.00694	-0.69121	4.94947
F	-4.58617	-4.03881	-2.18261	B	1.81519	-0.03415	0.35914
F	-0.27944	-2.86994	-3.71000	C	2.16528	1.53236	0.06449
F	-0.34755	-0.66528	-2.20543	C	2.54363	-1.06214	-0.67446
C	-3.13974	-0.34415	1.39790	C	1.38477	2.29170	-0.80041
C	-2.52021	-1.37703	2.13989	C	1.58486	3.64500	-1.04276
C	-3.01239	-1.65417	3.41142	C	2.63700	4.29263	-0.41328
C	-4.09753	-0.96661	3.95078	C	3.82375	-0.88069	-1.18981
C	-4.72091	0.00483	3.17099	C	4.41154	-1.74404	-2.10660
C	-4.26799	0.33798	1.89573	C	3.71205	-2.86224	-2.53897
C	-1.39846	-2.23047	1.60320	C	2.44102	-3.09973	-2.03976

C	1.89957	-2.20762	-1.12460	F	-4.13129	0.95198	1.70218
F	1.75245	-4.17576	-2.43578	F	-5.18242	3.38830	1.31604
C	3.46194	3.57642	0.44308	F	-3.88793	5.20377	-0.24839
C	3.21543	2.22554	0.65963	F	-1.51729	4.52570	-1.41761
F	0.33263	1.73066	-1.43278	F	-0.46259	2.12268	-1.04883
F	0.77901	4.32814	-1.86762	F	-4.22904	-0.09200	-0.94124
F	2.85217	5.59057	-0.62872	F	-5.63175	-2.26331	-1.50857
F	4.56125	0.16636	-0.80286	F	-4.77628	-4.72612	-0.71810
F	5.64014	-1.51507	-2.57276	F	-2.44249	-4.95448	0.67705
F	4.25865	-3.70165	-3.41819	F	-1.01114	-2.76959	1.26805
F	4.47804	4.19401	1.04701	H	4.57215	-1.03324	-1.66902
F	4.05029	1.59401	1.48992	H	7.26975	-2.25374	1.12024
F	0.66047	-2.52169	-0.67559	H	6.97503	-1.90246	-0.58480
H	2.33956	-1.71708	5.64146	H	7.35681	-0.58661	0.55136
H	0.62616	-0.15721	0.14722	H	5.57703	-1.55160	2.89972
				H	4.06403	-0.76179	2.43985
				H	5.59862	0.12365	2.33375
				H	4.75209	-3.20454	-0.34769
				H	5.12477	-3.45949	1.36396
				H	3.58312	-2.72587	0.90185
				H	6.79419	2.03745	-2.16759
				H	5.91825	0.65600	-2.83609
				H	7.12366	0.41700	-1.55117
				H	6.22223	3.00251	0.04111
				H	5.10891	2.19263	1.14840
				H	6.69393	1.47098	0.77602
				H	3.38178	2.48127	-0.72482
				H	4.59221	3.12336	-1.84810
				H	3.62569	1.71410	-2.30638
				H	-1.65518	-0.12763	1.96002
62				61			
<b>2H<sub>2</sub></b>				<b>[2H]<sup>+</sup></b>			
C	2.18830	0.60694	0.80619	C	2.12327	0.72290	0.56083
C	0.82925	0.64437	1.02897	C	0.74091	0.79313	0.61862
C	-0.07776	-0.17585	0.34791	C	-0.07477	-0.05359	-0.13277
C	0.49233	-1.03667	-0.58710	C	0.57930	-0.96999	-0.95406
C	1.85765	-1.09282	-0.82545	C	1.96412	-1.03940	-1.03340
C	2.74161	-0.26210	-0.13596	C	2.76407	-0.18775	-0.27343
P	4.48471	-0.32279	-0.46486	P	4.56042	-0.30686	-0.36856
C	5.32992	-1.40422	0.77624	C	5.16536	-1.38438	1.00899
C	5.24054	1.33314	-0.86226	C	5.40106	1.31897	-0.71151
C	6.81943	-1.53073	0.43328	C	6.68219	-1.57333	0.86534
C	5.12499	-0.84978	2.19212	C	4.80281	-0.76966	2.36726
C	4.64659	-2.77763	0.65422	C	4.44777	-2.73412	0.83300
C	6.33294	1.07783	-1.91619	C	6.61617	0.98879	-1.59916
C	5.84743	2.02622	0.36397	C	5.85979	2.03229	0.56669
C	4.13089	2.20606	-1.46958	C	4.41064	2.19655	-1.49248
B	-1.65903	-0.05867	0.74755	B	-1.66389	0.01727	-0.04986
C	-2.55293	-1.31562	0.22432	C	-2.46890	-1.31348	-0.05563
C	-2.24183	1.41637	0.37181	C	-2.34930	1.41031	0.03612
F	2.34266	-1.95621	-1.73039				
F	-0.25631	-1.85649	-1.32678				
F	3.01722	1.42679	1.48445				
F	0.38855	1.52620	1.92540				
C	-3.74054	-1.25869	-0.49432				
C	-4.49753	-2.38379	-0.81421				
C	-4.06732	-3.63754	-0.41507				
C	-2.88049	-3.74976	0.29724				
C	-2.16738	-2.60114	0.59700				
C	-3.45023	1.81584	0.93956				
C	-4.01915	3.06487	0.74694				
C	-3.36328	3.99323	-0.05208				
C	-2.16151	3.64525	-0.64350				
C	-1.63422	2.37595	-0.42486				

F	2.52860	-1.94779	-1.82952	C	2.84231	-0.27397	-0.24583
F	-0.11208	-1.82245	-1.70192	P	4.62017	-0.48985	-0.68796
F	2.85980	1.55335	1.30831	C	5.28238	-1.31521	0.88494
F	0.20919	1.70240	1.42825	C	5.35981	1.25831	-0.87372
C	-3.75080	-1.40758	-0.61435	C	6.80242	-1.46487	0.74109
C	-4.46770	-2.59315	-0.65827	C	4.93698	-0.64605	2.21727
C	-3.90815	-3.74540	-0.11749	C	4.65681	-2.71993	0.87321
C	-2.63765	-3.70429	0.44837	C	6.55361	1.05672	-1.82678
C	-1.94544	-2.50639	0.45825	C	5.86416	2.01506	0.35962
C	-3.56740	1.60368	0.70298	C	4.31197	2.11575	-1.59715
C	-4.17523	2.84436	0.81646	B	-1.58581	-0.04958	0.70866
C	-3.56782	3.95365	0.23888	C	-2.50184	-1.30471	0.19700
C	-2.35730	3.81490	-0.43287	C	-2.24246	1.41078	0.37381
C	-1.77226	2.56355	-0.51115	F	2.36584	-2.10481	-1.67430
F	-4.18009	0.58208	1.29501	F	-0.18838	-1.99130	-1.24574
F	-5.31907	2.98215	1.46986	F	3.04004	1.56079	1.25489
F	-4.13490	5.14014	0.33262	F	0.46510	1.66741	1.68476
F	-1.77635	4.87371	-0.98175	C	-3.63902	-1.24828	-0.59835
F	-0.60651	2.48551	-1.16313	C	-4.41463	-2.36146	-0.91531
F	-4.32288	-0.34048	-1.16560	C	-4.05459	-3.60684	-0.43299
F	-5.67077	-2.63852	-1.21034	C	-2.92001	-3.72078	0.35868
F	-4.57904	-4.88012	-0.14451	C	-2.18375	-2.58372	0.65093
F	-2.10319	-4.80377	0.96359	C	-3.46306	1.73903	0.96096
F	-0.72631	-2.52075	1.01048	C	-4.09297	2.96515	0.81542
H	4.75138	-1.05502	-1.53722	C	-3.49090	3.94764	0.04166
H	7.00764	-2.28872	1.62626	C	-2.28098	3.67324	-0.57046
H	6.95602	-1.98540	-0.11110	C	-1.68964	2.42384	-0.39886
H	7.23605	-0.64609	1.02974	F	-4.10519	0.82479	1.70455
H	5.13515	-1.46043	3.14774	F	-5.26891	3.21611	1.40612
H	3.72309	-0.63956	2.47954	F	-4.07646	5.14137	-0.11279
H	5.29352	0.19014	2.53935	F	-1.69308	4.61028	-1.32619
H	4.65874	-3.19501	-0.13645	F	-0.52542	2.24978	-1.04800
H	4.81082	-3.41164	1.61134	F	-4.06489	-0.08857	-1.12816
H	3.36492	-2.64173	0.95363	F	-5.50357	-2.23872	-1.68598
H	7.14151	1.92454	-1.81019	F	-4.78550	-4.68862	-0.72838
H	6.31662	0.55194	-2.55586	F	-2.55644	-4.92272	0.82536
H	7.32644	0.31724	-1.11010	F	-1.08866	-2.76167	1.40642
H	6.30615	2.98574	0.26877	H	7.18686	-2.09651	1.55162
H	5.03229	2.24845	1.24313	H	7.06596	-1.93888	-0.21067
H	6.62688	1.46780	1.10233	H	7.32069	-0.50343	0.79976
H	3.58454	2.53232	-0.86226	H	5.33200	-1.25759	3.03953
H	4.95026	3.08183	-1.84140	H	3.85505	-0.56862	2.35073
H	4.00522	1.68781	-2.37289	H	5.36321	0.35391	2.30727
				H	4.88963	-3.25569	-0.05188
				H	5.04818	-3.29968	1.71839
				H	3.56832	-2.67205	0.97391
61				H	7.01728	2.02696	-2.04511
[2H] <sup>-</sup>				H	6.23514	0.60428	-2.76987
C	2.26529	0.65695	0.61886	H	7.32075	0.41061	-1.38703
C	0.90331	0.70767	0.85241	H	6.26577	2.98365	0.03291
C	-0.01662	-0.16195	0.26742	H	5.07051	2.20548	1.07939
C	0.56154	-1.08795	-0.58953				
C	1.93120	-1.14800	-0.83765				

H 6.67752 1.48456 0.86304  
H 3.50171 2.40570 -0.92562  
H 4.78984 3.02956 -1.97185  
H 3.87784 1.58740 -2.45273  
H -1.57818 -0.12965 1.92153

60  
**2**

C 2.20158 0.73761 0.41498  
C 0.81999 0.82705 0.48510  
C -0.02653 -0.07698 -0.16021  
C 0.62557 -1.07051 -0.89221  
C 2.00829 -1.14291 -0.98754  
C 2.85056 -0.23689 -0.33898  
P 4.67904 -0.48999 -0.59149  
C 5.10518 -1.35629 1.03867  
C 5.46983 1.23851 -0.67267  
C 6.62777 -1.54830 1.07173  
C 4.62650 -0.67704 2.32380  
C 4.44556 -2.74190 0.93971  
C 6.76355 0.99430 -1.47620  
C 5.84627 1.97679 0.61569  
C 4.54592 2.12325 -1.52243  
B -1.58816 0.01507 -0.06505  
C -2.45316 -1.29227 -0.08895  
C -2.28438 1.41497 0.05469  
F 2.51988 -2.13762 -1.71567  
F -0.08101 -1.99270 -1.55307  
F 2.90146 1.64365 1.10978  
F 0.30834 1.81209 1.23127  
C -3.73000 -1.33289 -0.65797  
C -4.50269 -2.48279 -0.70167  
C -4.00693 -3.65390 -0.14316  
C -2.74740 -3.66370 0.44230  
C -1.99644 -2.49863 0.45150  
C -3.47201 1.60012 0.76989  
C -4.09319 2.83247 0.89954  
C -3.53175 3.94263 0.28191  
C -2.35720 3.80999 -0.44738  
C -1.75511 2.56484 -0.54032  
F -4.05552 0.57186 1.38795  
F -5.21363 2.96074 1.60273  
F -4.11554 5.12603 0.38824  
F -1.82339 4.87137 -1.04308  
F -0.63223 2.49917 -1.25635  
F -4.25682 -0.23980 -1.21244  
F -5.70550 -2.47491 -1.26678  
F -4.73464 -4.75950 -0.16816  
F -2.27590 -4.78275 0.98235  
F -0.79734 -2.56773 1.03076  
H 6.89232 -2.19431 1.91675

H 6.99018 -2.02676 0.15591  
H 7.16174 -0.60321 1.20151  
H 4.91126 -1.29700 3.18295  
H 3.53759 -0.57642 2.34005  
H 5.06459 0.31161 2.46477  
H 4.75687 -3.27496 0.03692  
H 4.73447 -3.34055 1.81126  
H 3.35327 -2.67041 0.93623  
H 7.27947 1.94914 -1.62959  
H 6.54903 0.55607 -2.45449  
H 7.45147 0.32482 -0.95022  
H 6.31256 2.93143 0.34202  
H 4.98374 2.19462 1.24239  
H 6.57942 1.42134 1.20643  
H 3.67225 2.45400 -0.95717  
H 5.09754 3.01583 -1.83931  
H 4.20533 1.60472 -2.42535

34  
**2B**

C 4.237201 -0.699882 1.023035  
C 3.430284 0.055686 1.857360  
C 2.096144 0.272311 1.543256  
C 1.499279 -0.264365 0.399112  
C 2.336128 -1.029129 -0.418283  
C 3.675830 -1.237831 -0.123081  
F 3.927826 0.590155 2.972525  
F 1.380054 1.013007 2.393885  
F 1.863777 -1.580848 -1.539654  
F 4.415987 -1.969212 -0.956172  
B -0.013473 -0.023883 0.054367  
C -0.836978 -1.139973 -0.675747  
C -0.698658 1.331895 0.440753  
C -1.869128 -0.842064 -1.571524  
C -2.596487 -1.815353 -2.238424  
C -2.310833 -3.154310 -2.004423  
C -2.049772 1.412594 0.793493  
C -2.668002 2.599639 1.153798  
C -1.929348 3.775878 1.153151  
C -0.585552 3.750489 0.802643  
C 0.002790 2.541766 0.465045  
F 0.119379 4.876872 0.796847  
C -1.300317 -3.502917 -1.117516  
C -0.582549 -2.501677 -0.482328  
F -2.185904 0.425692 -1.839616  
F -3.559253 -1.481772 -3.091502  
F -3.001053 -4.097234 -2.626043  
F -2.808485 0.315668 0.816451  
F -3.952150 2.622986 1.494915  
F -2.505556 4.919983 1.486210  
F -1.031024 -4.784057 -0.889782



F 0.373411 -2.896363 0.359266  
F 1.294266 2.579439 0.135499  
H 5.280657 -0.865863 1.260820

35  
[2BH]<sup>-</sup>

C 4.175757 -0.823843 1.188389  
C 3.297127 -0.034766 1.906597  
C 2.040856 0.289828 1.401943  
C 1.589722 -0.140306 0.159775  
C 2.497058 -0.938957 -0.535748  
C 3.749515 -1.277754 -0.050645  
F 3.652583 0.428485 3.117994  
F 1.268413 1.050691 2.199812  
F 2.152607 -1.435616 -1.736602  
F 4.559248 -2.055377 -0.791169  
B 0.183162 0.254568 -0.574258  
C -0.744376 -1.043965 -0.936742  
C -0.642580 1.441682 0.192561  
C -1.817851 -0.868504 -1.808175  
C -2.638277 -1.893946 -2.251603  
C -2.396472 -3.189619 -1.816623  
C -1.934518 1.378717 0.698499  
C -2.596216 2.466992 1.263156  
C -1.955136 3.689720 1.347482  
C -0.658189 3.804823 0.866540  
C -0.043593 2.695157 0.308260  
F -0.023460 4.981980 0.950294  
C -1.347377 -3.420570 -0.944960  
C -0.554130 -2.356054 -0.522787  
F -2.115978 0.363861 -2.248835  
F -3.657416 -1.655872 -3.088462  
F -3.172222 -4.199183 -2.230861  
F -2.637650 0.232930 0.679698  
F -3.845897 2.340503 1.730224  
F -2.572939 4.746695 1.889487  
F -1.108740 -4.665842 -0.511265  
F 0.425429 -2.681394 0.337683  
F 1.215875 2.867094 -0.122052  
H 5.151675 -1.081048 1.578716  
H 0.503989 0.728893 -1.646323

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2P

C 1.726228 -0.872785 0.300215  
P 0.603924 0.278126 -0.718751  
C 3.146315 -0.459954 -0.136851  
C 1.477740 -2.305869 -0.191655  
C 1.675647 -0.841952 1.831133  
C -1.042742 -0.577269 -0.879706  
C -1.691471 -0.432117 -2.108870

C -2.922964 -1.021166 -2.374560  
C -3.564325 -1.787435 -1.417660  
C -2.944244 -1.940528 -0.189186  
C -1.718634 -1.340523 0.069690  
F -1.146414 0.304986 -3.079350  
F -3.481001 -0.835024 -3.572026  
F -3.524325 -2.663081 0.771908  
F -1.200651 -1.530656 1.290579  
C 0.088901 1.790527 0.297956  
C -0.759195 2.642147 -0.661385  
C 1.364593 2.574265 0.636882  
C -0.726248 1.527079 1.566017  
H 3.880308 -1.106167 0.358445  
H 3.373832 0.574722 0.138479  
H 3.274345 -0.556212 -1.218252  
H 2.298048 -2.948684 0.148179  
H 0.546545 -2.711872 0.208718  
H 1.443076 -2.359560 -1.285274  
H 0.703177 -1.131634 2.224327  
H 2.418771 -1.552034 2.215128  
H 1.937774 0.141367 2.230447  
H -4.522237 -2.248988 -1.621012  
H -1.693880 2.138378 -0.927561  
H -0.218849 2.870642 -1.584437  
H -1.020079 3.587022 -0.170603  
H 1.090284 3.542098 1.072323  
H 1.990495 2.052410 1.365693  
H 1.964957 2.766124 -0.258581  
H -1.666512 1.018044 1.336473  
H -0.182865 0.929073 2.298267  
H -0.978325 2.486504 2.034861

39  
[2PH]<sup>+</sup>

C 2.02050 -1.09151 -1.04758  
P 1.08846 0.37398 -0.37425  
C 3.12292 -0.51093 -1.95394  
C 1.03758 -1.91801 -1.89090  
C 2.64474 -1.95731 0.05413  
C -0.68074 0.07794 -0.16918  
C -1.60385 0.96955 -0.71651  
C -2.97030 0.76284 -0.56020  
C -3.44067 -0.33286 0.14677  
C -2.53037 -1.22209 0.70052  
C -1.16726 -1.01389 0.54507  
F -1.17930 2.04049 -1.38514  
F -3.80898 1.63453 -1.09517  
F -2.94213 -2.27733 1.38430  
F -0.30277 -1.87935 1.08418  
C 1.72615 1.26537 1.11652  
C 0.89869 2.55822 1.22135



P	-2.238140	-1.088563	-0.813651	H	-2.849711	1.052690	-3.214033
C	-0.940488	-0.312844	-1.823249	H	-2.750985	1.926818	-1.684321
C	0.398248	-0.989945	-1.487393	H	-6.075386	1.624103	-2.480388
B	1.591078	0.136428	-1.579080	H	-8.791099	-0.717914	-1.562891
C	-3.985248	-0.649301	-1.080696	H	-8.388677	0.742634	-2.483584
C	-4.392191	0.502103	-1.790307	H	-8.535873	0.815549	-0.726240
C	-3.443525	1.498714	-2.412995	H	-7.037642	-1.935774	-0.320239
C	-5.759026	0.738733	-1.935242	H	-5.473041	-3.284869	0.579665
C	-6.726657	-0.114821	-1.411597	H	-3.897408	-2.618608	1.014530
C	-8.191696	0.194829	-1.559711	H	-4.098947	-3.527045	-0.493822
C	-6.299413	-1.250280	-0.728254	H	-2.401683	2.219823	1.779920
C	-4.948683	-1.538665	-0.551162	H	-3.276128	1.337574	0.524536
C	-4.578452	-2.806620	0.179089	H	-1.568606	1.798140	0.290540
C	-1.751519	-1.057512	0.930087	H	-1.422581	1.123657	3.505764
C	-1.833692	0.154578	1.645318	H	0.791905	-0.448316	4.880649
C	-2.306977	1.441691	1.020570	H	-0.195190	-1.807729	5.442070
C	-1.380372	0.184679	2.960134	H	-0.801106	-0.143557	5.575407
C	-0.814494	-0.931752	3.569709	H	-0.298778	-2.994777	3.302720
C	-0.229913	-0.833531	4.950360	H	-0.589609	-4.265193	1.496413
C	-0.745612	-2.117747	2.842460	H	-0.304547	-3.428298	-0.025611
C	-1.195187	-2.212211	1.527644	H	-1.945937	-3.936875	0.423689
C	-1.006265	-3.528331	0.808912				
C	1.290212	1.267273	-0.418816	71			
C	0.996744	2.599762	-0.700277	[3H] <sup>+</sup>			
F	0.912392	3.025154	-1.967333	P	-2.347415	-0.637362	-0.619403
C	0.752712	3.559323	0.279999	C	-0.827036	0.364083	-0.599225
F	0.466417	4.821667	-0.048694	C	0.411218	-0.522705	-0.750987
C	0.801697	3.193044	1.617130	B	1.820653	0.170385	-0.506866
F	0.559367	4.090102	2.574817	C	-3.889759	0.259356	-0.913145
C	1.096852	1.878755	1.950133	C	-4.041751	1.653760	-0.732761
F	1.138040	1.519905	3.241073	C	-2.959929	2.589744	-0.243583
C	1.313393	0.952270	0.938023	C	-5.283854	2.215975	-1.022202
F	1.545891	-0.312720	1.332624	C	-6.363331	1.462498	-1.480075
C	3.079320	-0.478499	-1.313864	C	-7.677354	2.114633	-1.808422
C	4.187602	0.336898	-1.533285	C	-6.183886	0.090506	-1.646394
F	4.006459	1.597840	-1.952247	C	-4.969181	-0.531708	-1.377012
C	5.499946	-0.070679	-1.336328	C	-4.856678	-2.018688	-1.616058
F	6.522536	0.756537	-1.568729	C	-2.365138	-1.818287	0.746559
C	5.747411	-1.359401	-0.883338	C	-2.739010	-1.386031	2.037474
F	6.999415	-1.775796	-0.684889	C	-3.090006	0.047476	2.347498
C	4.679513	-2.207220	-0.636952	C	-2.761702	-2.319349	3.069376
F	4.905019	-3.448676	-0.194061	C	-2.419508	-3.655432	2.865014
C	3.382378	-1.751532	-0.848065	C	-2.427377	-4.637098	4.003748
F	2.405366	-2.641226	-0.571162	C	-2.040288	-4.051983	1.582723
H	-2.179515	-2.438038	-1.169700	C	-1.999928	-3.165383	0.509060
H	-1.210704	-0.420288	-2.877566	C	-1.568047	-3.700338	-0.837772
H	-0.914625	0.755546	-1.592898	C	1.860534	1.635932	0.072377
H	0.556377	-1.836063	-2.164241	C	1.230557	2.715615	-0.539259
H	0.392346	-1.387763	-0.469377	F	0.635696	2.551581	-1.734234
H	1.565670	0.671361	-2.664883	C	1.197545	3.986837	0.014647
H	-4.009619	2.323857	-2.846756	F	0.575730	4.981038	-0.607389

C	1.825800	4.206293	1.234989	C	3.776927	-1.659971	-0.344832
F	1.799984	5.407654	1.784787	C	4.136333	-2.370699	0.822590
C	2.479393	3.159849	1.878034	C	3.146178	-3.142996	1.661782
F	3.076511	3.368577	3.042167	C	5.466426	-2.388055	1.244291
C	2.492431	1.906112	1.285179	C	6.480104	-1.736838	0.547893
F	3.129671	0.920977	1.921989	C	7.899029	-1.733757	1.055626
C	3.129601	-0.645384	-0.730623	C	6.129498	-1.088778	-0.629624
C	4.406272	-0.060002	-0.670699	C	4.812176	-1.048803	-1.092298
F	4.549407	1.239949	-0.431474	C	4.566171	-0.339847	-2.403999
C	5.578825	-0.772939	-0.869688	C	1.831511	0.286653	-1.170121
F	6.755621	-0.169064	-0.808753	C	2.188356	1.172680	-0.128021
C	5.511509	-2.134849	-1.138483	C	2.796387	0.743029	1.188843
F	6.616655	-2.826569	-1.328112	C	1.993959	2.544298	-0.303663
C	4.275020	-2.767149	-1.208142	C	1.426440	3.077257	-1.457337
F	4.205491	-4.066742	-1.462359	C	1.206445	4.562658	-1.584975
C	3.125379	-2.021412	-1.011587	C	1.055987	2.192835	-2.464112
F	1.971923	-2.697323	-1.091169	C	1.258343	0.815353	-2.347482
H	-2.185866	-1.425461	-1.761334	C	0.846942	-0.058001	-3.511739
H	-0.906880	1.072964	-1.424061	C	-1.279280	0.373628	1.024975
H	-0.791792	0.937288	0.330314	C	-0.528580	0.752443	2.131871
H	0.408813	-1.028425	-1.723749	F	-0.112046	-0.162384	3.026356
H	0.381042	-1.339407	-0.011883	C	-0.121178	2.060565	2.376925
H	-2.492776	2.240425	0.679738	F	0.654665	2.358793	3.431645
H	-2.173202	2.746049	-0.987687	C	-0.467632	3.059635	1.484386
H	-3.394313	3.567054	-0.031017	F	-0.027521	4.314809	1.666081
H	-5.411875	3.285693	-0.881625	C	-1.198926	2.734621	0.353350
H	-7.707000	2.389158	-2.867673	F	-1.481022	3.687379	-0.546603
H	-7.825602	3.025174	-1.225128	C	-1.567111	1.413902	0.142975
H	-8.513044	1.438360	-1.618421	F	-2.225939	1.161494	-1.000797
H	-7.014444	-0.515840	-1.997293	C	-3.276823	-1.231990	0.236854
H	-5.837413	-2.435932	-1.845433	C	-4.272352	-1.221111	1.210837
H	-4.467587	-2.555881	-0.745389	F	-3.944287	-1.139301	2.509930
H	-4.207967	-2.236091	-2.473183	C	-5.632803	-1.287311	0.933349
H	-3.385068	0.148273	3.392443	F	-6.543073	-1.280116	1.918231
H	-3.915002	0.415927	1.731109	C	-6.052949	-1.358687	-0.385661
H	-2.226567	0.705170	2.196600	F	-7.358394	-1.423550	-0.679498
H	-3.054733	-1.992191	4.063257	C	-5.104650	-1.358950	-1.395991
H	-1.444933	-4.663536	4.485880	F	-5.503283	-1.419121	-2.674833
H	-2.652244	-5.646720	3.654857	C	-3.754449	-1.289369	-1.068734
H	-3.161497	-4.358462	4.761964	F	-2.909852	-1.276987	-2.113446
H	-1.766318	-5.089261	1.410905	H	0.789715	-2.980331	0.461587
H	-1.318742	-4.758129	-0.750894	H	0.841282	-1.327009	1.057220
H	-0.678507	-3.190725	-1.220392	H	-0.981981	-2.589729	-0.998274
H	-2.360662	-3.617284	-1.588981	H	-0.587060	-0.902568	-1.251509
				H	-1.575579	-1.857142	1.678304
				H	3.666155	-3.655009	2.474928
				H	2.625547	-3.900985	1.070550
				H	2.384262	-2.497564	2.105406
				H	5.715688	-2.932928	2.153185
				H	8.611461	-1.593359	0.238312
				H	8.141089	-2.672220	1.562175
71							
[3H]							
P	2.068093	-1.561916	-1.090494				
C	0.728779	-1.934535	0.155300				
C	-0.650616	-1.680236	-0.482580				
B	-1.695514	-1.181320	0.677452				

H 8.058933 -0.923043 1.774968  
H 6.903462 -0.600774 -1.219786  
H 5.502849 -0.247675 -2.959990  
H 4.155631 0.663159 -2.253632  
H 3.850265 -0.888463 -3.024323  
H 2.591797 1.497031 1.953925  
H 3.881965 0.620901 1.103615  
H 2.395576 -0.205514 1.547036  
H 2.254911 3.216791 0.512892  
H 0.808275 4.970965 -0.652757  
H 0.495206 4.786542 -2.383278  
H 2.144746 5.082547 -1.807965  
H 0.590883 2.581148 -3.367701  
H 0.495914 0.562264 -4.340165  
H 0.041186 -0.744799 -3.236808  
H 1.678920 -0.673768 -3.865444

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**3PB**

P 1.130866 -0.301931 -0.614489  
C 0.793941 -0.043823 -2.426744  
C -0.545922 -0.805684 -2.322971  
B -0.971394 -0.328565 -0.820848  
C 2.243706 -1.775403 -0.694861  
C 1.807740 -3.068077 -0.341469  
C 0.425153 -3.358347 0.180284  
C 2.693515 -4.139620 -0.463029  
C 3.997555 -3.977320 -0.918833  
C 4.942859 -5.145940 -1.007800  
C 4.407509 -2.694946 -1.270733  
C 3.562961 -1.589290 -1.170028  
C 4.138498 -0.248128 -1.561386  
C 2.048396 0.968542 0.356797  
C 2.464165 0.591620 1.653791  
C 2.202855 -0.773017 2.241295  
C 3.147248 1.512267 2.447391  
C 3.420440 2.804254 2.013586  
C 4.123181 3.794072 2.903734  
C 2.987451 3.163713 0.741033  
C 2.305781 2.281116 -0.097747  
C 1.900814 2.813389 -1.450926  
C -2.054226 -1.180753 0.015280  
C -3.214405 -1.550296 -0.665623  
F -3.358817 -1.229113 -1.959048  
C -4.270817 -2.233055 -0.076935  
F -5.351602 -2.557749 -0.783891  
C -4.193631 -2.572715 1.265713  
F -5.190163 -3.229237 1.852166  
C -3.064114 -2.221243 1.989444  
F -2.973436 -2.546171 3.278384  
C -2.035649 -1.530007 1.360877

F -0.972682 -1.247843 2.132274  
C -1.259686 1.270180 -0.678442  
C -1.735800 2.078097 -1.710721  
F -1.981762 1.571896 -2.926319  
C -1.959560 3.443705 -1.568808  
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C -1.708130 4.054880 -0.348717  
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C -1.246539 3.291779 0.714978  
F -1.006521 3.867352 1.890912  
C -1.055059 1.928801 0.533957  
F -0.624452 1.236051 1.594711  
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H 1.559329 -0.457937 -3.086771  
H -0.356763 -1.885287 -2.349509  
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H 0.336386 -4.413666 0.444554  
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H 0.204699 -2.768880 1.071768  
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H 5.649393 -5.020994 -1.831627  
H 4.401212 -6.082575 -1.156735  
H 5.524702 -5.242247 -0.085368  
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H 5.033618 -0.392621 -2.169301  
H 4.416133 0.336803 -0.679247  
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H 2.327821 -0.739694 3.325161  
H 2.891337 -1.524072 1.842370  
H 1.182958 -1.104855 2.040469  
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H 4.699951 4.513720 2.318198  
H 4.800328 3.291113 3.597782  
H 3.184765 4.170765 0.381729  
H 2.238511 3.845514 -1.557293  
H 0.815274 2.807752 -1.579111  
H 2.339071 2.237824 -2.270900

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**3B**

C 2.178950 -0.344118 0.433983  
C 2.919314 0.950683 0.776340  
B 0.653791 -0.244398 0.064168  
C -0.208662 -1.525532 -0.233532  
C -0.028788 1.181502 0.058990  
C -1.562199 -1.472416 -0.603737  
C -2.328217 -2.600820 -0.857216  
C -1.749260 -3.857622 -0.746877  
C -1.037950 1.516032 0.953896

C	-1.587224	2.786792	1.023873	H	-1.44140	4.46759	-1.45268
C	-1.127480	3.769318	0.154002	H	-2.27680	2.93339	-1.18405
C	-0.130945	3.472462	-0.766415	H	-1.35227	3.17251	-2.66050
C	0.400842	2.190369	-0.792650	H	-0.11214	0.92562	-2.34177
F	0.298492	4.408634	-1.607574				
C	-0.413575	-3.970776	-0.387576	48			
C	0.323333	-2.820993	-0.144473	<b>3P</b>			
F	-2.193804	-0.308932	-0.747300	C	0.525517	-1.392824	-0.011033
F	-3.605062	-2.489506	-1.207316	P	-0.511792	-0.490262	1.238945
F	-2.467116	-4.942685	-0.986541	C	0.373703	-1.261540	-1.407798
F	-1.508711	0.579532	1.786191	C	1.175590	-2.028462	-2.255903
F	-2.544992	3.073091	1.900708	C	2.125889	-2.922480	-1.770594
F	-1.646144	4.989974	0.200193	C	-2.193494	-1.149931	0.684035
F	0.146476	-5.171411	-0.283219	C	-0.482199	1.284955	0.690195
F	1.599283	-3.015762	0.188884	C	-1.592752	2.114440	0.957723
F	1.350033	1.926224	-1.701216	C	-1.588735	3.441228	0.523721
H	2.232625	-1.038294	1.285693	C	-0.498232	4.001541	-0.130997
H	2.700715	-0.893013	-0.362105	C	0.640503	3.211756	-0.263461
H	3.933731	0.739652	1.123213	C	0.683185	1.880997	0.154763
H	2.996246	1.608604	-0.091313	C	-2.771611	1.672004	1.798303
H	2.406299	1.503406	1.568930	C	-0.530060	5.419105	-0.638757
				C	2.021062	1.179329	0.060584
				C	2.265648	-3.039294	-0.390688
				C	1.483938	-2.295773	0.494354
				C	-0.562606	-0.270034	-2.059156
				C	2.955838	-3.759533	-2.708762
				C	1.713685	-2.484105	1.977515
				C	-2.947873	-1.832104	1.824584
				H	1.056575	-1.914795	-3.331693
				H	-2.793359	-0.356162	0.235040
				H	-1.994052	-1.878868	-0.105884
				H	-2.460100	4.059343	0.732152
				H	1.542082	3.650373	-0.686931
				H	-3.601226	1.270946	1.208460
				H	-2.480685	0.910672	2.527151
				H	-3.157962	2.528428	2.355989
				H	-1.227999	6.030975	-0.062020
				H	0.458302	5.882255	-0.583393
				H	-0.850193	5.451778	-1.685551
				H	2.818270	1.926452	0.055889
				H	2.191846	0.514365	0.911511
				H	2.121831	0.573240	-0.844483
				H	3.004234	-3.729392	0.011378
				H	-1.493373	-0.133664	-1.509814
				H	-0.091739	0.717196	-2.124145
				H	-0.805438	-0.593485	-3.074097
				H	3.106157	-3.252233	-3.664708
				H	3.935805	-3.981150	-2.279206
				H	2.462815	-4.715130	-2.915884
				H	2.511090	-3.210995	2.146812
				H	1.994141	-1.545975	2.465142
31							
<b>[3BH]<sup>-</sup></b>							
C	-0.12101	2.78187	-0.91131				
C	-1.35859	3.38084	-1.58467				
B	-0.03397	1.16999	-1.15370				
C	-1.28784	0.42620	-0.38950				
C	1.34764	0.45178	-0.61705				
C	-2.35742	-0.16983	-1.04894				
C	-3.42481	-0.77455	-0.39115				
C	-3.44992	-0.79765	0.99411				
C	2.32236	1.02333	0.19323				
C	3.47871	0.36087	0.59661				
C	3.69176	-0.94842	0.19910				
C	2.74333	-1.57327	-0.59678				
C	1.60739	-0.86981	-0.97618				
F	2.93730	-2.84361	-0.98242				
C	-2.40865	-0.21407	1.70035				
C	-1.36579	0.37885	0.99963				
F	-2.41810	-0.18572	-2.38868				
F	-4.43296	-1.33500	-1.07653				
F	-4.47014	-1.37466	1.64449				
F	2.20130	2.28434	0.64071				
F	4.38808	0.97087	1.37216				
F	4.79795	-1.60370	0.57874				
F	-2.42789	-0.23075	3.04146				
F	-0.39007	0.92862	1.74525				
F	0.72647	-1.54236	-1.73484				
H	0.77656	3.26893	-1.31751				
H	-0.13436	3.03293	0.15731				

H 0.812697 -2.839140 2.485124  
H -2.356279 -2.650367 2.244911  
H -3.171694 -1.138881 2.639656  
H -3.894386 -2.249526 1.468570

H 2.166986 -2.023220 2.148998  
H 0.666620 -2.959166 2.241484  
H -1.509191 -1.077149 3.742202  
H -2.409468 0.243267 2.989019  
H -3.204812 -1.304750 3.304432

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[3PH]<sup>+</sup>

C 0.487004 -1.517426 -0.257639  
P -0.365941 -0.530793 0.989293  
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C 1.026633 -2.079444 -2.532257  
C 1.884128 -3.092616 -2.107115  
C -1.856669 -1.374566 1.616526  
C -0.512538 1.231639 0.638257  
C -1.722370 1.882814 0.307758  
C -1.674407 3.249134 0.040934  
C -0.488852 3.982408 0.083100  
C 0.689702 3.310510 0.402222  
C 0.708427 1.948034 0.685918  
C -3.069451 1.205342 0.211934  
C -0.486460 5.461095 -0.186992  
C 2.030923 1.305832 1.037248  
C 2.029699 -3.304496 -0.735500  
C 1.350403 -2.539062 0.206668  
C -0.584983 -0.207511 -2.192451  
C 2.611119 -3.957888 -3.098575  
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C -2.268007 -0.840648 2.992063  
H 0.477706 -0.570943 2.102927  
H 0.901363 -1.904135 -3.597216  
H -2.654158 -1.306325 0.876166  
H -1.571425 -2.430823 1.670575  
H -2.598595 3.759172 -0.216346  
H 1.625057 3.862581 0.431301  
H -3.068971 0.357158 -0.478005  
H -3.424952 0.851881 1.183479  
H -3.809722 1.914110 -0.160140  
H -1.287514 5.740376 -0.873885  
H -0.640499 6.013575 0.745409  
H 0.465914 5.785216 -0.610592  
H 2.844828 2.009164 0.860277  
H 2.071900 1.026898 2.096658  
H 2.237218 0.411355 0.440469  
H 2.694568 -4.090929 -0.388690  
H -1.580833 -0.238086 -1.742169  
H -0.175503 0.793462 -2.026964  
H -0.713171 -0.346659 -3.266461  
H 2.746621 -3.442760 -4.051095  
H 3.591216 -4.254774 -2.719919  
H 2.040083 -4.871704 -3.291318  
H 2.168706 -3.743767 1.780729

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3PHBH

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C -5.648225 -1.665501 -0.794323  
C -5.534758 -1.898058 -2.162651  
C -1.288582 -2.165661 1.196775  
C -2.237462 0.845849 1.293576  
C -2.034719 0.957109 2.685815  
C -2.356223 2.161921 3.307941  
C -2.854046 3.256444 2.606392  
C -3.043857 3.120700 1.235382  
C -2.750041 1.939290 0.556318  
C -1.474554 -0.139856 3.555570  
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C -3.048608 1.907607 -0.924367  
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C -3.153373 -1.376654 -2.032352  
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C -1.839484 -1.228634 -2.762781  
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H -6.617414 -1.775169 -0.314043  
H -0.497805 -1.900089 1.896051  
H -2.129864 -2.579036 1.759618  
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H -2.037260 -1.073230 3.468023  
H -0.428712 -0.340082 3.312959  
H -1.516598 0.163675 4.602483  
H -3.432188 4.392299 4.345698  
H -2.256198 5.195307 3.301981  
H -3.947291 5.104229 2.804979  
H -3.049248 2.926552 -1.314712  
H -2.309919 1.350632 -1.499428  
H -4.031672 1.464381 -1.115489  
H -4.180776 -1.921748 -3.826720  
H -3.974613 -1.378085 2.088744  
H -4.867056 0.067227 1.634791  
H -5.706164 -1.484660 1.781980  
H -7.661651 -2.043062 -2.493865  
H -6.700912 -1.883118 -3.974979  
H -6.730387 -3.415487 -3.102046

H	-1.974684	-1.448523	-3.822624	C	4.254194	-2.635625	1.599007
H	-1.419027	-0.220080	-2.683116	C	8.292335	-0.589477	-0.553858
H	-1.071725	-1.906500	-2.378629	C	3.840625	0.318453	-2.619161
H	-1.559465	-3.448554	-0.552995	C	1.542694	-0.651166	1.184310
H	0.079443	-2.764040	-0.393185	C	1.866168	0.680895	1.510757
H	-0.449290	-4.074625	0.672338	C	1.255156	1.259596	2.622610
C	2.376739	-1.303086	-2.843238	C	0.334933	0.566533	3.402255
C	2.003923	-2.783546	-2.960418	C	0.062189	-0.763256	3.077850
B	1.894745	-0.627293	-1.448102	C	0.647183	-1.399873	1.988508
C	2.178666	0.981446	-1.406175	C	2.848105	1.513499	0.724570
C	2.533905	-1.278898	-0.077962	C	-0.382854	1.230636	4.543564
C	1.185290	1.946397	-1.386303	C	0.293265	-2.848625	1.740315
C	1.423377	3.314402	-1.350197	C	-1.354400	1.220875	-1.109113
C	2.733482	3.766871	-1.332462	F	-2.600907	0.981683	0.917214
C	3.653437	-2.101001	0.013541	C	-1.632526	1.583417	0.209648
C	4.097029	-2.672491	1.204400	C	-0.936300	2.567301	0.905677
C	3.419199	-2.416580	2.386468	F	-1.236969	2.848897	2.179903
C	2.315867	-1.576859	2.354082	F	0.883374	4.071953	1.011593
C	1.928649	-1.020419	1.145585	C	0.136847	3.206226	0.311734
F	1.627683	-1.325701	3.480787	F	1.579146	3.393760	-1.547848
C	3.772040	2.844045	-1.346934	C	0.483872	2.862026	-0.984297
C	3.475237	1.487497	-1.381068	F	0.146121	1.627929	-2.907523
F	-0.124144	1.584981	-1.396377	C	-0.272941	1.911310	-1.654412
F	0.410753	4.188984	-1.330177	C	-3.496071	-0.445987	-1.250022
F	2.994364	5.074803	-1.298752	F	-4.572686	1.636391	-1.557005
F	4.368313	-2.410719	-1.074202	C	-4.615339	0.373706	-1.108116
F	5.166251	-3.469235	1.221336	F	-6.832928	0.818562	-0.393041
F	3.816524	-2.965948	3.534149	C	-5.796148	-0.018308	-0.494542
F	5.035106	3.274465	-1.323629	F	-7.020123	-1.700964	0.628386
F	4.515441	0.640084	-1.378415	C	-5.895877	-1.299806	0.030406
F	0.857626	-0.179914	1.205326	F	-4.881439	-3.386029	0.445940
H	3.454919	-1.185918	-2.999879	C	-4.809613	-2.151923	-0.067625
H	1.892622	-0.755617	-3.665102	F	-2.636698	-2.609382	-0.713337
H	2.296152	-3.222244	-3.920991	C	-3.648466	-1.708632	-0.693471
H	0.919641	-2.924767	-2.857289	H	2.107021	-2.781382	-0.100263
H	2.483601	-3.377733	-2.175864	H	-2.594230	0.765144	-2.993616
H	0.684739	-0.795058	-1.348426	H	1.661790	-1.592773	-2.618151
				H	1.174078	-0.025810	-1.967587
75				H	-0.192711	-2.724689	-1.523620
<b>4H<sub>2</sub></b>				H	-0.568462	-1.315793	-0.532031
P	2.231219	-1.404359	-0.307531	H	-0.612461	-0.707571	-3.444626
B	-2.180500	0.131044	-2.045738	H	-1.812303	-1.885812	-2.970543
C	1.193480	-1.095975	-1.762210	H	6.816939	-2.023123	1.231986
C	-0.227905	-1.627932	-1.526215	H	6.441408	0.416143	-2.256716
C	-1.195454	-1.066549	-2.587697	H	5.044368	-2.931380	2.289918
C	4.016674	-1.147016	-0.481776	H	3.820450	-3.555167	1.189268
C	4.821229	-1.759250	0.506490	H	3.477882	-2.127188	2.179363
C	6.198983	-1.557925	0.468581	H	8.738184	-0.748873	0.429830
C	6.799994	-0.777678	-0.515073	H	8.554080	0.414441	-0.895304
C	5.984271	-0.194686	-1.482746	H	8.748374	-1.303374	-1.247196
C	4.599726	-0.358073	-1.499303	H	3.370059	-0.408211	-3.285412



H	4.534118	0.906285	-3.221636
H	3.060490	1.004464	-2.277086
H	1.469444	2.300943	2.849392
H	-0.644040	-1.320770	3.687374
H	2.715525	2.570742	0.959218
H	2.705253	1.413515	-0.353674
H	3.881634	1.232624	0.952488
H	-0.365365	0.602651	5.438083
H	-1.427495	1.400334	4.268557
H	0.061125	2.198157	4.783020
H	-0.343439	-3.211506	2.547869
H	1.182033	-3.489315	1.716975
H	-0.259723	-2.988012	0.807342

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[4H]<sup>+</sup>

P	-2.915781	-0.521822	-0.425326
B	2.420460	-0.596966	-0.094587
C	-1.446759	-1.602374	-0.270699
C	-0.195361	-0.717147	-0.357679
C	1.094377	-1.464508	-0.017674
C	-4.525095	-1.287960	-0.727831
C	-5.516210	-0.424290	-1.254473
C	-6.779118	-0.945382	-1.518340
C	-7.090445	-2.283652	-1.284806
C	-6.094709	-3.109824	-0.765852
C	-4.811423	-2.648869	-0.480488
C	-5.261564	1.032119	-1.560738
C	-8.454843	-2.826387	-1.606762
C	-3.818042	-3.643643	0.069160
C	-2.861816	0.724661	0.882330
C	-3.269898	0.380157	2.187811
C	-3.165802	1.340769	3.191071
C	-2.660292	2.615013	2.944197
C	-2.249477	2.924451	1.646847
C	-2.341646	2.012361	0.599617
C	-3.779168	-0.992256	2.552307
C	-2.569855	3.641988	4.038307
C	-1.881153	2.461903	-0.769443
C	3.823714	-1.232983	0.129054
F	5.003486	0.811964	-0.182769
C	5.018780	-0.495278	0.062509
C	6.270610	-1.060109	0.251998
F	7.366015	-0.318088	0.178868
F	7.554222	-2.970159	0.708450
C	6.370937	-2.419177	0.525234
F	5.314195	-4.492967	0.872747
C	5.221701	-3.196933	0.607813
F	2.926391	-3.402084	0.515239
C	3.987710	-2.598830	0.413779
C	2.268605	0.935566	-0.464738

F	3.476726	0.636742	-2.458118
C	2.767666	1.439880	-1.661374
F	3.021095	3.180990	-3.237194
C	2.546512	2.744905	-2.079017
F	1.558509	4.839097	-1.651222
C	1.803772	3.595610	-1.267409
F	0.575995	3.946953	0.711954
C	1.308081	3.136651	-0.053802
F	1.033344	1.406865	1.492816
C	1.544704	1.822764	0.322475
H	-2.648524	0.187445	-1.599443
H	-1.473514	-2.352993	-1.065833
H	-1.486823	-2.121219	0.690553
H	-0.123233	-0.295842	-1.368259
H	-0.314261	0.119412	0.335199
H	1.026247	-1.907682	0.985875
H	1.223043	-2.329153	-0.682404
H	-7.543019	-0.283857	-1.917585
H	-6.323992	-4.154266	-0.573345
H	-6.192546	1.523288	-1.844526
H	-4.568555	1.147733	-2.402724
H	-4.852796	1.574174	-0.702047
H	-9.224768	-2.063145	-1.478596
H	-8.701535	-3.680825	-0.973973
H	-8.490376	-3.161989	-2.648098
H	-3.035428	-3.880735	-0.656624
H	-4.326329	-4.578115	0.308589
H	-3.340397	-3.293192	0.986559
H	-3.480911	1.079701	4.197595
H	-1.836601	3.907955	1.443658
H	-4.137365	-1.001300	3.582291
H	-2.978859	-1.738626	2.489965
H	-4.603879	-1.316101	1.911562
H	-1.651905	4.227247	3.950783
H	-2.593963	3.176573	5.024973
H	-3.412107	4.338095	3.974596
H	-1.493565	3.479870	-0.708413
H	-2.699618	2.465912	-1.497253
H	-1.076753	1.834820	-1.167500

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[4H]<sup>-</sup>

P	2.912571	-0.754937	-1.177308
B	-2.533884	-0.334328	-0.879401
C	1.297766	-1.124227	-0.307422
C	0.026208	-0.759278	-1.075789
C	-1.257327	-1.232404	-0.379248
C	3.652021	0.902476	-0.757658
C	5.027185	1.032017	-1.068598
C	5.699146	2.224043	-0.785872
C	5.055869	3.318457	-0.224314

C	3.688212	3.205344	0.008555	H	1.085236	1.275446	0.552737
C	2.972179	2.037808	-0.258062	H	0.948545	2.099529	-0.998251
C	5.841041	-0.068777	-1.712382	H	1.215055	3.032352	0.465762
C	5.797553	4.586744	0.110279	H	5.543545	-2.324053	2.843984
C	1.480149	2.101394	-0.041093	H	5.458800	-4.938043	-0.535423
C	3.979385	-1.888449	-0.147399	H	4.126979	-0.546100	3.005975
C	4.402735	-1.619726	1.170533	H	3.018801	-0.037555	1.723597
C	5.218773	-2.545594	1.828784	H	4.698502	0.467385	1.669013
C	5.618313	-3.738434	1.237054	H	7.165430	-5.242451	1.308591
C	5.170318	-4.005415	-0.053989	H	5.853314	-5.500149	2.459426
C	4.360390	-3.108384	-0.749250	H	7.054529	-4.243399	2.767490
C	4.038124	-0.365761	1.931639	H	4.300918	-4.470005	-2.413071
C	6.471885	-4.732224	1.982620	H	4.260052	-2.758550	-2.886169
C	3.914285	-3.483874	-2.144015	H	2.823597	-3.511768	-2.224921
C	-2.397083	1.136133	-0.147756				
F	-3.281716	0.337883	1.903167		73		
C	-2.749492	1.341635	1.184544		<b>4PB</b>		
C	-2.565188	2.539708	1.864010	P	0.378938	1.198788	-0.763567
F	-2.929604	2.674170	3.146549	B	-0.556237	-0.671818	-0.886807
F	-1.767962	4.767889	1.842934	C	-0.301288	1.784397	-2.383070
C	-1.977767	3.609247	1.204713	C	-0.817608	0.538787	-3.151166
F	-0.977921	4.466682	-0.748008	C	-0.293946	-0.751388	-2.499167
C	-1.593147	3.455876	-0.117132	C	0.196656	2.622268	0.402444
F	-1.367132	2.172611	-2.025866	C	0.840371	3.847763	0.095572
C	-1.813366	2.241094	-0.758334	C	0.713933	4.920135	0.973645
C	-4.009430	-0.977228	-0.554342	C	-0.032193	4.836987	2.148642
F	-5.011824	0.381078	-2.220383	C	-0.648803	3.628390	2.435195
C	-5.126656	-0.568934	-1.278889	C	-0.550112	2.518025	1.591161
F	-7.439558	-0.655284	-1.831054	C	1.661210	4.078562	-1.151233
C	-6.404144	-1.085800	-1.095066	C	-0.170194	6.027784	3.059366
F	-7.830571	-2.576761	0.062582	C	-1.251685	1.270613	2.063830
C	-6.609208	-2.061635	-0.132402	C	2.189640	0.815343	-0.814882
F	-5.725474	-3.432149	1.567419	C	2.983567	0.747261	-1.985782
C	-5.534359	-2.494837	0.627445	C	4.266010	0.200472	-1.901426
F	-3.298365	-2.408041	1.204772	C	4.800470	-0.288021	-0.716119
C	-4.275633	-1.945099	0.408823	C	4.035480	-0.152156	0.435464
H	-2.477636	-0.169103	-2.080481	C	2.752965	0.392310	0.415036
H	1.350333	-2.218497	-0.220812	C	2.577551	1.234143	-3.360092
H	1.262885	-0.756977	0.723321	C	6.141025	-0.968832	-0.673202
H	0.079520	-1.191045	-2.083078	C	2.040351	0.482441	1.743258
H	-0.019485	0.320973	-1.233282	C	-2.174947	-0.638416	-0.678682
H	-1.130483	-1.152443	0.710872	C	-3.003121	0.464456	-0.527596
H	-1.399872	-2.303927	-0.577207	F	-2.480224	1.705582	-0.434539
H	6.759236	2.292465	-1.023690	C	-4.389787	0.393927	-0.445987
H	3.147179	4.061682	0.406133	F	-5.115798	1.500957	-0.287730
H	6.723857	0.359190	-2.194161	C	-5.012720	-0.838988	-0.542403
H	5.263166	-0.603683	-2.472643	F	-6.337790	-0.932877	-0.474729
H	6.177965	-0.811025	-0.982206	C	-4.234820	-1.976874	-0.712652
H	6.787095	4.600035	-0.353543	F	-4.818652	-3.169725	-0.812302
H	5.934560	4.689231	1.192071	C	-2.855620	-1.852393	-0.783512
H	5.247932	5.468130	-0.232330	C	0.212668	-1.744899	0.067831

C	1.469860	-2.275899	-0.231604
F	2.090962	-2.000680	-1.385664
C	2.199197	-3.087014	0.630898
F	3.425666	-3.490238	0.294017
C	1.654045	-3.463319	1.846214
F	2.333280	-4.241619	2.683653
C	0.384135	-3.012795	2.175301
F	-0.167830	-3.371925	3.333914
C	-0.297770	-2.183101	1.295280
F	-1.509856	-1.788346	1.720415
F	-2.160887	-2.986383	-0.953980
H	-1.112830	2.461291	-2.108509
H	0.421256	2.358432	-2.952659
H	-0.529329	0.607501	-4.205274
H	-1.911437	0.542798	-3.128181
H	0.761504	-0.891813	-2.743447
H	-0.820698	-1.627011	-2.896203
H	1.216356	5.853656	0.730767
H	-1.228681	3.528390	3.350333
H	1.021597	4.187509	-2.032401
H	2.367541	3.266674	-1.336051
H	2.234675	5.001830	-1.051941
H	-0.532132	5.732488	4.046240
H	-0.880503	6.749805	2.644201
H	0.786166	6.542588	3.182383
H	-0.870987	0.975341	3.047078
H	-1.137263	0.424095	1.395130
H	-2.324165	1.459977	2.169528
H	4.859125	0.134957	-2.809879
H	4.435347	-0.503672	1.384044
H	3.376280	1.014048	-4.069919
H	2.423070	2.317396	-3.377487
H	1.672094	0.754476	-3.734136
H	6.004383	-2.045799	-0.532788
H	6.746190	-0.601731	0.159889
H	6.697903	-0.815138	-1.599681
H	2.540278	-0.157181	2.474020
H	1.001509	0.155851	1.685661
H	2.042926	1.507957	2.125975

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P	2.907227	0.229575	-0.486444
B	-2.530254	-0.428933	-0.239406
C	1.439639	-0.902728	-0.247120
C	0.110002	-0.172644	-0.465499
C	-1.093266	-1.062062	-0.144099
C	3.551300	0.888073	1.126707
C	4.772942	1.592605	1.000070
C	5.373353	2.157563	2.127355
C	4.797016	2.080533	3.388099

C	3.572564	1.426457	3.492585
C	2.939283	0.833750	2.400033
C	5.484395	1.768025	-0.321769
C	5.450611	2.695212	4.598094
C	1.627887	0.141052	2.692841
C	4.186511	-1.036328	-0.955039
C	4.812703	-1.924771	-0.057061
C	5.778109	-2.813713	-0.537460
C	6.141751	-2.861701	-1.879126
C	5.495921	-1.997698	-2.759889
C	4.531362	-1.089956	-2.324332
C	4.499045	-1.976829	1.418993
C	7.209078	-3.807562	-2.364721
C	3.882912	-0.191455	-3.353129
C	-2.659575	1.084632	-0.676508
F	-3.596162	1.690006	1.395209
C	-3.144133	2.057205	0.189816
C	-3.184339	3.402715	-0.140563
F	-3.646007	4.306578	0.718282
F	-2.778307	5.085160	-1.733698
C	-2.739904	3.802653	-1.395849
F	-1.852071	3.241765	-3.503355
C	-2.262444	2.860690	-2.297657
F	-1.777077	0.634511	-2.814880
C	-2.227403	1.525261	-1.920295
C	-3.816550	-1.243485	0.152694
F	-5.333948	0.502972	-0.422870
C	-5.116834	-0.723993	0.046164
F	-7.460136	-0.894243	0.275871
C	-6.253459	-1.435983	0.400508
F	-7.198922	-3.420510	1.229826
C	-6.124149	-2.729467	0.887362
F	-4.734717	-4.534864	1.473960
C	-4.863191	-3.295797	1.011014
F	-2.575908	-3.174056	0.786563
C	-3.748621	-2.556426	0.643725
H	1.566294	-1.650192	-1.039761
H	1.446064	-1.457702	0.692677
H	0.070518	0.165553	-1.505429
H	0.065291	0.741197	0.140819
H	-0.996980	-1.439374	0.887060
H	-1.061067	-1.982667	-0.745355
H	6.317523	2.683686	2.005029
H	3.087615	1.370346	4.465316
H	6.253615	2.537989	-0.234064
H	4.789097	2.069212	-1.112164
H	5.966577	0.842090	-0.650095
H	6.394042	3.178322	4.335143
H	5.659233	1.937560	5.359533
H	4.801235	3.447216	5.056288
H	1.743901	-0.947411	2.734747

H 0.856709 0.367200 1.956337  
H 1.253980 0.459874 3.667950  
H 6.253172 -3.496730 0.163865  
H 5.749034 -2.029922 -3.817455  
H 4.819608 -2.934720 1.834986  
H 3.430296 -1.863725 1.611679  
H 5.008896 -1.178346 1.967151  
H 6.987369 -4.171354 -3.371069  
H 7.305964 -4.670034 -1.701245  
H 8.182636 -3.307576 -2.403404  
H 4.279988 -0.406950 -4.347470  
H 4.059003 0.864877 -3.131285  
H 2.797457 -0.326209 -3.385921

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**4B**

C -0.626626 -2.480994 -2.775451  
C -0.565206 -2.848363 -1.437681  
C -1.121174 -2.008385 -0.482302  
C -1.731602 -0.804201 -0.805532  
C -1.758816 -0.467269 -2.153343  
C -1.228342 -1.282116 -3.141253  
B -2.434220 0.092940 0.291007  
C -1.938467 1.565876 0.531279  
C -0.831718 2.122540 -0.129781  
C -0.396988 3.424056 0.074132  
C -1.073906 4.236468 0.973442  
C -2.173305 3.738246 1.658329  
C -2.578825 2.431226 1.431656  
F -2.316038 0.691809 -2.524221  
F -1.035410 -2.380684 0.802440  
F -0.105945 -3.271652 -3.705465  
F -3.638352 2.028102 2.132822  
F -0.116564 1.410834 -0.998744  
F -0.671065 5.479678 1.178905  
C -3.660818 -0.503417 1.072310  
C -4.129050 -1.917703 0.718741  
C -5.408631 -2.298509 1.458827  
F -1.281669 -0.930551 -4.422515  
F 0.022089 -3.988739 -1.087118  
F 0.659464 3.896773 -0.578398  
F -2.822612 4.511037 2.522847  
H -3.470164 -0.423140 2.153072  
H -4.492249 0.202920 0.918731  
H -4.295131 -1.989812 -0.362997  
H -3.341515 -2.638411 0.958347  
H -5.733617 -3.310526 1.204710  
H -5.259043 -2.255515 2.542239  
H -6.223169 -1.610743 1.210516

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**[4BH]<sup>-</sup>**

C -0.955087 -1.956518 -3.134267  
C -0.447601 -2.494367 -1.962446  
C -0.817153 -1.945142 -0.737873  
C -1.683293 -0.864365 -0.611758  
C -2.166759 -0.366335 -1.818655  
C -1.825865 -0.879141 -3.063920  
B -2.147761 -0.219265 0.829509  
C -1.767592 1.381965 0.780636  
C -0.427507 1.763808 0.817561  
C 0.009306 3.082181 0.793628  
C -0.925591 4.103603 0.716920  
C -2.271305 3.780951 0.663304  
C -2.659933 2.444343 0.686978  
F -3.017362 0.676049 -1.820909  
F -0.286412 -2.532324 0.344869  
F -0.611212 -2.473065 -4.322258  
F -3.984604 2.233535 0.616135  
F 0.534021 0.828125 0.876836  
F -0.531573 5.384564 0.693429  
C -3.724170 -0.548729 1.100225  
C -3.966347 -2.042353 1.324212  
C -5.431347 -2.395551 1.581284  
F -2.322442 -0.355122 -4.194255  
F 0.391677 -3.539044 -2.027544  
F 1.315815 3.383731 0.839253  
F -3.182012 4.762760 0.581171  
H -1.465945 -0.712169 1.705924  
H -4.077230 -0.002078 1.988136  
H -4.362833 -0.207635 0.272807  
H -3.609302 -2.605725 0.450321  
H -3.351842 -2.385164 2.166846  
H -5.582973 -3.469623 1.739472  
H -5.805657 -1.869652 2.466937  
H -6.056353 -2.089116 0.735136

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**4P**

C 4.048110 -0.979870 -0.064889  
C 3.053307 -1.584794 0.692796  
C 1.839066 -0.952324 0.968352  
C 1.582527 0.337774 0.446919  
C 2.611603 0.986073 -0.270471  
C 3.809463 0.315266 -0.516142  
P -0.067329 1.056160 0.911843  
C -1.248238 -0.185925 0.184883  
C -2.366961 -0.537725 0.976330  
C -3.292880 -1.460149 0.494339  
C -3.151538 -2.058904 -0.756408  
C -2.051946 -1.701377 -1.526229  
C -1.097085 -0.777944 -1.085491

C	2.507069	2.400903	-0.788756
C	0.853003	-1.703988	1.833087
C	5.336653	-1.691531	-0.384322
C	0.066871	-0.511156	-2.012704
C	-2.601262	0.051272	2.349140
C	-4.166563	-3.057486	-1.248771
C	-0.518055	2.503165	-0.188799
C	-1.941231	2.964753	0.147487
C	-2.358606	4.163150	-0.702606
H	3.223691	-2.580534	1.097037
H	4.586522	0.829643	-1.077798
H	-4.148532	-1.720760	1.114012
H	-1.925133	-2.152535	-2.508186
H	2.288924	3.108779	0.015620
H	3.453600	2.701894	-1.242017
H	1.728982	2.510302	-1.548564
H	1.370807	-2.485900	2.392940
H	0.362556	-1.041199	2.553351
H	0.064821	-2.176066	1.238643
H	5.550353	-2.471463	0.350322
H	5.286218	-2.168829	-1.368637
H	6.179603	-0.995962	-0.400312
H	-0.209962	-0.765566	-3.038536
H	0.393750	0.529233	-1.995308
H	0.936663	-1.116018	-1.735344
H	-1.760783	-0.144720	3.020720
H	-2.721762	1.137583	2.309458
H	-3.504064	-0.373898	2.793132
H	-5.165956	-2.613862	-1.288200
H	-3.915874	-3.417523	-2.248804
H	-4.220776	-3.922491	-0.580857
H	0.168560	3.329765	0.008207
H	-0.461615	2.261817	-1.255210
H	-2.644595	2.139195	-0.011134
H	-1.994468	3.228896	1.210575
H	-3.371304	4.491936	-0.455295
H	-1.682319	5.009359	-0.546618
H	-2.337797	3.911446	-1.767315

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**[4PH]<sup>+</sup>**

C	-3.622904	-1.901754	0.185827
C	-2.625464	-2.031120	1.150179
C	-1.532124	-1.171130	1.200542
C	-1.436231	-0.141967	0.232054
C	-2.430129	0.012334	-0.761180
C	-3.501872	-0.877702	-0.753056
P	0.040282	0.885351	0.371393
C	1.601108	0.062990	-0.008693
C	1.720227	-0.820110	-1.100867
C	2.954013	-1.427133	-1.324499

C	4.058095	-1.187750	-0.508455
C	3.913273	-0.298428	0.557597
C	2.706406	0.336275	0.832319
C	-2.418618	1.069101	-1.841273
C	-0.511085	-1.374077	2.296567
C	-4.809932	-2.823952	0.171892
C	2.639610	1.271568	2.018224
C	0.581343	-1.131780	-2.038810
C	5.370546	-1.877805	-0.756969
C	-0.041403	2.553480	-0.355733
C	-1.059968	3.446542	0.367955
C	-1.249350	4.771387	-0.366290
H	-2.699006	-2.825484	1.887791
H	-4.270115	-0.769500	-1.513710
H	0.116224	1.163664	1.738653
H	3.055378	-2.104189	-2.168208
H	4.769559	-0.090624	1.193632
H	-3.267206	0.917652	-2.508914
H	-2.508169	2.079918	-1.433991
H	-1.518399	1.030745	-2.460462
H	-0.718489	-2.301256	2.831116
H	0.512377	-1.439810	1.913597
H	-0.548926	-0.563198	3.033471
H	-5.618477	-2.405573	0.779756
H	-5.193822	-2.960832	-0.840795
H	-4.556948	-3.802252	0.584624
H	3.639816	1.434002	2.420459
H	2.232619	2.255729	1.763661
H	2.029161	0.854289	2.827658
H	0.087780	-0.222226	-2.393206
H	0.953864	-1.658236	-2.918249
H	-0.177527	-1.760325	-1.563445
H	5.448226	-2.225600	-1.788342
H	6.211190	-1.212375	-0.549456
H	5.469303	-2.748720	-0.101317
H	-0.238079	2.478672	-1.427105
H	0.973901	2.954726	-0.252803
H	-0.705705	3.628769	1.388707
H	-2.021335	2.928256	0.463987
H	-1.946199	5.415544	0.172583
H	-1.648130	4.608544	-1.372039
H	-0.300353	5.305599	-0.462551

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**4PHBH**

C	0.456892	-4.184194	0.021302
C	-0.146256	-3.479475	-1.017847
C	-0.867502	-2.308484	-0.801852
C	-1.012203	-1.842722	0.527978
C	-0.434789	-2.550543	1.601783
C	0.288345	-3.708871	1.317520

P	-1.766786	-0.204512	0.715464	C	2.777966	3.915411	-0.734634
C	-3.316142	-0.011530	-0.205240	B	1.830302	0.555825	1.123780
C	-4.308333	-1.010530	-0.178663	C	2.042102	-0.445106	-0.184007
C	-5.490945	-0.790281	-0.883223	C	1.450704	-0.188683	-1.419789
C	-5.711896	0.380491	-1.605229	C	1.640302	-0.938189	-2.572353
C	-4.712043	1.351330	-1.613985	C	2.459801	-2.053705	-2.523960
C	-3.510715	1.187230	-0.926295	C	3.071567	-2.370595	-1.322808
C	-0.514806	-2.126479	3.045781	C	2.845794	-1.585628	-0.195832
C	-1.434213	-1.608294	-2.016754	F	3.880089	1.889603	-0.452257
C	1.315624	-5.384986	-0.263618	F	-0.395697	2.568238	1.468047
C	-2.475531	2.287164	-1.011224	F	1.626199	5.956372	-1.046619
C	-4.131529	-2.333979	0.527785	F	3.471223	-2.009265	0.912927
C	-7.008584	0.606594	-2.335665	F	0.579502	0.846209	-1.562864
C	-2.124421	0.492198	2.370837	F	2.628703	-2.822699	-3.600932
C	-3.380414	-0.007366	3.088343	C	3.008535	0.437114	2.250167
C	-3.601009	0.787828	4.374350	C	2.745076	-0.600262	3.346239
H	-0.018675	-3.829159	-2.039910	C	3.971503	-0.894548	4.206503
H	0.752077	-4.243173	2.142226	F	3.804067	4.372946	-1.454037
H	-0.868733	0.682557	0.124329	F	-0.480309	4.993635	0.416138
H	-6.258745	-1.559939	-0.869307	F	0.994447	-0.630959	-3.703964
H	-4.868828	2.268287	-2.176276	F	3.852192	-3.456420	-1.247878
H	-0.097967	-2.908489	3.682220	H	0.745408	0.281388	1.637316
H	0.076352	-1.222919	3.214290	H	3.977154	0.225644	1.778161
H	-1.541440	-1.950620	3.372812	H	3.137292	1.412011	2.742272
H	-0.978532	-2.019763	-2.918640	H	1.929126	-0.234868	3.987418
H	-2.518607	-1.734487	-2.092769	H	2.387320	-1.537180	2.899987
H	-1.221530	-0.534789	-2.023261	H	3.754701	-1.597754	5.017318
H	2.324042	-5.057453	-0.535610	H	4.767683	-1.324765	3.590365
H	1.395959	-6.033954	0.610716	H	4.361981	0.026007	4.653055
H	0.917962	-5.967852	-1.097714				
H	-2.880240	3.134230	-1.566625	78			
H	-2.161366	2.660258	-0.031774	5H <sub>2</sub>			
H	-1.571348	1.952941	-1.532947	P	3.685517	-0.816736	-0.637007
H	-3.638966	-2.237609	1.498299	B	-2.903207	-0.036710	-1.299200
H	-5.103390	-2.802880	0.692313	C	2.204120	-0.103910	-1.414144
H	-3.520051	-3.018600	-0.069923	C	0.963967	-0.914841	-1.006933
H	-7.489879	-0.339480	-2.591659	C	-0.322619	-0.222919	-1.460957
H	-7.704578	1.177013	-1.712246	C	-1.582871	-0.971813	-1.039380
H	-6.849123	1.173948	-3.255276	C	5.321367	-0.306884	-1.237133
H	-2.254734	1.553779	2.131657	C	6.393373	-1.174812	-0.921241
H	-1.220706	0.429700	2.979248	C	7.672970	-0.843518	-1.357901
H	-3.304870	-1.070827	3.332789	C	7.924456	0.308942	-2.098508
H	-4.245906	0.103498	2.425893	C	6.850959	1.144612	-2.397968
H	-4.504754	0.453202	4.888103	C	5.547329	0.867082	-1.989220
H	-3.708078	1.854979	4.160566	C	6.211867	-2.458487	-0.147570
H	-2.756553	0.665652	5.058449	C	9.311381	0.629541	-2.584477
C	1.670018	4.728176	-0.528881	C	4.470036	1.846617	-2.388291
C	0.610169	4.242136	0.219453	C	3.515010	-0.807515	1.163880
C	0.690032	2.960547	0.749015	C	3.737211	0.387718	1.879078
C	1.753573	2.094944	0.555303	C	3.571613	0.375995	3.261198
C	2.794510	2.635133	-0.196131	C	3.180987	-0.771499	3.948074



F	-7.654414	-3.359628	-0.988900	C	5.476873	1.355484	-1.911103
C	-6.592558	-2.587657	-0.858486	C	6.517595	-2.027150	-0.422476
F	-5.175537	-4.384070	-1.410805	C	9.224062	2.023529	-1.559317
C	-5.322660	-3.108810	-1.073374	C	4.317345	2.142971	-2.473046
F	-3.034955	-2.852800	-1.164947	C	3.721268	-1.297204	0.605812
C	-4.220286	-2.281370	-0.934871	C	4.033026	-0.363770	1.616224
H	3.547874	-0.976661	-1.811015	C	3.963668	-0.758136	2.955890
H	2.060924	1.014466	0.581641	C	3.587588	-2.041731	3.334047
H	2.104340	1.383139	-1.147568	C	3.275333	-2.951433	2.327357
H	0.978360	-0.786776	-1.663547	C	3.333311	-2.604077	0.978377
H	1.003423	-1.236273	0.045424	C	4.474273	1.056893	1.347489
H	-0.443112	1.199666	-1.112480	C	3.478831	-2.426843	4.786708
H	-0.446535	0.727299	0.581233	C	2.968383	-3.657439	-0.042233
H	-1.488665	-1.496503	-0.087199	C	-2.963122	1.305092	0.106946
H	-1.558560	-0.974523	-1.731668	F	-3.383376	-0.400040	1.697230
H	8.327164	0.178966	-2.030924	C	-3.190677	0.902068	1.419918
H	6.598310	3.738789	-0.416785	C	-3.236006	1.771077	2.502842
H	7.233143	-1.787388	-2.116723	F	-3.461539	1.324608	3.746841
H	5.574969	-1.592495	-2.665522	F	-3.075946	3.987322	3.314760
H	5.910784	-2.108989	-0.999076	C	-3.040971	3.127414	2.287801
H	9.755033	2.126240	-1.443732	F	-2.610917	4.892625	0.790270
H	9.022291	3.613586	-0.814290	C	-2.805351	3.582147	1.000203
H	8.881688	3.211526	-2.527403	F	-2.526417	3.196617	-1.263950
H	3.722987	2.370947	1.008116	C	-2.770722	2.673111	-0.053377
H	3.398982	3.081022	-0.581856	C	-4.323351	-0.609778	-1.112827
H	4.574643	3.817099	0.494646	F	-5.453295	1.351718	-1.810043
H	4.598361	-2.146138	3.896573	C	-5.495508	0.052200	-1.474240
H	3.459417	-4.999736	0.922909	F	-7.838700	0.145580	-1.877865
H	4.788829	0.071212	3.470180	C	-6.748596	-0.545706	-1.513284
H	3.548562	0.678506	2.386964	F	-8.068356	-2.484668	-1.195639
H	5.234822	0.572816	1.839671	C	-6.871572	-1.882578	-1.165134
H	4.013339	-5.781128	3.096416	F	-5.852089	-3.877327	-0.440189
H	3.445937	-4.661509	4.344022	C	-5.740717	-2.585731	-0.784705
H	5.169752	-4.789676	4.000319	F	-3.472327	-2.702606	-0.363526
H	2.918152	-4.451098	-1.171386	C	-4.506796	-1.941552	-0.758109
H	3.901463	-3.183662	-1.890120	H	-2.864064	0.830368	-2.174378
H	2.209575	-2.869974	-1.467752	H	2.266786	0.979481	-0.604619
				H	2.184149	0.573893	-2.325716
				H	0.975161	-1.530335	-1.797655
				H	1.046969	-1.157366	-0.075608
				H	-0.324676	0.584604	-2.187561
				H	-0.252797	0.937753	-0.471680
				H	-1.506820	-1.198320	0.001912
				H	-1.584222	-1.522486	-1.718563
				H	8.645936	-0.502081	-0.697334
				H	6.810046	2.956342	-2.397956
				H	7.521311	-2.453097	-0.494802
				H	5.834292	-2.663515	-0.994006
				H	6.200412	-2.074615	0.623697
				H	10.046045	1.303491	-1.540450
				H	9.347643	2.689569	-0.698545

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[5H]<sup>-</sup>

P	3.773901	-0.927182	-1.218576
B	-2.901360	0.217455	-1.126063
C	2.251987	0.151323	-1.320461
C	1.001300	-0.703734	-1.074213
C	-0.289084	0.110588	-1.196546
C	-1.562110	-0.707435	-0.979812
C	5.344546	0.064325	-1.352449
C	6.521101	-0.609507	-0.946824
C	7.757921	0.035058	-1.025540
C	7.888469	1.327263	-1.517448
C	6.733969	1.957099	-1.973382



H 9.324718 2.633569 -2.461171  
H 3.569149 2.382010 -1.713835  
H 3.809598 1.595668 -3.271652  
H 4.675282 3.084813 -2.894335  
H 4.204893 -0.028821 3.726941  
H 2.971587 -3.960500 2.598212  
H 4.287503 1.675608 2.228530  
H 3.951885 1.504559 0.501221  
H 5.544245 1.102975 1.117916  
H 3.766505 -3.470059 4.942332  
H 2.449030 -2.313538 5.141154  
H 4.115792 -1.797088 5.412801  
H 2.733809 -4.600792 0.456237  
H 3.781638 -3.831145 -0.752604  
H 2.095532 -3.357968 -0.629052

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**5PB**

P -0.437669 1.199087 0.749870  
B 0.587137 -0.638945 0.850278  
C 0.223980 2.105326 2.238307  
C 0.563881 1.362688 3.539945  
C 1.203788 -0.015615 3.376077  
C 0.392199 -0.929735 2.451475  
C -0.353448 2.579112 -0.500416  
C -1.103928 3.761356 -0.272790  
C -1.000444 4.819126 -1.176038  
C -0.183839 4.767843 -2.300918  
C 0.514615 3.590440 -2.528015  
C 0.440709 2.496086 -1.664026  
C -2.046597 4.003888 0.887896  
C -0.062192 5.945896 -3.230064  
C 1.193991 1.270596 -2.112519  
C -2.235072 0.724269 0.766853  
C -3.059797 0.652618 1.910394  
C -4.317985 0.053701 1.815906  
C -4.800294 -0.488448 0.633667  
C -4.014244 -0.337820 -0.502838  
C -2.757561 0.262641 -0.469758  
C -2.695567 1.166923 3.280926  
C -6.108401 -1.227866 0.571578  
C -2.042768 0.368534 -1.795575  
C 2.199275 -0.566114 0.579849  
C 3.006364 0.546632 0.391808  
F 2.465468 1.779754 0.290213  
C 4.391555 0.499775 0.273601  
F 5.091171 1.618355 0.081922  
C 5.039902 -0.719785 0.365362  
F 6.363935 -0.791704 0.261710  
C 4.285358 -1.868446 0.563543  
F 4.890586 -3.051282 0.652410

C 2.906530 -1.767330 0.669976  
C -0.165485 -1.724871 -0.118060  
C -1.390465 -2.309701 0.213032  
F -1.998972 -2.047101 1.376847  
C -2.101728 -3.162258 -0.624089  
F -3.304403 -3.610384 -0.258669  
C -1.565628 -3.529951 -1.845772  
F -2.226912 -4.347308 -2.660094  
C -0.322800 -3.029769 -2.204661  
F 0.223444 -3.382337 -3.368165  
C 0.340124 -2.160065 -1.348818  
F 1.528589 -1.728484 -1.804253  
F 2.242177 -2.917841 0.855621  
H 1.150270 2.494493 1.807261  
H -0.399550 2.974612 2.445385  
H 1.238303 2.018947 4.101830  
H -0.330388 1.260539 4.154952  
H 1.289063 -0.461240 4.373531  
H 2.229257 0.091893 3.004646  
H -0.659165 -0.904846 2.758601  
H 0.709770 -1.970752 2.591846  
H -1.587816 5.715667 -0.989083  
H 1.134705 3.500388 -3.417594  
H -1.550334 4.566600 1.685856  
H -2.462670 3.092483 1.311097  
H -2.886291 4.613242 0.546344  
H 0.210471 5.628118 -4.238799  
H 0.713064 6.634165 -2.878218  
H -0.999253 6.505040 -3.285153  
H 0.808054 0.932347 -3.080049  
H 1.124053 0.438581 -1.422093  
H 2.255153 1.500965 -2.243887  
H -4.928273 -0.005882 2.713898  
H -4.379487 -0.719691 -1.453708  
H -3.606986 1.385563 3.841108  
H -2.101865 2.079671 3.252441  
H -2.141006 0.413427 3.847081  
H -5.920914 -2.298013 0.438411  
H -6.715129 -0.891557 -0.273382  
H -6.687094 -1.095308 1.487899  
H -2.484838 -0.333395 -2.506568  
H -0.982815 0.131212 -1.726036  
H -2.128822 1.378072 -2.209957

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**5**

P 3.718932 -0.539672 -1.220936  
B -2.984495 0.005516 -0.477627  
C 2.180113 0.468341 -0.867158  
C 0.951848 -0.440305 -0.985311  
C -0.350641 0.316979 -0.725736

C	-1.579959	-0.584216	-0.864825	H	7.487483	-2.148860	-1.163878
C	5.261551	0.457670	-0.939223	H	5.807707	-2.173567	-1.717454
C	6.448496	-0.302278	-0.830424	H	6.164820	-2.287656	0.004461
C	7.670668	0.342771	-0.620761	H	9.893698	1.683399	-0.145104
C	7.773643	1.724515	-0.541044	H	9.051113	3.072728	0.555387
C	6.605770	2.464569	-0.713168	H	9.374030	3.022510	-1.176716
C	5.363964	1.867160	-0.920107	H	3.442903	2.706336	-0.334452
C	6.475808	-1.810332	-0.929868	H	3.688581	2.600521	-2.080243
C	9.095740	2.409714	-0.313733	H	4.532169	3.830559	-1.143228
C	4.189688	2.794067	-1.127805	H	4.103956	-1.689454	3.675709
C	3.666181	-1.610617	0.300901	H	2.958265	-4.859762	1.051478
C	3.955047	-1.153788	1.606865	H	4.200341	0.468470	2.988896
C	3.878971	-2.050700	2.673820	H	3.868178	1.009777	1.337883
C	3.526307	-3.386883	2.501188	H	5.457281	0.394775	1.743472
C	3.238582	-3.821223	1.212116	H	3.190810	-5.333909	3.369541
C	3.303227	-2.961525	0.113366	H	2.709139	-3.982988	4.405266
C	4.387584	0.257749	1.933396	H	4.417014	-4.367574	4.202273
C	3.456284	-4.321442	3.680976	H	2.760433	-4.598316	-1.170170
C	2.982158	-3.531853	-1.249875	H	3.814771	-3.403495	-1.946952
C	-3.061213	1.502456	0.026310	H	2.117316	-3.039041	-1.703255
F	-3.845056	0.837818	2.142561				
C	-3.443668	1.818058	1.324477	36			
C	-3.431133	3.114106	1.816148	<b>5B</b>			
F	-3.794179	3.376293	3.068122	C	4.422188	0.781540	2.117374
F	-3.026080	5.398955	1.425994	C	3.629104	-0.293327	2.494972
C	-3.037892	4.150242	0.976641	C	2.415592	-0.502980	1.856246
F	-2.300663	4.872690	-1.139914	C	1.929811	0.324652	0.831118
C	-2.663330	3.879858	-0.332913	C	2.776594	1.389970	0.487995
F	-2.326664	2.335586	-2.052829	C	3.994655	1.630649	1.106341
C	-2.677828	2.565592	-0.779986	C	-1.851489	-2.070510	2.283816
C	-4.287732	-0.873487	-0.518120	C	-2.214700	-3.074861	1.393616
F	-5.742189	0.905692	0.117096	C	-1.677227	-3.097215	0.113449
C	-5.562911	-0.372588	-0.210254	C	-0.786692	-2.099916	-0.260341
F	-7.894291	-0.618470	0.065015	C	-0.399086	-1.079495	0.597318
C	-6.712950	-1.147852	-0.234238	C	-0.948998	-1.101793	1.873117
F	-7.712418	-3.241613	-0.605763	B	0.548616	0.091525	0.116287
C	-6.624209	-2.489804	-0.578300	C	0.047665	1.031360	-1.039760
F	-5.299729	-4.321861	-1.228984	F	4.039036	-1.111138	3.458562
C	-5.389712	-3.038527	-0.895924	C	-1.350747	0.791160	-1.613163
F	-3.116103	-2.834779	-1.187718	C	-1.758330	1.855836	-2.629906
C	-4.260686	-2.233169	-0.864356	C	-3.150592	1.612957	-3.205192
H	2.192371	0.929839	0.125520	F	2.442642	2.246589	-0.477100
H	2.094688	1.264175	-1.610490	F	1.727066	-1.564173	2.272057
H	0.919433	-0.883494	-1.989605	F	5.582234	0.993948	2.716730
H	1.032745	-1.272618	-0.274275	F	-0.272880	-2.152462	-1.497183
H	-0.422791	1.159009	-1.422566	F	-0.597361	-0.154607	2.751064
H	-0.319520	0.750020	0.282725	F	-3.071917	-4.015444	1.770407
H	-1.444981	-1.479387	-0.236993	F	4.752216	2.658710	0.738498
H	-1.634241	-1.003777	-1.880308	F	-2.015004	-4.065255	-0.733453
H	8.568603	-0.264166	-0.526045	F	-2.364565	-2.054127	3.510471
H	6.661923	3.551103	-0.689377	H	0.109386	2.059451	-0.649600

H	0.796747	1.031178	-1.846035	C	3.757653	-1.973695	-0.180799
H	-1.394884	-0.193367	-2.091745	C	3.829222	-0.585843	-0.154531
H	-2.087796	0.770732	-0.799105	C	2.730481	0.208440	0.178297
H	-1.719782	2.843520	-2.153250	C	1.484815	-0.396982	0.452674
H	-1.019778	1.878714	-3.441117	C	1.437477	-1.805478	0.568733
H	-3.425654	2.381487	-3.931715	C	2.562095	-2.558226	0.227752
H	-3.200419	0.642146	-3.707890	C	-3.711552	-1.044142	0.680161
H	-3.905650	1.614549	-2.412881	C	-3.813398	-1.607677	-0.588082

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[5BH]<sup>-</sup>

C	2.506644	-2.992343	-0.774961	C	-2.556482	-0.384279	1.102424
C	1.491882	-3.070215	0.164343	P	0.016147	0.668754	0.854141
C	0.675715	-1.964945	0.385926	C	0.018484	2.014321	-0.469423
C	0.796507	-0.759380	-0.299754	C	-0.052270	3.421420	0.124170
C	1.842307	-0.734107	-1.221956	C	-0.031738	4.507708	-0.950065
C	2.685395	-1.809708	-1.475416	C	-0.131455	5.913165	-0.363396
C	1.569377	3.818493	1.458221	C	0.245515	-2.566044	1.109003
C	1.986221	3.376047	2.703284	C	2.980328	1.693852	0.332661
C	1.743778	2.060640	3.069258	C	4.937792	-2.813924	-0.592608
C	1.089118	1.220144	2.177556	C	-0.395053	-0.869840	-2.044564
C	0.653068	1.609404	0.913902	C	-2.536670	0.189038	2.502098
C	0.918667	2.938372	0.598152	C	-5.080873	-2.286303	-1.038255
B	-0.144485	0.582013	-0.093315	H	4.777185	-0.097389	-0.372490
C	-1.636661	0.278607	0.505588	H	2.503598	-3.642024	0.308547
F	1.315485	-4.208129	0.852256	H	-4.554829	-1.118479	1.363292
C	-2.475541	-0.727837	-0.292693	H	-2.771842	-1.941948	-2.432111
C	-2.630606	-0.375914	-1.771525	H	0.886963	1.915478	-1.125625
C	-3.573818	-1.328032	-2.503504	H	-0.864991	1.845048	-1.093063
F	2.096200	0.378389	-1.928798	H	-0.968026	3.514801	0.722857
F	-0.270847	-2.137306	1.323990	H	0.779160	3.587296	0.820489
F	3.305967	-4.043728	-1.001957	H	0.892551	4.414048	-1.535080
F	0.881961	-0.039650	2.599893	H	-0.857380	4.337671	-1.652202
F	0.544947	3.456009	-0.581574	H	-0.110380	6.677818	-1.143963
F	2.612699	4.209781	3.545046	H	-1.061381	6.034249	0.200686
F	3.670459	-1.721444	-2.381884	H	0.699028	6.109325	0.321864
F	2.141199	1.625307	4.273978	H	0.585080	-3.519415	1.520788
F	1.798300	5.091498	1.101687	H	-0.258453	-2.017108	1.909044
H	-0.220112	1.118869	-1.176514	H	-0.506840	-2.778405	0.343736
H	-1.588201	-0.061483	1.548046	H	4.013612	1.854217	0.649353
H	-2.182033	1.235519	0.525994	H	2.835342	2.260800	-0.592127
H	-2.021684	-1.725377	-0.218679	H	2.331870	2.130393	1.097090
H	-3.481911	-0.826548	0.146189	H	5.879381	-2.287993	-0.416980
H	-2.996909	0.655533	-1.861790	H	4.964240	-3.757334	-0.041466
H	-1.644907	-0.385686	-2.247934	H	4.890052	-3.057793	-1.659180
H	-3.667662	-1.079893	-3.565721	H	0.280393	-1.706559	-1.834250
H	-3.213306	-2.360177	-2.432117	H	-0.776533	-0.993926	-3.060811
H	-4.577211	-1.302721	-2.063215	H	0.212196	0.034077	-2.013434

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5P

H	-3.480251	-0.022355	3.009874
H	-1.722641	-0.231403	3.099628

H -5.623395 -2.713305 -0.191459  
H -5.748757 -1.573134 -1.532706  
H -4.869700 -3.087483 -1.750648

55  
[5PH]<sup>+</sup>

C 2.897301 -2.947665 0.154623  
C 3.002828 -1.938171 -0.801116  
C 2.161040 -0.827750 -0.818851  
C 1.169054 -0.733106 0.184632  
C 1.038801 -1.743195 1.169290  
C 1.908461 -2.828872 1.128945  
C -4.026760 0.267354 0.700936  
C -4.414862 -0.365229 -0.480294  
C -3.433598 -0.657339 -1.426991  
C -2.091482 -0.356667 -1.215286  
C -1.724018 0.256022 0.000707  
C -2.699419 0.590933 0.969628  
P 0.005139 0.640928 0.348582  
C 0.512912 2.236584 -0.368321  
C 1.759753 2.803369 0.325555  
C 2.300842 4.033288 -0.404298  
C 3.508135 4.635163 0.308343  
C 0.013896 -1.690465 2.278214  
C 2.376399 0.184988 -1.918911  
C 3.806004 -4.144614 0.116456  
C -1.095463 -0.655275 -2.306101  
C -2.384625 1.288207 2.273815  
C -5.852664 -0.733105 -0.720026  
H 3.769832 -2.017328 -1.566579  
H 1.810570 -3.603848 1.884162  
H -4.784288 0.522641 1.436856  
H -3.722029 -1.127745 -2.363011  
H 0.027210 0.920525 1.716271  
H 0.647768 2.134644 -1.447096  
H -0.351864 2.894100 -0.218493  
H 1.502964 3.070407 1.358033  
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H 2.572829 3.750833 -1.429244  
H 1.503540 4.780800 -0.490116  
H 3.885706 5.506346 -0.229951  
H 3.246735 4.954248 1.321171  
H 4.322088 3.908329 0.383927  
H -0.000826 -2.638047 2.817056  
H 0.255101 -0.909496 3.009262  
H -0.999585 -1.511443 1.905099  
H 3.139594 -0.179781 -2.606877  
H 1.472010 0.356107 -2.507080  
H 2.724702 1.148235 -1.535835  
H 4.775479 -3.892446 -0.317144  
H 3.966539 -4.551814 1.116414

H 3.362676 -4.935309 -0.497205  
H -0.294110 -1.318035 -1.966882  
H -1.588976 -1.134987 -3.151963  
H -0.645243 0.270157 -2.682861  
H -1.844897 2.229215 2.126098  
H -3.310179 1.528813 2.797222  
H -1.789450 0.657733 2.943913  
H -6.055423 -1.734823 -0.327787  
H -6.528750 -0.037984 -0.218684  
H -6.087708 -0.740661 -1.785921

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5PHBH

C -3.797642 -3.893512 -0.701367  
C -2.426637 -3.831134 -0.503726  
C -1.884500 -2.705742 0.102125  
C -2.626330 -1.616334 0.533501  
C -3.993523 -1.722627 0.298029  
C -4.590026 -2.827010 -0.299095  
C -2.470664 3.180873 -0.703691  
C -1.891032 2.896431 -1.928689  
C -1.356171 1.636779 -2.139333  
C -1.404776 0.710107 -1.111640  
C -1.979471 0.923770 0.137805  
C -2.523890 2.198636 0.284554  
B -1.968296 -0.299235 1.252557  
C -2.668354 0.033995 2.680912  
F -1.646264 -4.843375 -0.900229  
C -1.837982 0.948893 3.583658  
C -2.528343 1.328544 4.892194  
C -1.661589 2.207790 5.790002  
F -4.808366 -0.714357 0.641654  
F -0.532789 -2.714793 0.239340  
F -4.347213 -4.962786 -1.279248  
F -0.781735 -0.469360 -1.374032  
F -3.125990 2.571654 1.422783  
F -1.791998 3.836521 -2.873007  
F -5.909099 -2.874823 -0.497141  
F -0.761124 1.347094 -3.305121  
F -2.952953 4.407599 -0.480221  
C 5.412966 -1.019164 2.674080  
C 4.187548 -1.664086 2.834976  
C 3.119867 -1.449859 1.967300  
C 3.297794 -0.549657 0.891747  
C 4.528938 0.107452 0.698977  
C 5.562833 -0.145706 1.600651  
C 1.509106 3.177326 -2.403536  
C 1.015991 4.056598 -1.447518  
C 0.922992 3.610334 -0.127661  
C 1.254796 2.312672 0.238014  
C 1.699536 1.419282 -0.771431

C	1.856265	1.857793	-2.097578	H	1.126122	6.197518	-1.251745
P	1.884633	-0.296679	-0.219005	H	0.666656	5.638083	-2.872430
C	1.863604	-1.609064	-1.497041	H	-0.498411	5.564579	-1.544270
C	3.226848	-2.220180	-1.824631				
C	3.124841	-3.191917	-2.999670				
C	4.459266	-3.862723	-3.310649				
C	4.789603	1.087740	-0.419207	69			
C	1.823782	-2.182603	2.214086	6H <sub>2</sub>	0.052241	-0.247989	-1.078465
C	6.535226	-1.253241	3.649318	P	-1.514319	-0.318479	-0.219013
C	1.115386	1.910491	1.685127	B	1.191116	-0.268875	0.145464
C	2.331337	0.997862	-3.243795	C	2.662163	-0.702957	-0.384815
C	0.557592	5.443937	-1.804213	C	1.189510	1.229873	0.803766
H	-0.787352	-0.573534	1.459524	C	-2.899839	0.433192	-1.123729
H	-2.825809	-0.913862	3.217303	C	-1.999425	-1.861713	0.601839
H	-3.666684	0.468000	2.550881	C	-2.956944	-1.722456	1.632302
H	-0.878477	0.457963	3.815116	C	-3.423231	-2.869001	2.272130
H	-1.583651	1.874887	3.049006	C	-2.956806	-4.137857	1.941143
H	-2.812320	0.413940	5.428444	C	-1.985645	-4.242532	0.948365
H	-3.465085	1.848676	4.656158	C	-1.484591	-3.132169	0.270158
H	-2.175069	2.480727	6.716252	C	-3.126023	1.817048	-0.949388
H	-1.385683	3.134546	5.275427	C	-4.177624	2.407861	-1.646983
H	-0.733411	1.693198	6.061020	C	-4.996454	1.679545	-2.508778
H	4.055994	-2.357720	3.661566	C	-4.737938	0.321202	-2.676338
H	6.515447	0.357006	1.454614	C	-3.698276	-0.318945	-2.004228
H	1.599174	3.509429	-3.434585	C	3.106010	-0.612460	-1.699314
H	0.554506	4.288757	0.638038	C	4.373788	-1.005091	-2.111288
H	0.733114	-0.521606	0.553623	C	5.266190	-1.507089	-1.175987
H	1.185292	-2.364180	-1.086491	C	4.876768	-1.606316	0.152220
H	1.357290	-1.203463	-2.374410	C	3.597968	-1.204159	0.516843
H	3.967653	-1.444530	-2.060681	C	0.590915	1.538119	2.020986
H	3.612300	-2.741460	-0.940334	C	0.517795	2.826161	2.540712
H	2.366944	-3.951015	-2.773181	C	1.076587	3.876950	1.828189
H	2.763888	-2.648405	-3.881840	C	1.682291	3.625962	0.603490
H	4.370142	-4.548730	-4.155787	C	1.721039	2.322906	0.122243
H	5.222802	-3.119531	-3.560298	C	-2.282727	2.687242	-0.042944
H	4.818692	-4.434597	-2.450102	C	-3.461012	-1.787261	-2.253581
H	5.861614	1.271167	-0.509032	C	-6.104938	2.356668	-3.269948
H	4.435635	0.723294	-1.387004	C	-3.462211	-0.381608	2.112579
H	4.293726	2.045546	-0.235298	C	-0.399453	-3.366426	-0.750936
H	1.947186	-2.893497	3.032151	C	-3.451153	-5.359231	2.668751
H	1.010387	-1.499689	2.486167	F	2.298072	-0.126303	-2.658319
H	1.484500	-2.744922	1.339660	F	4.740674	-0.902123	-3.390756
H	6.606782	-2.309353	3.920230	F	6.486955	-1.889235	-1.549209
H	7.494456	-0.936070	3.235764	F	5.731117	-2.084501	1.059136
H	6.363973	-0.688700	4.571283	F	3.282556	-1.312933	1.814131
H	2.049714	1.505091	2.087988	F	-0.028412	0.579497	2.738440
H	0.838025	2.775523	2.289432	F	-0.093598	3.062695	3.703201
H	0.327160	1.161648	1.820577	F	1.019151	5.118247	2.306218
H	1.478691	0.509805	-3.725894	F	2.208083	4.633686	-0.092493
H	2.815052	1.624999	-3.995250	F	2.278772	2.142631	-1.083905
H	3.047693	0.230005	-2.947820	H	0.133660	-1.049943	-1.810841

H 0.047693 0.697320 -1.633294  
H -1.358967 0.549619 0.856095  
H 0.839835 -1.060353 0.995323  
H -4.164146 -2.762502 3.060317  
H -1.594166 -5.224141 0.694003  
H -4.359061 3.471824 -1.516282  
H -5.358036 -0.258891 -3.355307  
H -2.426465 2.435048 1.014674  
H -1.210664 2.603678 -0.255911  
H -2.561403 3.734317 -0.169364  
H -2.404918 -1.989605 -2.459518  
H -3.753844 -2.398666 -1.394832  
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H -6.559919 3.154456 -2.678557  
H -5.718069 2.806962 -4.189702  
H -6.884990 1.645860 -3.550375  
H -2.650054 0.187112 2.580698  
H -3.885228 0.225007 1.305740  
H -4.240927 -0.522978 2.863109  
H -0.157627 -4.429393 -0.793259  
H -0.699110 -3.062224 -1.758037  
H 0.511641 -2.821763 -0.486932  
H -2.809900 -5.575352 3.529236  
H -4.467790 -5.214789 3.040603  
H -3.440506 -6.237783 2.019897

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[6H]<sup>+</sup>

C -0.261511 -1.370100 -0.901158  
P -1.703978 -0.417305 -0.305974  
B 1.139261 -0.597869 -0.839605  
C 2.468766 -1.329269 -0.519128  
C 1.075173 0.956390 -1.066693  
C -3.191135 -1.426749 -0.180612  
C -1.368545 0.780375 1.011376  
C -2.069549 2.008196 0.895544  
C -1.722880 3.051645 1.747533  
C -0.709547 2.927658 2.701340  
C -0.063501 1.699880 2.813983  
C -0.373148 0.614163 1.993177  
C -4.049712 -1.466335 -1.305825  
C -5.216077 -2.220552 -1.210586  
C -5.551562 -2.930255 -0.057444  
C -4.676873 -2.883054 1.027976  
C -3.495278 -2.149539 0.991602  
C 2.545053 -2.589956 0.096641  
C 3.739917 -3.231987 0.370920  
C 4.937132 -2.620218 0.010297  
C 4.923446 -1.371905 -0.601410  
C 3.708255 -0.751379 -0.846084  
C 1.631606 1.824031 -0.126094

C 1.299894 3.168854 -0.059211  
C 0.419034 3.700291 -0.993307  
C -0.111212 2.884733 -1.988076  
C 0.223770 1.540712 -2.002086  
C -3.775136 -0.737172 -2.602542  
C -2.579374 -2.176774 2.187652  
C -6.807483 -3.754670 -0.000385  
C -3.167302 2.245766 -0.117205  
C 0.410191 -0.653858 2.233064  
C -0.312397 4.098223 3.556327  
F 1.436648 -3.227390 0.495820  
F 3.752922 -4.413123 0.969734  
F 6.081382 -3.221440 0.257633  
F 6.061652 -0.788466 -0.940232  
F 3.762411 0.440351 -1.432135  
F 2.441480 1.348967 0.823229  
F 1.776813 3.935239 0.912751  
F 0.066896 4.970703 -0.921960  
F -0.978132 3.378060 -2.865104  
F -0.365035 0.768018 -2.932695  
H -1.987324 0.421567 -1.375613  
H -2.255951 3.994973 1.660164  
H 0.716015 1.575351 3.561780  
H -5.884885 -2.256403 -2.066211  
H -4.920392 -3.436926 1.930487  
H -3.869641 0.349111 -2.489849  
H -2.779118 -0.944836 -3.006486  
H -4.497674 -1.044806 -3.358766  
H -1.626321 -2.658611 1.943140  
H -2.369088 -1.172635 2.567193  
H -3.029563 -2.751604 2.997749  
H -7.594276 -3.321443 -0.620815  
H -6.611527 -4.765958 -0.370895  
H -7.178080 -3.842001 1.022553  
H -2.762377 2.450539 -1.117159  
H -3.859319 1.400531 -0.192205  
H -3.753113 3.119003 0.171990  
H 0.214487 -1.021146 3.245466  
H 0.176690 -1.469775 1.552391  
H 1.481871 -0.445681 2.163049  
H 0.405085 4.721647 3.013911  
H -1.175538 4.719311 3.803700  
H 0.161004 3.771854 4.483774  
H -0.256729 -2.350559 -0.428559  
H -0.494299 -1.533721 -1.964056

68

[6H]<sup>-</sup>

C -0.152638 -1.138008 -0.289573  
P 1.278650 -1.501792 0.828235  
B -1.227077 -0.091147 0.452222

C	-1.094346	1.358111	-0.292290	H	5.382241	-1.566791	1.879190	
C	-2.737293	-0.736899	0.395132	H	3.673321	-1.492851	2.333566	
C	2.718052	-2.133942	-0.195439	H	5.908517	-4.473822	-3.049066	
C	1.842690	0.230692	1.228794	H	6.368250	-2.788185	-3.294430	
C	1.810658	0.607280	2.589986	H	7.013362	-3.679403	-1.914856	
C	2.229463	1.880954	2.971208	H	0.274846	-0.617112	3.472634	
C	2.658543	2.820098	2.038667	H	1.891402	-1.251909	3.714738	
C	2.689292	2.440859	0.701964	H	1.359621	0.164969	4.644014	
C	2.287508	1.170321	0.277720	H	3.091050	1.517886	-1.683712	
C	2.536585	-2.962406	-1.328745	H	2.456616	-0.120404	-1.474821	
C	3.641876	-3.403998	-2.058948	H	1.347000	1.243963	-1.647688	
C	4.947370	-3.091989	-1.696598	H	2.175334	4.896842	2.209259	
C	5.122440	-2.373813	-0.520002	H	3.209036	4.296641	3.516815	
C	4.047159	-1.911742	0.241893	H	3.887607	4.593049	1.904567	
C	-1.326808	1.498937	-1.658877					
C	-1.065316	2.656124	-2.377251					
C	-0.521426	3.750627	-1.715432	67				
C	-0.283183	3.667859	-0.354419	<b>6</b>	C	0.456784	-1.092311	-1.154261
C	-0.595158	2.494949	0.329208	P	1.345700	-1.241290	0.514616	
C	-2.927999	-1.991830	0.974911	B	-0.987569	-0.539935	-0.884646	
C	-4.144257	-2.658477	1.020324	C	-1.214410	1.020346	-0.985379	
C	-5.266228	-2.056826	0.469233	C	-2.167428	-1.492270	-0.462473	
C	-5.139492	-0.805889	-0.109013	C	3.151443	-1.490794	0.135809	
C	-3.897107	-0.176359	-0.129631	C	1.240732	0.556107	0.988387	
C	1.184239	-3.471116	-1.775933	C	0.492875	0.843464	2.150002	
C	4.392546	-1.236516	1.550946	C	0.296028	2.171386	2.538267	
C	6.121532	-3.534520	-2.530988	C	0.822263	3.232553	1.810301	
C	1.310697	-0.325694	3.668119	C	1.573918	2.933637	0.675010	
C	2.301416	0.925507	-1.212984	C	1.789188	1.624769	0.242135	
C	3.009109	4.227402	2.444349	C	3.608488	-2.290739	-0.933898	
F	-1.822013	0.459768	-2.353491	C	4.980225	-2.422521	-1.157593	
F	-1.315337	2.735338	-3.691847	C	5.929748	-1.824403	-0.336743	
F	-0.240152	4.873901	-2.387999	C	5.465051	-1.137861	0.779884	
F	0.257846	4.713895	0.288833	C	4.105167	-0.975351	1.045475	
F	-0.348129	2.510497	1.644110	C	-0.714772	1.780852	-2.038258	
F	-1.887205	-2.628494	1.539447	C	-0.746196	3.168516	-2.051824	
F	-4.253447	-3.865784	1.591654	C	-1.292861	3.841075	-0.968040	
F	-6.453209	-2.676240	0.499612	C	-1.811765	3.123421	0.101016	
F	-6.217745	-0.211020	-0.637764	C	-1.777571	1.739499	0.067159	
F	-3.892136	1.044297	-0.692886	C	-1.969201	-2.838427	-0.115195	
H	0.173929	-0.754284	-1.261458	C	-2.997391	-3.688936	0.266716	
H	-0.650961	-2.091775	-0.471484	C	-4.300900	-3.214689	0.288755	
H	-0.971063	0.051180	1.630179	C	-4.559995	-1.898876	-0.070017	
H	2.189259	2.156876	4.023253	C	-3.507987	-1.073957	-0.437416	
H	3.009027	3.164557	-0.047135	C	2.694105	-3.088097	-1.836760	
H	3.469380	-4.028441	-2.934218	C	3.742454	-0.291544	2.345605	
H	6.132588	-2.175015	-0.164600	C	7.402674	-1.941074	-0.627609	
H	0.596827	-3.832135	-0.927229	C	-0.153695	-0.237135	2.988250	
H	0.590668	-2.704252	-2.277135	C	2.576089	1.467833	-1.041274	
H	1.317940	-4.304422	-2.470731	C	0.549481	4.664643	2.188129	
H	4.404042	-0.146143	1.470716	F	-0.158714	1.177820	-3.099486	

F	-0.240582	3.850609	-3.076577	F	-0.47936	-1.11742	1.41125
F	-1.291876	5.170092	-0.934512	F	-2.44249	2.25718	-1.26081
F	-2.286851	3.768214	1.163978	F	-4.78704	0.99273	-1.11511
F	-2.271726	1.090325	1.126989	F	-5.01083	-1.31736	0.29564
F	-0.754961	-3.388350	-0.134834	F	-2.84450	-2.35904	1.55770
F	-2.746348	-4.952020	0.594954	F	0.37492	-1.22664	-1.17250
F	-5.293917	-4.015239	0.641125	F	2.61133	2.32666	1.03039
F	-5.809907	-1.447061	-0.069289	F	4.90272	1.00200	0.80367
F	-3.849481	0.161075	-0.801210	F	4.96753	-1.42662	-0.41104
H	1.018402	-0.440544	-1.825618	F	2.68632	-2.51924	-1.39335
H	0.402469	-2.093111	-1.575680	H	-0.94329	3.43709	0.06614
H	-0.303509	2.378531	3.421438	H	0.26291	3.14807	1.32467
H	1.993188	3.751120	0.089530	H	0.80363	3.47536	-0.30007
H	5.312512	-3.033780	-1.994133				
H	6.182919	-0.725141	1.485887	28			
H	1.886102	-3.564237	-1.273403	<b>[6BH]<sup>-</sup></b>			
H	2.245177	-2.476916	-2.624432	C	1.43745	-1.06225	-0.28106
H	3.265424	-3.881068	-2.323687	C	1.31897	-0.19021	0.79772
H	3.541573	0.775482	2.216404	C	2.37637	0.70188	0.93736
H	4.568874	-0.398416	3.052013	C	3.47516	0.73108	0.08304
H	2.854186	-0.735078	2.804947	C	3.54361	-0.16173	-0.97421
H	7.627562	-2.861459	-1.171881	C	2.51256	-1.07035	-1.16086
H	7.745751	-1.102143	-1.242158	C	-1.50156	1.24192	0.28703
H	7.989977	-1.935198	0.293864	C	-2.59081	1.57355	-0.50817
H	-0.892915	-0.801683	2.411548	C	-3.56319	0.61623	-0.75654
H	0.576081	-0.961713	3.359695	C	-3.41953	-0.64602	-0.20579
H	-0.665165	0.208619	3.843855	C	-2.30760	-0.93138	0.58264
H	3.351526	2.236119	-1.094342	C	-1.31183	-0.00672	0.87718
H	3.059792	0.497467	-1.138197	B	0.02366	-0.25600	1.81293
H	1.926245	1.611479	-1.912860	C	0.03461	-1.66443	2.63349
H	-0.038568	5.161398	1.409194	F	-0.59325	2.21400	0.47341
H	-0.011782	4.728884	3.122322	F	-2.25480	-2.18606	1.05997
H	1.480559	5.226555	2.304497	F	-4.35262	-1.58018	-0.44591
				F	-4.62589	0.90925	-1.51974
				F	-2.71735	2.79840	-1.04130
				F	0.47004	-1.96578	-0.52219
				F	2.39524	1.59913	1.93443
				F	4.47159	1.61124	0.26628
				F	4.59482	-0.14917	-1.80632
				F	2.57170	-1.93672	-2.18351
				H	0.08787	0.68744	2.57403
				H	-0.84647	-1.76883	3.27849
				H	0.91538	-1.70565	3.28715
				H	0.06418	-2.54945	1.98861
				45			
				<b>6P</b>			
				P	0.03396	1.60269	0.52680
				C	0.21536	2.77447	-0.90968
				C	-1.46062	0.52511	0.31492
				C	1.42723	0.47147	0.03898
27							
<b>6B</b>							
C	1.45782	-0.63931	-0.66160				
C	1.36648	0.61888	-0.05383				
C	2.57517	1.14009	0.42141				
C	3.78520	0.46780	0.32108				
C	3.82087	-0.77460	-0.29643				
C	2.65057	-1.33307	-0.79500				
C	-1.51859	-0.56425	0.77987				
C	-2.73251	-1.22674	0.87028				
C	-3.84360	-0.69353	0.22806				
C	-3.72796	0.48988	-0.48819				
C	-2.49910	1.13409	-0.53913				
C	-1.35488	0.63701	0.08666				
B	0.01558	1.41530	0.07075				
C	0.01908	2.96919	0.26732				



C	2.60649	0.56196	0.81071	C	2.72029	-1.05169	-1.46766
C	3.69636	-0.25266	0.50756	C	1.56368	-0.33306	-1.17757
C	3.66151	-1.16230	-0.54644	C	-1.68146	-0.68854	1.13633
C	2.49847	-1.23358	-1.30549	C	-2.83996	-1.45101	1.02897
C	1.38181	-0.43497	-1.04058	C	-3.84133	-1.14903	0.10701
C	-1.47182	-0.66271	1.08099	C	-3.66506	-0.03750	-0.71535
C	-2.56497	-1.52849	1.00109	C	-2.52775	0.76563	-0.65920
C	-3.67053	-1.25329	0.20586	C	-0.66522	-1.06939	2.18772
C	-3.67706	-0.04512	-0.48665	C	-2.47082	1.95406	-1.58922
C	-2.60855	0.84937	-0.43971	C	-5.06791	-2.01059	-0.00593
C	-0.34324	-1.05746	2.00605	C	2.60068	1.12289	2.25179
C	-2.76496	2.14739	-1.19677	C	5.05833	-1.84262	-0.95218
C	-4.82415	-2.21613	0.10054	C	0.42782	-0.35182	-2.16985
C	2.73395	1.51874	1.97475	H	0.13222	1.53966	1.84543
C	4.85968	-2.01553	-0.87270	H	1.07856	3.40772	0.14624
C	0.17416	-0.63531	-1.92816	H	-0.69271	3.60465	0.08842
H	1.22681	3.17414	-0.78858	H	0.19606	2.95195	-1.32120
H	-0.48137	3.60989	-0.84750	H	4.57391	-0.37034	1.27580
H	0.15757	2.31251	-1.89675	H	2.77099	-1.60333	-2.40246
H	4.59655	-0.17585	1.11373	H	-2.96565	-2.30444	1.68963
H	2.45232	-1.93427	-2.13682	H	-4.44414	0.21845	-1.42789
H	-2.54859	-2.44211	1.59185	H	-0.59506	-0.30559	2.97144
H	-4.54989	0.21851	-1.08057	H	-0.96288	-1.99799	2.67500
H	0.06018	-0.19340	2.54418	H	0.33474	-1.22428	1.77038
H	-0.70364	-1.77625	2.74530	H	-3.33036	1.93643	-2.25964
H	0.48879	-1.51583	1.46267	H	-2.50991	2.90057	-1.04371
H	-3.78425	2.23505	-1.57813	H	-1.57780	1.95931	-2.21860
H	-2.57842	3.01197	-0.55387	H	-5.37965	-2.38218	0.97234
H	-2.08673	2.21615	-2.05143	H	-5.89956	-1.46241	-0.45154
H	-4.84911	-2.89844	0.95335	H	-4.86186	-2.87947	-0.63904
H	-5.77937	-1.68637	0.05781	H	2.37815	2.18828	2.13325
H	-4.74510	-2.82293	-0.80760	H	1.87669	0.70206	2.95896
H	2.59638	2.55860	1.66373	H	3.58347	1.05285	2.71837
H	1.98096	1.32222	2.74327	H	5.55317	-2.22754	-0.05844
H	3.72282	1.43078	2.42999	H	4.83788	-2.67975	-1.61687
H	5.38726	-2.31927	0.03500	H	5.76710	-1.18602	-1.46680
H	4.56824	-2.91614	-1.41801	H	0.76493	-0.76887	-3.11945
H	5.57097	-1.46504	-1.49727	H	-0.41278	-0.95480	-1.81348
H	0.48249	-1.07432	-2.87992	H	0.05113	0.65464	-2.37891
H	-0.55158	-1.31000	-1.46176				
H	-0.35753	0.29421	-2.13645				

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**6PHBH**

46				C	4.015409	0.446559	0.806564
<b>[6PH]<sup>+</sup></b>				C	2.843983	1.108197	0.455389
P	0.03024	1.31592	0.47129	C	3.022801	2.363343	-0.112252
C	0.14468	2.98487	-0.23357	C	4.272400	2.935019	-0.323912
C	-1.52411	0.42517	0.27384	C	5.411579	2.233062	0.040977
C	1.50827	0.37915	0.03832	C	5.285028	0.975008	0.614149
C	2.60010	0.37710	0.93709	C	1.340409	-1.037695	-1.430903
C	3.72900	-0.36014	0.59263	C	1.226811	-2.194064	-2.190614
C	3.81073	-1.08156	-0.59929	C	1.054945	-3.408863	-1.542969



C	0.489601	-2.684908	-1.425478	C	-1.216311	1.309319	-0.567909
C	3.253159	-1.728094	-5.450589	C	2.993628	0.694850	0.673502
F	-2.688023	-0.622052	2.567952	C	2.179395	-1.909759	-0.769646
F	-4.823496	-2.166981	2.769576	C	3.538595	-2.261504	-0.967246
F	-5.839656	-3.433744	0.580744	C	3.820337	-3.541223	-1.446173
F	-4.638628	-3.095459	-1.841639	C	2.831083	-4.467614	-1.762383
F	-2.507406	-1.549470	-2.089098	C	1.504251	-4.058601	-1.654238
F	0.228950	1.773151	-1.836775	C	1.153207	-2.797762	-1.181946
F	-0.249120	4.354380	-2.191953	C	3.245588	1.982240	0.141359
F	-2.204835	5.616075	-0.765419	C	4.232415	2.756535	0.744691
F	-3.657068	4.204542	1.054419	C	4.963462	2.310759	1.847460
F	-3.178296	1.623702	1.458301	C	4.677283	1.047493	2.359995
H	1.589977	1.366686	0.045225	C	3.700850	0.228232	1.798075
H	-0.745304	-1.592706	2.661069	C	-3.028990	-0.843856	1.949065
H	0.993464	-1.795940	2.478910	C	-4.304133	-1.342251	2.174883
H	-0.134503	-2.524850	1.313317	C	-5.105202	-1.672555	1.087026
H	0.163539	1.798651	1.821654	C	-4.631383	-1.496007	-0.209905
H	-0.896159	0.746608	2.749283	C	-3.361002	-0.974178	-0.392613
H	0.858506	0.639195	2.990885	C	-0.908685	1.462415	-1.915119
H	4.035481	0.428189	-3.998793	C	-1.097510	2.653900	-2.603541
H	1.503711	-3.006525	-3.789622	C	-1.624952	3.751581	-1.933932
H	5.244565	1.487473	3.312063	C	-1.961440	3.643436	-0.588635
H	5.223199	-2.677016	2.355687	C	-1.764498	2.431009	0.055382
H	3.118003	2.651831	0.855872	C	2.499693	2.575320	-1.034019
H	2.187859	2.396390	2.332923	C	3.450876	-1.116725	2.436617
H	3.852925	2.959783	2.424257	C	6.042828	3.168180	2.447586
H	2.080641	-2.771640	0.672024	C	4.731137	-1.351727	-0.767728
H	3.506282	-2.709442	-0.364923	C	-0.316011	-2.449073	-1.198946
H	3.539198	-3.634696	1.144712	C	3.181199	-5.851496	-2.232186
H	7.206872	0.034856	3.857742	F	-2.292091	-0.526479	3.019979
H	6.201148	-0.979743	4.893295	F	-4.759054	-1.503450	3.407784
H	7.116967	-1.712398	3.573197	F	-6.315007	-2.160125	1.284171
H	2.725315	2.246413	-1.533668	F	-5.389696	-1.822189	-1.245080
H	4.028419	1.369261	-0.694212	F	-2.918716	-0.822555	-1.647520
H	4.241534	1.896413	-2.362005	F	-0.388221	0.438858	-2.612965
H	0.902261	-3.695407	-1.333961	F	-0.777443	2.746119	-3.885636
H	0.159233	-2.346338	-0.451971	F	-1.803648	4.893387	-2.572187
H	-0.403267	-2.729795	-2.054602	F	-2.466719	4.681382	0.058167
H	2.784930	-1.065864	-6.185382	F	-2.109251	2.341261	1.347433
H	4.335900	-1.639909	-5.572570	H	1.233637	0.466763	-1.126712
H	2.961208	-2.752806	-5.688085	H	-0.822248	-2.093907	2.004752
H	-0.697571	-0.388963	-1.086276	H	0.578164	-1.563591	2.920622
				H	0.790255	-2.503391	1.443208
				H	0.509663	1.775326	1.582645
				H	-0.523080	0.892651	2.721287
				H	1.229274	0.666839	2.757198
				H	4.861365	-3.813191	-1.597277
				H	0.712623	-4.733651	-1.968209
				H	4.438366	3.744389	0.341562
				H	5.229655	0.684789	3.223122
				H	2.582871	1.965038	-1.939437

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[7H]<sup>+</sup>

C	0.224021	-0.385360	1.115241
P	1.681978	-0.305793	-0.059259
B	-1.128389	0.013167	0.354008
C	0.195223	-1.714356	1.909738
C	0.371497	0.821619	2.099420
C	-2.515187	-0.645498	0.668791

H 1.433645 2.708747 -0.813750  
H 2.905890 3.559217 -1.269809  
H 2.770052 -1.022571 3.289111  
H 3.030651 -1.854153 1.747777  
H 4.385763 -1.529346 2.822562  
H 5.748317 4.219750 2.460520  
H 6.275484 2.859492 3.467990  
H 6.960331 3.090519 1.855800  
H 4.549650 -0.331752 -1.109371  
H 5.046696 -1.298304 0.277270  
H 5.570644 -1.747116 -1.340935  
H -0.834303 -3.082978 -1.920665  
H -0.796219 -2.612542 -0.230190  
H -0.496376 -1.423525 -1.531021  
H 4.160234 -5.871339 -2.714240  
H 3.214453 -6.540407 -1.382113  
H 2.437840 -6.230628 -2.936166

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[7H]<sup>-</sup>

C 0.088293 -0.790641 0.673631  
P 1.589990 -0.085421 -0.343094  
B -1.251874 -0.618280 -0.307313  
C 0.254682 -2.246104 1.181573  
C -0.053970 0.165397 1.878343  
C -2.718170 -1.103849 0.309484  
C -1.415078 0.940668 -0.810211  
C 2.580925 0.794459 0.978121  
C 2.795339 -1.387325 -0.929434  
C 4.191866 -1.131111 -0.990320  
C 5.067256 -2.149764 -1.374026  
C 4.628523 -3.407446 -1.772325  
C 3.255538 -3.579456 -1.896170  
C 2.342436 -2.588238 -1.529640  
C 2.595487 2.204319 0.887426  
C 3.338975 2.955713 1.799282  
C 4.071644 2.357186 2.819126  
C 4.019675 0.970994 2.926330  
C 3.284023 0.182272 2.037166  
C -3.071576 -1.645724 1.541678  
C -4.362179 -2.045148 1.884544  
C -5.389695 -1.914718 0.969406  
C -5.101483 -1.386296 -0.279797  
C -3.800079 -1.005966 -0.573961  
C -0.941781 1.352463 -2.054683  
C -1.021725 2.661507 -2.514271  
C -1.623094 3.628450 -1.721718  
C -2.129797 3.268600 -0.483279  
C -2.019858 1.946422 -0.063095  
C 1.817523 2.952289 -0.172761  
C 3.258783 -1.304090 2.293929

C 4.903314 3.182385 3.767684  
C 4.828717 0.228271 -0.775359  
C 0.905260 -2.791870 -1.933803  
C 5.597159 -4.509266 -2.113989  
F -2.166812 -1.833129 2.523070  
F -4.615780 -2.557926 3.096458  
F -6.635465 -2.293621 1.279610  
F -6.080113 -1.257547 -1.185649  
F -3.613973 -0.520501 -1.812312  
F -0.365212 0.479619 -2.893038  
F -0.539372 3.003789 -3.716282  
F -1.718574 4.892531 -2.151617  
F -2.725063 4.191779 0.283887  
F -2.543744 1.673386 1.145760  
H -1.145798 -1.286294 -1.304199  
H -0.577611 -2.875933 0.847371  
H 0.245523 -2.281352 2.275897  
H 1.181015 -2.723900 0.847946  
H -0.022886 1.218216 1.577658  
H -1.017863 -0.001428 2.359647  
H 0.729022 0.022244 2.630537  
H 6.134386 -1.932414 -1.387390  
H 2.869760 -4.502247 -2.326007  
H 3.341607 4.040385 1.708676  
H 4.562783 0.481747 3.733214  
H 2.109738 2.650062 -1.182572  
H 0.743667 2.750657 -0.095236  
H 1.971788 4.029428 -0.066964  
H 2.277613 -1.608736 2.668085  
H 3.456626 -1.889244 1.394100  
H 4.002127 -1.570384 3.050024  
H 4.440124 4.154683 3.956216  
H 5.031868 2.673226 4.726505  
H 5.901755 3.368851 3.356717  
H 4.167359 1.034790 -1.100174  
H 5.093385 0.427683 0.266049  
H 5.743261 0.281843 -1.373080  
H 0.840396 -3.607498 -2.659200  
H 0.239946 -3.025803 -1.104095  
H 0.510229 -1.885420 -2.400316  
H 6.544895 -4.104925 -2.480781  
H 5.821639 -5.125288 -1.235911  
H 5.188546 -5.171970 -2.882006

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7

C -0.208143 -1.105132 -0.482891  
P -1.628413 0.177141 -0.425321  
B 1.198087 -0.421721 -0.337378  
C -0.384918 -2.425883 0.275082  
C -0.164875 -1.460972 -2.011517

C	2.456810	-1.125650	0.322127	H	-4.715835	1.040562	-0.311542
C	1.518436	0.985912	-0.989399	H	-4.728938	2.759980	0.104294
C	-2.103592	0.839815	1.248752	H	0.598082	0.611352	3.213113
C	-3.079376	-0.920165	-0.821695	H	-0.280721	-0.923087	3.248074
C	-3.758324	-1.731393	0.121626	H	0.350639	-0.293402	1.732384
C	-4.854789	-2.490062	-0.291605	H	-3.482937	3.808263	4.828110
C	-5.325551	-2.473750	-1.601418	H	-4.724785	2.563065	4.954681
C	-4.673200	-1.650188	-2.510271	H	-3.159093	2.336174	5.750325
C	-3.569208	-0.873792	-2.149190	H	-3.781200	-2.750128	2.007455
C	-3.285256	1.630392	1.214521	H	-2.348818	-1.737491	1.787845
C	-3.765575	2.207658	2.387721	H	-3.892745	-0.987588	2.143929
C	-3.112184	2.070077	3.610053	H	-2.180218	-0.525189	-3.774808
C	-1.929832	1.345362	3.618144	H	-3.747116	0.254246	-3.966459
C	-1.412352	0.740449	2.469096	H	-2.546916	0.919519	-2.840635
C	3.162735	-0.440183	1.310808	H	-6.161910	-4.342913	-2.265195
C	4.286942	-0.957799	1.936571	H	-7.229238	-3.411838	-1.213647
C	4.762473	-2.202920	1.545292	H	-6.990701	-2.918610	-2.898846
C	4.107311	-2.909553	0.545848				
C	2.973496	-2.364911	-0.042393	33			
C	2.265879	1.017342	-2.159260	<b>7B</b>			
C	2.614865	2.199324	-2.796202	B	-0.06096	1.11880	0.23498
C	2.222200	3.405471	-2.229631	C	-0.04098	2.66457	0.55587
C	1.490892	3.415875	-1.047941	C	-1.40765	0.32709	0.02213
C	1.153256	2.210348	-0.449136	C	1.30963	0.33635	0.14063
C	-4.082998	1.892164	-0.044210	C	2.33028	0.73720	-0.71224
C	-0.118623	-0.007161	2.667717	C	3.56164	0.09889	-0.76588
C	-3.648240	2.726406	4.855106	C	3.79758	-0.98194	0.07343
C	-3.417318	-1.806594	1.593302	C	2.80262	-1.41870	0.94052
C	-2.976646	-0.002002	-3.235591	C	1.58183	-0.76237	0.94921
C	-6.493276	-3.329178	-2.017205	C	-1.44234	-0.97716	-0.49790
F	2.737612	0.766202	1.706877	C	-2.61236	-1.70106	-0.67446
F	4.911220	-0.277109	2.892057	C	-3.82715	-1.13030	-0.32176
F	5.841205	-2.713790	2.122745	C	-3.85539	0.15700	0.19526
F	4.570960	-4.092989	0.157648	C	-2.66615	0.85462	0.35062
F	2.400923	-3.079948	-1.018821	F	-0.32643	-1.59801	-0.87843
F	2.655699	-0.143079	-2.709688	F	-2.79177	2.08651	0.84749
F	3.316897	2.189561	-3.925921	F	-2.57984	-2.92984	-1.17879
F	2.548369	4.550789	-2.816802	F	-4.95218	-1.80753	-0.48281
F	1.129835	4.573971	-0.504280	F	-5.01542	0.71143	0.53168
F	0.467377	2.246475	0.696234	F	2.13083	1.76628	-1.54832
H	-1.362581	-2.863992	0.053588	F	4.50744	0.50750	-1.60644
H	-0.295485	-2.309432	1.356893	F	4.97001	-1.60215	0.04395
H	0.371918	-3.146393	-0.046757	F	3.02810	-2.45768	1.73904
H	-1.066314	-2.031135	-2.260651	F	0.63303	-1.21904	1.77545
H	-0.126152	-0.571696	-2.645522	C	1.30005	3.22840	1.03982
H	0.698916	-2.091680	-2.238791	C	-0.54568	3.45512	-0.67295
H	-5.362935	-3.111008	0.443397	H	-0.77535	2.82153	1.35529
H	-5.036157	-1.597235	-3.534541	H	1.17660	4.26453	1.36998
H	-4.678778	2.797401	2.338784	H	1.70460	2.65615	1.87993
H	-1.376123	1.240839	4.549646	H	2.04505	3.22802	0.24018
H	-3.435102	2.096320	-0.902137	H	-0.58140	4.52358	-0.43919

H	-1.54737	3.14541	-0.97986	C	-2.52909	0.47724	-0.62995
H	0.13307	3.32335	-1.52046	C	-3.64897	-0.35427	-0.75008
				C	-3.81535	-1.50845	0.00228
34				C	-2.81853	-1.81981	0.92147
<b>[7BH]<sup>-</sup></b>				C	-1.69430	-1.01641	1.09357
B	-0.00619	1.29534	-0.72115	C	-2.50102	1.66391	-1.56691
C	-0.11345	2.76465	0.00386	C	-0.70691	-1.43197	2.15863
C	1.39650	0.46654	-0.44790	C	-5.03017	-2.38550	-0.15111
C	-1.29348	0.37831	-0.26050	C	2.50125	0.33463	2.40991
C	-1.32224	-0.39452	0.89612	C	4.77125	-2.42741	-1.09649
C	-2.41961	-1.14243	1.30598	C	0.43459	-0.22128	-2.25114
C	-3.57285	-1.13090	0.53701	C	1.65567	3.07422	-0.32188
C	-3.60313	-0.37044	-0.62105	C	-0.61646	3.77165	0.48152
C	-2.47791	0.35874	-0.99080	H	-0.19322	2.57823	-1.26997
C	1.50565	-0.86078	-0.86782	H	4.33541	-1.22708	1.30839
C	2.65115	-1.63490	-0.74723	H	2.59777	-1.71322	-2.56362
C	3.79026	-1.08001	-0.18376	H	-4.41602	-0.08436	-1.47246
C	3.74765	0.23547	0.24133	H	-2.92192	-2.71106	1.53699
C	2.57264	0.97051	0.09954	H	-1.71656	1.56108	-2.32193
F	0.45549	-1.47307	-1.44264	H	-3.45207	1.73228	-2.09872
F	2.65724	2.24122	0.53912	H	-2.34813	2.61275	-1.05225
F	2.67667	-2.90617	-1.17333	H	-1.08034	-2.30391	2.69926
F	4.91124	-1.80377	-0.05860	H	0.26992	-1.68900	1.73703
F	4.84251	0.79154	0.78155	H	-0.54971	-0.62250	2.87867
F	-0.24355	-0.45056	1.69934	H	-5.67269	-2.03413	-0.96138
F	-2.38322	-1.86984	2.43212	H	-4.74410	-3.41892	-0.36782
F	-4.64680	-1.83944	0.91290	H	-5.62326	-2.39785	0.76857
F	-4.71798	-0.34974	-1.36723	H	2.49563	1.42771	2.41423
F	-2.59664	1.07455	-2.12111	H	1.63362	0.01630	2.99329
C	-1.34743	3.52666	-0.49101	H	3.40447	-0.00216	2.92349
C	-0.14037	2.70953	1.53512	H	5.26896	-2.87548	-0.23342
H	-0.06792	1.43214	-1.92980	H	4.45640	-3.23082	-1.76713
H	0.76760	3.34804	-0.29465	H	5.51285	-1.82472	-1.63120
H	-1.40268	4.53967	-0.06723	H	0.71770	-0.68276	-3.19945
H	-1.35540	3.60802	-1.58242	H	-0.54796	-0.60267	-1.96210
H	-2.27017	3.00758	-0.20005	H	0.33652	0.85481	-2.42352
H	-0.15738	3.71354	1.98282	H	1.75066	4.07671	-0.75213
H	0.72324	2.17551	1.94066	H	2.23351	2.37765	-0.93363
H	-1.04135	2.18766	1.88400	H	2.10540	3.09990	0.67756
				H	-0.63595	4.69611	-0.10542
51				H	-1.64935	3.47578	0.68870
<b>7P</b>				H	-0.14590	3.98792	1.44589
P	0.02140	1.10201	0.75188				
C	0.17663	2.68210	-0.25032	52			
C	-1.51520	0.14812	0.29881	<b>[7PH]<sup>+</sup></b>			
C	1.40850	0.04158	0.10322	P	0.00379	0.94096	0.41772
C	2.46543	-0.22204	1.00394	C	0.05343	2.67548	-0.19376
C	3.53289	-1.02799	0.60165	C	-1.55488	0.04365	0.18188
C	3.59934	-1.58106	-0.67247	C	1.50560	0.01277	0.03054
C	2.56228	-1.29977	-1.55776	C	2.49424	-0.16255	1.02878
C	1.47771	-0.49861	-1.19924	C	3.62844	-0.90231	0.70103

C	3.82098	-1.45692	-0.56404	C	-1.965323	1.310852	0.768658
C	2.83884	-1.24957	-1.53172	C	-2.610568	-1.179256	-0.001494
C	1.68484	-0.52053	-1.26338	C	-3.977484	-1.160489	0.258224
C	-2.51161	0.34342	-0.81741	C	-4.905596	-1.926838	-0.437208
C	-3.67393	-0.42544	-0.86083	C	-4.473372	-2.755472	-1.463248
C	-3.92539	-1.46515	0.03169	C	-3.123329	-2.796465	-1.776864
C	-2.96243	-1.74413	0.99882	C	-2.240959	-2.009263	-1.050060
C	-1.78275	-1.01333	1.09862	C	-1.958212	2.215899	1.826544
C	-2.37948	1.43234	-1.85711	C	-2.266593	3.567509	1.694289
C	-0.81107	-1.38272	2.19384	C	-2.594160	4.078884	0.449510
C	-5.20638	-2.24895	-0.03275	C	-2.602180	3.226297	-0.645073
C	2.40269	0.40307	2.42818	C	-2.297436	1.885504	-0.459292
C	5.07157	-2.22659	-0.88624	F	-1.624458	1.830411	3.071276
C	0.68594	-0.30058	-2.36956	F	-2.290554	1.130951	-1.576489
C	1.47049	3.23294	-0.01959	F	-2.237283	4.378535	2.755441
C	-0.98093	3.49355	0.59097	F	-2.881020	5.372878	0.301361
H	0.07323	1.13624	1.80037	F	-2.888119	3.704038	-1.860079
H	-0.19387	2.66401	-1.25654	F	-4.464587	-0.359925	1.218154
H	4.39088	-1.04817	1.46123	F	-6.204927	-1.872241	-0.138213
H	2.97563	-1.66530	-2.52628	F	-5.345812	-3.501477	-2.142320
H	-4.41069	-0.20277	-1.62756	F	-2.690751	-3.578207	-2.772254
H	-3.13247	-2.55715	1.69925	F	-0.939860	-2.082101	-1.443946
H	-1.45442	1.35266	-2.43127	C	-0.411057	-2.219246	2.131300
H	-3.20234	1.35696	-2.56843	C	-2.377321	-1.112129	3.207220
H	-2.42784	2.43282	-1.41949	H	-0.507686	-0.323793	0.138650
H	-1.13391	-2.30109	2.68457	H	-0.488433	-0.202510	2.803994
H	0.20080	-1.55367	1.81333	H	-0.985392	-2.936636	1.529133
H	-0.76410	-0.60624	2.96660	H	0.551061	-2.063257	1.626992
H	-5.62138	-2.24968	-1.04220	H	-0.199201	-2.696513	3.096914
H	-5.05361	-3.28289	0.28266	H	-2.947162	-0.191274	3.349170
H	-5.95267	-1.80571	0.63421	H	-2.071855	-1.479083	4.195529
H	2.29779	1.49168	2.43104	H	-3.058533	-1.858664	2.781154
H	1.56514	-0.01847	2.99319	P	2.427064	-0.877262	-0.506728
H	3.31279	0.16762	2.98021	C	2.546535	-2.517685	-1.336047
H	5.47671	-2.71473	0.00202	C	3.080842	-0.797359	1.191418
H	4.88360	-2.98659	-1.64691	C	2.996851	0.451129	-1.607936
H	5.84068	-1.55120	-1.27439	C	2.036025	1.259770	-2.260320
H	1.00418	-0.80917	-3.28017	C	2.495888	2.264827	-3.111105
H	-0.30735	-0.67730	-2.10725	C	3.850994	2.492309	-3.338027
H	0.60271	0.76545	-2.61181	C	4.773733	1.674239	-2.690103
H	1.48592	4.26424	-0.38057	C	4.374104	0.652214	-1.833455
H	2.21232	2.66088	-0.58087	C	3.970817	-1.735802	1.762715
H	1.76474	3.25148	1.03440	C	4.259751	-1.623431	3.123693
H	-1.06371	4.49072	0.15234	C	3.709478	-0.632059	3.929646
H	-1.97496	3.03820	0.59430	C	2.872755	0.306807	3.332524
H	-0.66000	3.61206	1.63045	C	2.548029	0.254037	1.980446
				C	4.668556	-2.853452	1.019871
				C	1.650148	1.329558	1.422224
				C	4.000026	-0.575130	5.404407
				C	0.546923	1.123126	-2.067967
				C	4.300189	3.575374	-4.281310

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**7PHBH**

B	-1.525440	-0.272239	0.820435
C	-1.169515	-0.897740	2.290378

C	5.433815	-0.213101	-1.202347
C	2.024068	-2.380809	-2.772399
C	1.726343	-3.550744	-0.550213
H	1.034017	-0.692948	-0.342312
H	3.601388	-2.800953	-1.364978
H	1.762469	2.893243	-3.609458
H	5.836172	1.832802	-2.855828
H	4.941028	-2.344553	3.567390
H	2.451272	1.107060	3.934882
H	5.163670	-2.504468	0.112718
H	5.439533	-3.284381	1.660217
H	3.990328	-3.663997	0.744762
H	1.408801	2.056586	2.199077
H	2.127176	1.863730	0.593214
H	0.699600	0.914280	1.072654
H	4.888253	-1.156654	5.658867
H	4.151336	0.454753	5.736156
H	3.156815	-0.982082	5.971126
H	0.172986	0.105656	-2.211179
H	0.246997	1.423997	-1.058755
H	0.013849	1.767959	-2.767653
H	3.672437	4.464219	-4.186179
H	5.337004	3.861191	-4.093573
H	4.229374	3.231949	-5.318288
H	6.428596	0.165131	-1.442269
H	5.340346	-0.246309	-0.113127
H	5.377682	-1.238256	-1.585785
H	2.107596	-3.353800	-3.263958
H	2.593357	-1.651537	-3.353449
H	0.967129	-2.100937	-2.776722
H	1.911169	-4.543586	-0.969817
H	1.966143	-3.574643	0.515213
H	0.661674	-3.328551	-0.643693

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**8H<sub>2</sub>**

C	0.617878	-1.407299	0.463737
B	-0.353607	-0.498745	-0.545085
P	2.304132	-1.226145	-0.108263
C	3.418938	-0.674210	1.270294
C	2.870633	-2.679762	-1.114757
C	4.063334	-2.283035	-1.997271
C	1.700502	-3.070435	-2.035453
C	3.237204	-3.857038	-0.204100
C	3.327517	-1.635455	2.463300
C	2.885824	0.707423	1.696714
C	4.871386	-0.540251	0.801008
C	-1.936656	-0.727201	-0.262249
C	0.027769	1.076443	-0.316900
C	-0.232635	1.714869	0.891737

C	0.088789	3.039348	1.154230
C	0.707667	3.789797	0.162270
C	1.002924	3.198693	-1.058028
C	0.656944	1.867450	-1.271768
C	-2.502326	-1.348531	0.843442
C	-3.872914	-1.498387	1.023547
C	-4.742843	-0.995242	0.068936
C	-4.228797	-0.352281	-1.049117
C	-2.852840	-0.229495	-1.185970
F	-1.723656	-1.856258	1.818670
F	-4.356475	-2.114793	2.104609
F	-6.059841	-1.126425	0.223076
F	-5.059097	0.140271	-1.970192
F	-2.408749	0.413554	-2.275053
F	-0.764201	1.010600	1.907878
F	-0.169778	3.591667	2.340117
F	1.031098	5.061348	0.387073
F	1.614127	3.909704	-2.006715
F	1.016770	1.345090	-2.455823
H	0.357909	-2.469999	0.452643
H	0.554357	-1.064774	1.499369
H	-0.112264	-0.795325	-1.693116
H	2.364544	-0.163667	-1.026611
H	4.310780	-3.132100	-2.642667
H	4.955978	-2.035587	-1.421190
H	3.817692	-1.435954	-2.644594
H	2.030800	-3.905763	-2.661627
H	0.817318	-3.390865	-1.478799
H	1.404083	-2.245176	-2.687537
H	2.433768	-4.097685	0.499687
H	3.411385	-4.741192	-0.825499
H	4.153382	-3.664183	0.361070
H	3.898090	-1.209453	3.294937
H	3.748541	-2.618126	2.240718
H	2.296203	-1.767064	2.801062
H	3.545699	1.104183	2.474909
H	2.869655	1.422507	0.866567
H	1.877169	0.645885	2.114301
H	4.959299	0.076382	-0.099379
H	5.452256	-0.056712	1.592977
H	5.327828	-1.514662	0.607756

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**[8H]<sup>+</sup>**

C	-0.794043	-1.126060	-0.890881
B	0.325661	-0.083238	-0.431594
P	-2.354970	-1.146457	0.030558
C	-3.666781	-1.917853	-1.027642
C	-2.086018	-1.810471	1.738928
C	-3.280754	-1.436644	2.631412
C	-0.824838	-1.118093	2.285539



C	-1.875886	-3.329776	1.703328	B	-0.310316	-0.379949	-0.759968
C	-3.133835	-3.217582	-1.649485	P	2.548399	-0.720321	-0.235569
C	-3.989422	-0.900419	-2.136661	C	3.328226	-1.213077	1.437643
C	-4.932414	-2.194875	-0.205764	C	3.210095	-1.897261	-1.576753
C	1.808660	-0.558841	-0.362505	C	4.567884	-1.373027	-2.065407
C	-0.075329	1.407218	-0.170336	C	2.219632	-1.776626	-2.745186
C	-1.132132	2.036418	-0.835878	C	3.340694	-3.372891	-1.196160
C	-1.486110	3.359733	-0.630620	C	2.897046	-2.558272	2.033082
C	-0.770348	4.110183	0.297074	C	2.870795	-0.094156	2.391536
C	0.280722	3.529335	1.000536	C	4.856722	-1.165290	1.352273
C	0.610815	2.205620	0.753920	C	-1.868270	-0.784194	-0.404154
C	2.181631	-1.871299	-0.041095	C	-0.082567	1.177298	-0.290502
C	3.493382	-2.311436	-0.016790	C	-0.230575	1.571367	1.034070
C	4.508751	-1.422010	-0.355382	C	0.027468	2.855247	1.498042
C	4.197685	-0.109326	-0.692799	C	0.449483	3.821536	0.598106
C	2.872433	0.297948	-0.684378	C	0.614186	3.481122	-0.736028
F	1.249377	-2.771883	0.319251	C	0.349686	2.180664	-1.150460
F	3.784337	-3.558570	0.320041	C	-2.310954	-1.764248	0.477270
F	5.762443	-1.823113	-0.350303	C	-3.654789	-2.049031	0.706820
F	5.161488	0.734626	-1.021478	C	-4.631662	-1.326391	0.043740
F	2.636140	1.560208	-1.033254	C	-4.246751	-0.330586	-0.842135
F	-1.862885	1.349799	-1.733967	C	-2.894634	-0.085516	-1.039664
F	-2.492400	3.905000	-1.297269	F	-1.444835	-2.523726	1.173194
F	-1.096120	5.367007	0.516803	F	-4.015378	-3.013780	1.565517
F	0.948485	4.239034	1.894530	F	-5.929348	-1.585768	0.251813
F	1.611004	1.687100	1.462542	F	-5.183670	0.376935	-1.489337
H	-0.426261	-2.153547	-0.914877	F	-2.594967	0.894191	-1.907723
H	-1.060295	-0.845837	-1.918913	F	-0.622753	0.674244	1.963149
H	-2.761592	0.180119	0.237664	F	-0.129281	3.173686	2.790714
H	-3.048741	-1.750275	3.653399	F	0.699858	5.070354	1.013496
H	-4.204114	-1.935908	2.337892	F	1.030730	4.413737	-1.604510
H	-3.453667	-0.356191	2.650694	F	0.558750	1.926468	-2.450009
H	-0.705841	-1.405536	3.334497	H	0.713530	-2.374704	-0.235278
H	0.076525	-1.441651	1.759165	H	0.616773	-1.236785	1.086924
H	-0.900186	-0.025746	2.252852	H	-0.209395	-0.435385	-1.965173
H	-1.049143	-3.616418	1.046447	H	4.909366	-1.968388	-2.923371
H	-1.622216	-3.666150	2.713050	H	5.340037	-1.430231	-1.293531
H	-2.779949	-3.862626	1.397413	H	4.486278	-0.329494	-2.384029
H	-3.933321	-3.657985	-2.252450	H	2.631778	-2.290206	-3.624611
H	-2.842154	-3.955786	-0.898290	H	1.252761	-2.223879	-2.503053
H	-2.284972	-3.036492	-2.313792	H	2.033493	-0.729859	-3.007673
H	-4.748848	-1.342267	-2.788391	H	2.413744	-3.760990	-0.762160
H	-4.392083	0.033179	-1.734327	H	3.567354	-3.969571	-2.091024
H	-3.122393	-0.663730	-2.758851	H	4.152153	-3.537737	-0.480362
H	-5.298079	-1.301374	0.309580	H	3.301894	-2.655824	3.050313
H	-5.718072	-2.522595	-0.892829	H	3.265653	-3.405063	1.450527
H	-4.782218	-2.993636	0.524485	H	1.809172	-2.641544	2.099021
				H	3.280412	-0.270234	3.395319
				H	3.216562	0.884278	2.043346
				H	1.779974	-0.049658	2.478325
				H	5.200642	-0.242779	0.871124
54							
[8H] <sup>-</sup>							
C	0.803802	-1.307601	0.010491				

H 5.290126 -1.203592 2.361037  
H 5.258251 -2.015266 0.791208

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**8**

C 0.843767 -1.125497 -0.869957  
B -0.273925 -0.107445 -0.467052  
P 2.452038 -0.936849 0.082123  
C 2.037920 -1.839018 1.698274  
C 3.585226 -2.022705 -0.987250  
C 4.822768 -2.429929 -0.178712  
C 4.046074 -1.092795 -2.123334  
C 2.946701 -3.268566 -1.610273  
C 3.192585 -1.595914 2.683747  
C 0.798343 -1.126109 2.263809  
C 1.744248 -3.337368 1.602178  
C 0.115837 1.401871 -0.220705  
C -1.791697 -0.537730 -0.382197  
C -2.831860 0.349926 -0.683883  
C -4.170751 -0.012402 -0.677622  
C -4.521920 -1.313977 -0.346423  
C -3.531604 -2.232633 -0.028067  
C -2.202417 -1.836542 -0.063522  
C -0.494326 2.161080 0.778720  
C -0.126615 3.464630 1.072446  
C 0.885328 4.063286 0.332405  
C 1.516282 3.352787 -0.679589  
C 1.130768 2.043930 -0.930847  
F -1.469069 1.624484 1.520202  
F -0.728176 4.143136 2.045340  
F 1.246592 5.312225 0.591453  
F 2.478755 3.928802 -1.393587  
F 1.767600 1.414905 -1.924215  
F -2.570950 1.613834 -1.022055  
F -5.115347 0.869604 -0.987389  
F -5.795604 -1.676137 -0.329513  
F -3.861262 -3.477657 0.301180  
F -1.309732 -2.775148 0.274350  
H 0.500218 -2.159627 -0.916725  
H 1.125298 -0.827311 -1.891758  
H 5.580233 -2.841939 -0.855998  
H 4.592020 -3.200460 0.562085  
H 5.267948 -1.573138 0.338502  
H 4.713131 -1.641789 -2.798593  
H 3.205253 -0.721640 -2.718606  
H 4.586083 -0.225593 -1.733232  
H 2.142716 -3.006189 -2.303411  
H 3.705893 -3.813050 -2.185262  
H 2.541972 -3.953928 -0.862761  
H 2.919885 -1.992389 3.669003  
H 4.116049 -2.089288 2.374489

H 3.398459 -0.526736 2.792359  
H 0.631741 -1.445251 3.299126  
H -0.105593 -1.384841 1.704216  
H 0.920574 -0.036815 2.268654  
H 2.633689 -3.909366 1.324279  
H 1.409428 -3.708340 2.579200  
H 0.950855 -3.552733 0.880775

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**8P**

C -2.900428 0.664447 -1.033563  
P -2.683403 -0.564010 0.399671  
C -2.468207 2.108883 -0.759605  
C -2.184521 0.138779 -2.282920  
C -4.412675 0.659239 -1.317708  
C -0.833098 -0.880922 0.683605  
C 0.104446 0.321114 0.553591  
C -0.725139 -1.431965 2.115546  
C -0.385285 -1.991576 -0.278159  
C -3.070117 0.549163 1.838393  
H -2.666953 2.720938 -1.648403  
H -3.030378 2.548521 0.069289  
H -1.404055 2.193516 -0.531720  
H -2.500796 0.719105 -3.158186  
H -2.427288 -0.912446 -2.472530  
H -1.097860 0.232549 -2.203127  
H -4.761324 -0.339219 -1.595755  
H -4.992723 0.989783 -0.449573  
H -4.634937 1.345610 -2.143734  
H 1.116248 0.031249 0.864474  
H 0.170852 0.679872 -0.476978  
H -0.206954 1.155828 1.189747  
H 0.281918 -1.834834 2.274837  
H -1.442111 -2.241394 2.292171  
H -0.892856 -0.652801 2.864406  
H -1.014774 -2.879914 -0.170173  
H -0.422489 -1.676156 -1.323446  
H 0.649785 -2.277193 -0.054090  
H -2.328502 1.337963 1.999023  
H -3.152772 -0.050033 2.747093  
H -4.042418 1.019779 1.669377

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**[8PH]<sup>+</sup>**

C -2.899758 0.702065 -1.079616  
P -2.515467 -0.314993 0.418138  
C -2.489309 2.161195 -0.829404  
C -2.180419 0.137409 -2.311796  
C -4.422260 0.609845 -1.288081  
C -0.777017 -0.879369 0.708731  
C 0.198053 0.298643 0.580086

C -0.734159 -1.447225 2.138994  
 C -0.429611 -1.995332 -0.289204  
 C -3.145427 0.535438 1.892108  
 H -3.267386 -1.493248 0.285547  
 H -2.724549 2.738848 -1.728032  
 H -3.043844 2.608815 -0.000015  
 H -1.418793 2.270321 -0.639351  
 H -2.528806 0.688488 -3.190238  
 H -2.407470 -0.920482 -2.476267  
 H -1.096991 0.265732 -2.253044  
 H -4.744064 -0.411499 -1.509840  
 H -4.991348 0.982324 -0.431757  
 H -4.685098 1.235065 -2.146321  
 H 1.194529 -0.048608 0.868447  
 H 0.263569 0.670527 -0.445409  
 H -0.061291 1.130246 1.243103  
 H 0.252268 -1.892862 2.295781  
 H -1.477223 -2.236183 2.297068  
 H -0.869398 -0.671963 2.897163  
 H -1.115696 -2.843577 -0.206609  
 H -0.417278 -1.650453 -1.323937  
 H 0.574099 -2.360140 -0.052340  
 H -2.467831 1.349540 2.160665  
 H -3.214595 -0.165674 2.724753  
 H -4.135910 0.947106 1.690656

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**8PHBH**

C -2.790120 2.254986 -1.363403  
 P -1.527045 1.850499 -0.070658  
 C -2.054319 2.122368 -2.711487  
 C -3.926187 1.221388 -1.302985  
 C -3.338125 3.680869 -1.223886  
 C -2.122727 1.724857 1.692739  
 C -2.459824 0.239762 1.913015  
 C -1.006143 2.161818 2.656307  
 C -3.347407 2.610204 1.958708  
 C -0.110120 2.970288 -0.231055  
 H -1.059460 0.580324 -0.418529  
 H -2.792902 2.246492 -3.509953  
 H -1.296578 2.900824 -2.838681  
 H -1.581240 1.144309 -2.827294  
 H -4.610133 1.420812 -2.134353  
 H -4.506737 1.288215 -0.379987  
 H -3.556247 0.199996 -1.418797  
 H -3.964968 3.809408 -0.340516  
 H -2.540743 4.430175 -1.203813  
 H -3.956793 3.891285 -2.102062  
 H -2.821260 0.106994 2.937552  
 H -3.241512 -0.113863 1.231792  
 H -1.573450 -0.388886 1.775855

H -0.084648 1.593627 2.531485  
 H -1.368431 1.998889 3.676230  
 H -0.783723 3.228282 2.552686  
 H -3.129445 3.668944 1.788642  
 H -4.216637 2.327539 1.362360  
 H -3.621064 2.496486 3.012247  
 H 0.588509 2.773960 0.583259  
 H -0.428056 4.014427 -0.206473  
 H 0.388044 2.743422 -1.176796  
 C 0.249977 -2.439372 0.375425  
 C -0.073194 -1.682574 -0.748908  
 C -1.417813 -1.747724 -1.098035  
 C -2.388614 -2.443409 -0.389770  
 C -2.013836 -3.170138 0.729755  
 C -0.678454 -3.171071 1.111002  
 C 2.043941 0.356168 0.456491  
 C 3.013135 0.972821 1.226532  
 C 4.323187 0.971580 0.769882  
 C 4.602024 0.356134 -0.440804  
 C 3.576589 -0.232265 -1.181053  
 C 2.245266 -0.250278 -0.774465  
 B 0.961253 -0.774564 -1.658155  
 C 1.322178 -1.570893 -3.023884  
 F 0.783447 0.392450 0.982443  
 F 3.953583 -0.781363 -2.342236  
 F 5.856104 0.345349 -0.895092  
 F 5.289989 1.555951 1.477471  
 F 2.685315 1.580122 2.376630  
 F 1.511921 -2.481860 0.824340  
 F -1.867819 -1.049346 -2.168010  
 F -3.676929 -2.377425 -0.751013  
 F -2.921221 -3.847625 1.433439  
 F -0.302575 -3.870691 2.182596  
 H 0.349860 0.263804 -1.931122  
 H 0.401468 -1.870610 -3.538405  
 H 1.901189 -2.482636 -2.838278  
 H 1.901536 -0.960082 -3.722245

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**9H<sub>2</sub>**

C -0.030303 -0.742016 0.614752  
 B 1.138464 -0.281769 -0.520963  
 P -1.633259 -0.416082 -0.091599  
 C -2.416591 -1.965991 -0.754814  
 C -2.695490 0.634752 1.013829  
 C -4.103110 0.823828 0.438944  
 C -1.984635 2.000471 1.074596  
 C -2.773397 0.037116 2.424575  
 C -3.485391 -1.621751 -1.802428  
 C -1.309534 -2.778827 -1.449882

C	-3.025733	-2.788538	0.386734	C	1.691289	-1.065835	1.599362
C	1.093998	1.343754	-0.568910	C	3.230585	-0.271405	-1.069885
C	2.584480	-0.852384	-0.081414	C	4.500469	-0.142829	-0.218922
C	2.895883	-1.310659	1.205381	C	3.156364	0.908748	-2.055498
C	4.172997	-1.757944	1.548408	C	3.231747	-1.597826	-1.843612
C	5.187235	-1.760186	0.598017	C	2.642511	-0.383262	2.595426
C	4.910313	-1.308857	-0.692565	C	0.253499	-0.960295	2.138462
C	3.633180	-0.865398	-1.016344	C	2.073703	-2.537231	1.396312
C	0.527079	2.059525	-1.633501	C	-1.160994	1.590759	-0.168823
C	0.383777	3.448786	-1.606850	C	-2.417496	-0.816617	-0.453049
C	0.818032	4.169840	-0.499055	C	-2.365411	-2.222141	-0.371842
C	1.416219	3.491731	0.564260	C	-3.519277	-2.992676	-0.339877
C	1.551002	2.107376	0.519593	C	-4.766041	-2.371784	-0.416271
H	0.024298	-1.803517	0.879019	C	-4.851782	-0.985458	-0.517650
H	0.075977	-0.154938	1.533341	C	-3.691621	-0.219572	-0.527257
H	0.807332	-0.722180	-1.616036	C	-1.927283	2.080634	0.903822
H	-1.482691	0.390200	-1.231446	C	-1.907109	3.428895	1.250351
H	-4.624700	1.579663	1.035373	C	-1.140070	4.325005	0.510401
H	-4.693038	-0.095724	0.484559	C	-0.381490	3.869418	-0.567623
H	-4.079097	1.178347	-0.596589	C	-0.382290	2.517028	-0.888064
H	-2.570121	2.662156	1.721794	H	0.223574	-1.663348	-1.094728
H	-0.974219	1.928693	1.485797	H	0.429134	-0.174749	-1.999751
H	-1.898484	2.468531	0.088751	H	1.611596	1.200085	0.345789
H	-1.780534	-0.108715	2.857460	H	5.359595	-0.078983	-0.893350
H	-3.318413	0.735794	3.067930	H	4.653225	-1.013039	0.423964
H	-3.303685	-0.917881	2.445656	H	4.497570	0.761052	0.398199
H	-3.856160	-2.555677	-2.237579	H	4.035184	0.868306	-2.705841
H	-4.340586	-1.091650	-1.381159	H	2.275108	0.861133	-2.702185
H	-3.067559	-1.021005	-2.615802	H	3.164415	1.874407	-1.541031
H	-1.768543	-3.679441	-1.871603	H	2.367278	-1.686670	-2.506980
H	-0.519665	-3.088340	-0.762455	H	4.129854	-1.630333	-2.467575
H	-0.839346	-2.215024	-2.258659	H	3.257699	-2.467594	-1.182640
H	-3.903059	-2.299396	0.819557	H	2.536481	-0.885019	3.561841
H	-3.347520	-3.757330	-0.008962	H	3.690195	-0.455363	2.302494
H	-2.300704	-2.978774	1.184747	H	2.387748	0.670655	2.742062
H	2.123442	-1.323389	1.973636	H	0.234912	-1.388297	3.145286
H	4.373749	-2.105690	2.558341	H	-0.462462	-1.519490	1.530348
H	6.182560	-2.109004	0.856606	H	-0.083914	0.079606	2.214535
H	5.694333	-1.305550	-1.445024	H	3.121697	-2.653882	1.107889
H	3.431993	-0.514536	-2.026726	H	1.931602	-3.065854	2.343634
H	0.197887	1.509173	-2.514398	H	1.444508	-3.031154	0.648360
H	-0.060224	3.967320	-2.452635	H	-1.405174	-2.731292	-0.316259
H	0.710679	5.250015	-0.469865	H	-3.453456	-4.072636	-0.263053
H	1.781169	4.048000	1.423568	H	-5.670235	-2.971654	-0.401750
H	2.031426	1.592175	1.351649	H	-5.821260	-0.504252	-0.588611
				H	-3.768675	0.859931	-0.615143
				H	-2.539787	1.390033	1.478337
				H	-2.497416	3.782349	2.089115
				H	-1.135082	5.378635	0.769362
				H	0.204688	4.569226	-1.154092
				H	0.213655	2.182050	-1.736584
54							
[9H] <sup>+</sup>							
C	0.249434	-0.574000	-0.991116				
B	-1.146542	0.067086	-0.506640				
P	1.712535	-0.153109	-0.012422				

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[9H]<sup>-</sup>

C	-0.175280	-0.606171	0.348019
B	1.110797	-0.267169	-0.642325
P	-1.788682	-0.071117	-0.395212
C	-2.585261	-1.743464	-0.850946
C	-2.708219	0.641390	1.121719
C	-4.196834	0.825830	0.812404
C	-2.074761	2.036389	1.280418
C	-2.564551	-0.110434	2.449521
C	-3.832443	-1.483640	-1.707491
C	-1.556395	-2.453896	-1.745427
C	-2.954409	-2.667260	0.310784
C	1.285155	1.358529	-0.609584
C	2.474893	-0.997723	-0.124571
C	2.633620	-1.561046	1.150868
C	3.827701	-2.152891	1.568670
C	4.921006	-2.202236	0.710258
C	4.801059	-1.649690	-0.565702
C	3.603359	-1.063892	-0.962139
C	0.697463	2.194581	-1.572576
C	0.737661	3.585616	-1.480244
C	1.380600	4.197930	-0.406901
C	1.982458	3.398926	0.563790
C	1.931677	2.010273	0.454909
H	-0.233306	-1.664138	0.645722
H	-0.038448	-0.041205	1.280526
H	0.887639	-0.619992	-1.797272
H	-4.661801	1.472940	1.569306
H	-4.733702	-0.128763	0.824360
H	-4.345038	1.291430	-0.168474
H	-2.526766	2.556120	2.136698
H	-0.992913	1.980560	1.445525
H	-2.228942	2.642576	0.382554
H	-1.516381	-0.292661	2.699002
H	-3.002157	0.488327	3.261350
H	-3.080040	-1.073205	2.437410
H	-4.229103	-2.435148	-2.088847
H	-4.630696	-0.994121	-1.143171
H	-3.586978	-0.847689	-2.563513
H	-2.007101	-3.364390	-2.164628
H	-0.655336	-2.734557	-1.194812
H	-1.239133	-1.809923	-2.571459
H	-3.811904	-2.283059	0.872799
H	-3.231841	-3.660259	-0.071372
H	-2.117641	-2.796452	1.004591
H	1.793256	-1.538352	1.843116
H	3.903351	-2.577445	2.567848
H	5.852985	-2.663549	1.027315
H	5.646706	-1.679404	-1.249945

H	3.524407	-0.636519	-1.960643
H	0.181769	1.729357	-2.409774
H	0.263952	4.195174	-2.247153
H	1.415129	5.281821	-0.328714
H	2.493662	3.861298	1.405880
H	2.411633	1.401119	1.220927

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C	0.413284	0.048043	-0.924317
B	-1.079736	0.185924	-0.424396
P	1.724714	0.243909	0.416733
C	2.025250	-1.543937	0.974511
C	3.191195	0.815075	-0.656712
C	4.496506	0.648439	0.130677
C	2.957962	2.322012	-0.862775
C	3.335965	0.154491	-2.031682
C	2.893253	-1.494660	2.242130
C	0.649748	-2.098845	1.373072
C	2.653481	-2.495155	-0.045787
C	-1.662582	1.591432	-0.037404
C	-2.022542	-1.071336	-0.403080
C	-1.938127	-2.064475	-1.392814
C	-2.750554	-3.193301	-1.362257
C	-3.649731	-3.372604	-0.313207
C	-3.743644	-2.411307	0.690065
C	-2.950613	-1.268896	0.633087
C	-3.044262	1.839567	-0.132366
C	-3.580837	3.097195	0.127490
C	-2.743647	4.142784	0.505784
C	-1.370471	3.927864	0.609034
C	-0.841168	2.673000	0.330934
H	0.598042	-0.876279	-1.484582
H	0.609397	0.889771	-1.600900
H	5.302876	1.187126	-0.381469
H	4.798807	-0.399699	0.204764
H	4.411358	1.056798	1.143481
H	3.773637	2.742143	-1.463352
H	2.021632	2.527801	-1.393247
H	2.928372	2.852786	0.093797
H	2.449125	0.305756	-2.652989
H	4.184670	0.606125	-2.560572
H	3.523412	-0.918239	-1.962901
H	2.996610	-2.507232	2.650516
H	3.897732	-1.111476	2.050334
H	2.430438	-0.864828	3.007620
H	0.784317	-3.020743	1.951227
H	0.040356	-2.339695	0.499454
H	0.087838	-1.393443	1.997586
H	3.694297	-2.239131	-0.261668
H	2.644298	-3.516266	0.355862

H 2.096913 -2.509598 -0.988661  
H -1.228070 -1.947787 -2.208093  
H -2.677356 -3.938076 -2.148658  
H -4.274416 -4.259762 -0.277651  
H -4.438897 -2.549662 1.512189  
H -3.038394 -0.518194 1.414640  
H -3.707824 1.034187 -0.433754  
H -4.649968 3.261245 0.035841  
H -3.158473 5.123922 0.716500  
H -0.713888 4.740325 0.904303  
H 0.230337 2.521556 0.425067

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**9B**

C 3.75632 0.23595 0.41098  
C 2.54189 0.91137 0.44507  
C 1.35929 0.32680 -0.04062  
C 1.45643 -0.96269 -0.59125  
C 2.67225 -1.63735 -0.65302  
C 3.82264 -1.04129 -0.14309  
C -2.71508 -1.55956 0.73716  
C -3.83634 -1.00663 0.12324  
C -3.73448 0.21732 -0.53449  
C -2.51637 0.88764 -0.56357  
C -1.36295 0.34483 0.02730  
C -1.49351 -0.89635 0.67527  
B 0.00293 1.11369 -0.00356  
C 0.02997 2.68941 0.06397  
H 4.65224 0.70398 0.80672  
H 2.50630 1.91330 0.86565  
H 0.56411 -1.43626 -0.99159  
H 2.72320 -2.62735 -1.09531  
H 4.77115 -1.56827 -0.18160  
H -2.79295 -2.50872 1.25812  
H -4.78875 -1.52657 0.16007  
H -4.60639 0.65073 -1.01435  
H -2.45531 1.84739 -1.06965  
H -0.62272 -1.33906 1.15156  
H 0.83095 3.13349 -0.53379  
H 0.24022 2.96137 1.10932  
H -0.91721 3.17082 -0.18909

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**[9BH]<sup>-</sup>**

C 4.066633 1.397372 -1.125306  
C 3.364397 0.233343 -0.817977  
C 2.095036 0.247781 -0.215604  
C 1.568076 1.522276 0.056014  
C 2.253552 2.698523 -0.243920  
C 3.512498 2.643793 -0.838974  
C -2.235603 -0.462672 -1.334608

C -3.101657 -0.653818 -0.256564  
C -2.565361 -0.994129 0.981025  
C -1.184504 -1.141809 1.132239  
C -0.282931 -0.964639 0.071868  
C -0.863742 -0.615382 -1.162386  
B 1.336967 -1.138334 0.211764  
C 1.793591 -1.534292 1.738206  
H 5.046893 1.335638 -1.594995  
H 3.807627 -0.733627 -1.052545  
H 0.580785 1.586235 0.512130  
H 1.804325 3.663618 -0.016357  
H 4.051107 3.557359 -1.079608  
H -2.636737 -0.192582 -2.309806  
H -4.175453 -0.536529 -0.382009  
H -3.224909 -1.143268 1.834263  
H -0.790733 -1.407148 2.111682  
H -0.200781 -0.456070 -2.012127  
H 1.694373 -2.018306 -0.572593  
H 1.510697 -0.764763 2.473513  
H 2.883555 -1.647123 1.811268  
H 1.351878 -2.481460 2.081407

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**9P**

C -1.54981 -0.25359 0.01386  
C -1.83142 0.09414 1.47948  
C -2.71296 0.28014 -0.84045  
P 0.00092 0.53190 -0.75335  
C -1.50063 -1.77626 -0.15589  
C 1.55031 -0.24975 0.01677  
C -0.01781 2.18266 0.10295  
C 2.68909 0.75044 -0.24507  
C 1.50319 -0.55076 1.51609  
C 1.87238 -1.53604 -0.75835  
H -2.76106 -0.39570 1.79554  
H -1.03790 -0.23914 2.15087  
H -1.96766 1.17022 1.62042  
H -2.78471 1.37207 -0.79655  
H -3.66074 -0.12796 -0.46899  
H -2.60077 -0.00843 -1.88923  
H -2.48538 -2.20247 0.07106  
H -0.77861 -2.24148 0.52103  
H -1.24237 -2.05781 -1.18253  
H -0.99480 2.64892 -0.05034  
H 0.72880 2.83520 -0.35353  
H 0.17146 2.12459 1.17942  
H 2.71312 1.07026 -1.29271  
H 2.60167 1.63977 0.38538  
H 3.65010 0.27464 -0.01721  
H 2.49476 -0.87669 1.85516  
H 1.22983 0.33137 2.10391

H	0.79879	-1.35302	1.75141
H	2.82928	-1.94490	-0.41149
H	1.95611	-1.33599	-1.83075
H	1.11222	-2.30784	-0.61699

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**[9PH]<sup>+</sup>**

C	-1.047209	-1.214272	-0.163508
C	-2.249642	-0.565557	0.538982
C	-1.517219	-1.988472	-1.408365
P	0.100369	0.104365	-0.771417
C	-0.312592	-2.170528	0.785435
C	1.263578	0.913111	0.419404
C	-0.858576	1.366310	-1.654903
C	1.866990	2.125521	-0.312667
C	0.510880	1.376296	1.673965
C	2.387931	-0.070113	0.781414
H	-2.909586	-1.364456	0.889393
H	-1.958727	0.026355	1.410204
H	-2.832263	0.064385	-0.138867
H	-2.034062	-1.353355	-2.133200
H	-2.229669	-2.752186	-1.083237
H	-0.689900	-2.497796	-1.910369
H	0.922957	-0.513126	-1.727092
H	-0.987521	-2.998169	1.022495
H	-0.040319	-1.689627	1.727941
H	0.585264	-2.599080	0.329438
H	-1.606771	0.889426	-2.290427
H	-0.195776	1.968956	-2.277112
H	-1.362822	2.012845	-0.932579
H	2.341520	1.847226	-1.259741
H	1.126805	2.907275	-0.500068
H	2.643744	2.553811	0.327199
H	1.204798	1.946347	2.298640
H	-0.330455	2.035443	1.437132
H	0.145799	0.536458	2.270289
H	3.098656	0.452515	1.428213
H	2.935294	-0.406669	-0.104120
H	2.028524	-0.943236	1.327528

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**9PHBH**

C	4.842037	-2.184415	-0.578310
C	3.505751	-1.886363	-0.324974
C	3.085357	-0.617402	0.102044
C	4.090680	0.348273	0.257502
C	5.433271	0.068598	0.006734
C	5.816579	-1.202152	-0.413553
C	0.742956	3.125317	-1.293837
C	0.477847	3.975610	-0.218372
C	0.551055	3.470129	1.076246

C	0.861957	2.123766	1.287657
C	1.131016	1.236728	0.231801
C	1.067398	1.790692	-1.061737
B	1.525790	-0.334407	0.454616
C	1.197700	-0.844455	1.981590
H	5.126100	-3.180390	-0.909102
H	2.754528	-2.663955	-0.464182
H	3.811425	1.350056	0.580000
H	6.182955	0.845034	0.136754
H	6.860862	-1.424410	-0.613372
H	0.714617	3.512525	-2.309675
H	0.235789	5.020357	-0.389735
H	0.365860	4.124810	1.924296
H	0.913316	1.752382	2.309525
H	1.311986	1.148837	-1.908245
H	1.897891	-0.402845	2.703135
H	1.309180	-1.933101	2.077673
H	0.190777	-0.587321	2.357687
C	-3.252910	0.780237	0.011206
C	-2.556531	2.153244	0.000317
C	-4.310482	0.728706	-1.098624
P	-1.906067	-0.458537	-0.276517
C	-3.895118	0.560814	1.386809
C	-2.302836	-2.234504	0.093000
C	-1.372022	-0.313526	-2.000412
C	-1.219533	-3.100754	-0.574447
C	-2.242611	-2.458658	1.611661
C	-3.680362	-2.617201	-0.461637
H	-2.050305	2.367970	-0.944947
H	-3.318918	2.924261	0.153855
H	-1.808955	2.241491	0.793138
H	-3.874191	0.930050	-2.081154
H	-5.051814	1.510246	-0.903480
H	-4.838162	-0.226911	-1.138351
H	-0.852155	-0.079662	0.562606
H	-4.575686	1.394466	1.587333
H	-3.146032	0.545731	2.185148
H	-4.479167	-0.362033	1.432686
H	-1.263506	0.740990	-2.258323
H	-2.103707	-0.792904	-2.655552
H	-0.395936	-0.794548	-2.086028
H	-1.266150	-3.044677	-1.665744
H	-0.215639	-2.813377	-0.249485
H	-1.399839	-4.141597	-0.286630
H	-2.445699	-3.516436	1.808364
H	-1.249398	-2.225344	2.005003
H	-2.986540	-1.872895	2.155983
H	-3.819952	-3.693782	-0.321045
H	-3.766912	-2.412911	-1.534078
H	-4.494861	-2.107487	0.059624
H	0.863102	-0.998642	-0.362981

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10H<sub>2</sub>

C	1.163374	-3.234128	2.292235
C	1.043182	-1.778392	2.791150
C	0.613608	-0.803009	1.673938
C	-0.814102	-1.306111	1.252526
C	-0.312926	-3.647511	2.005850
C	-1.098485	-2.368424	2.340410
C	-0.305109	-1.834212	3.544457
P	1.561754	-0.530458	0.130094
B	-1.890658	-0.068721	1.197019
C	-1.205862	1.273040	0.516324
C	-3.273661	-0.435415	0.406172
C	2.372218	1.085518	-0.079340
C	2.592394	-1.907264	-0.457759
C	2.097092	-2.768062	-1.462173
C	2.923717	-3.806423	-1.898816
C	4.195726	-4.018730	-1.377385
C	4.651444	-3.160715	-0.375824
C	3.873445	-2.111019	0.098017
C	2.511427	1.532455	-1.417822
C	3.010447	2.809790	-1.648883
C	3.365675	3.664523	-0.605835
C	3.238133	3.196486	0.696740
C	2.745428	1.922893	0.989926
C	-0.699522	2.312211	1.293139
C	-0.103096	3.456058	0.774029
C	-0.004528	3.605131	-0.599694
C	-0.473892	2.592929	-1.423854
C	-1.043421	1.461982	-0.852973
C	-3.605367	-1.644911	-0.193106
C	-4.817252	-1.886045	-0.832880
C	-5.766879	-0.879855	-0.897458
C	-5.488439	0.349787	-0.316443
C	-4.266298	0.539406	0.312898
C	4.399752	-1.257127	1.222051
C	5.064122	-5.146054	-1.867552
C	0.725203	-2.654678	-2.089613
C	2.608561	1.573403	2.452218
C	3.817347	5.071249	-0.882640
C	2.092368	0.709290	-2.612288
F	-1.365686	0.464716	-1.708430
F	-0.296799	2.685382	-2.746744
F	0.586247	4.680531	-1.126115
F	0.423281	4.380937	1.581375
F	-0.701853	2.220624	2.636709
F	-4.055553	1.748952	0.855432
F	-2.748476	-2.691188	-0.183379
F	-5.070184	-3.075113	-1.388097
F	-6.933465	-1.089556	-1.508747
F	-6.394723	1.328614	-0.371512

H	1.590410	-3.845075	3.093180
H	1.815358	-3.350228	1.424774
H	1.896048	-1.436218	3.385227
H	0.520453	0.196841	2.106838
H	-0.752953	-1.814441	0.286070
H	-0.473350	-3.957144	0.968700
H	-0.612836	-4.481153	2.648366
H	-2.166038	-2.525203	2.507628
H	-0.275233	-2.530154	4.389020
H	-0.649023	-0.854025	3.885453
H	0.564653	-0.474365	-0.839121
H	-2.177448	0.232000	2.337546
H	2.551925	-4.474217	-2.671108
H	5.637616	-3.319016	0.053919
H	3.099334	3.157159	-2.674834
H	3.508489	3.847558	1.524233
H	5.390168	-1.596355	1.529050
H	4.475087	-0.203406	0.937826
H	3.744241	-1.327984	2.097136
H	4.556059	-5.736621	-2.631766
H	5.994025	-4.760455	-2.295463
H	5.334962	-5.812746	-1.043940
H	0.566417	-1.690770	-2.582573
H	0.605140	-3.429798	-2.847595
H	-0.079358	-2.785745	-1.360187
H	3.394846	2.071977	3.022986
H	1.646205	1.929479	2.837427
H	2.679954	0.504611	2.651505
H	4.347810	5.139527	-1.834855
H	2.942443	5.726211	-0.937361
H	4.469665	5.444429	-0.090485
H	2.526601	-0.294665	-2.598674
H	1.001192	0.616656	-2.666836
H	2.414068	1.200307	-3.531479

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[10H]<sup>+</sup>

C	-1.013688	-3.734764	-1.084742
C	-0.649896	-2.486202	-1.916603
C	-0.406835	-1.249586	-1.020680
C	0.859680	-1.665173	-0.178450
C	0.323236	-4.103959	-0.377513
C	1.282301	-2.997538	-0.846514
C	0.814820	-2.788661	-2.297221
P	-1.774654	-0.551800	0.006753
B	1.878297	-0.490287	0.051531
C	1.271635	0.964400	0.232692
C	3.424861	-0.644202	0.178958
C	-2.245803	1.156836	-0.380151
C	-3.204767	-1.609937	0.343874



C	-3.233010	-2.335358	1.559710	H	-5.150820	-1.264340	-2.478429
C	-4.366489	-3.087437	1.850284	H	-4.293479	0.114469	-1.782646
C	-5.459508	-3.151446	0.983690	H	-3.393917	-1.244679	-2.480047
C	-5.390110	-2.449697	-0.217477	H	-6.407689	-4.865671	1.879188
C	-4.282774	-1.676933	-0.561393	H	-7.331139	-3.368018	2.004583
C	-2.736065	1.903446	0.723728	H	-7.255766	-4.222754	0.460801
C	-3.082251	3.235891	0.525745	H	-1.905919	-1.395172	3.012917
C	-2.964106	3.856465	-0.718954	H	-2.290967	-3.082117	3.335497
C	-2.492852	3.097321	-1.786015	H	-1.150711	-2.684037	2.057256
C	-2.130146	1.755331	-1.651589	H	-2.113868	1.491131	-3.775158
C	1.245816	1.784610	-0.886040	H	-0.540216	1.261156	-3.023161
C	0.712137	3.064305	-0.874950	H	-1.777365	-0.001843	-2.913214
C	0.195265	3.557948	0.316724	H	-4.102831	5.614597	-0.215398
C	0.190026	2.762943	1.457259	H	-2.421097	5.919718	-0.661162
C	0.716471	1.480160	1.394150	H	-3.603662	5.530915	-1.915816
C	4.089608	-0.103004	1.280781	H	-3.429318	0.403973	2.143883
C	5.464248	-0.180159	1.438198	H	-1.877301	1.159838	2.571271
C	6.221564	-0.792223	0.443704	H	-3.376548	2.053089	2.762606
C	5.602478	-1.321461	-0.684182				
C	4.222261	-1.243069	-0.794717				
C	-4.277456	-0.973609	-1.893616				
C	-6.679304	-3.951671	1.346818				
C	-2.082421	-2.367533	2.538858				
C	-1.613672	1.075430	-2.898426				
C	-3.300770	5.310654	-0.890672				
C	-2.861021	1.339000	2.120098				
F	0.618829	0.697918	2.482051				
F	-0.382087	3.209958	2.569233				
F	-0.338035	4.770429	0.357281				
F	0.642891	3.785622	-1.985813				
F	1.706717	1.285620	-2.048850				
F	3.660945	-1.723366	-1.909854				
F	3.377473	0.484264	2.247394				
F	6.057793	0.319780	2.511644				
F	7.533265	-0.867012	0.568840				
F	6.329909	-1.883075	-1.638550				
H	-1.331701	-4.532543	-1.760215				
H	-1.836003	-3.569595	-0.387351				
H	-1.325045	-2.291458	-2.753781				
H	-0.121542	-0.416505	-1.666435				
H	0.581623	-1.868610	0.876186				
H	0.235229	-4.142175	0.712509				
H	0.681883	-5.082418	-0.706287				
H	2.336050	-3.238103	-0.712039				
H	0.907413	-3.692297	-2.905251				
H	1.315013	-1.958415	-2.803956				
H	-1.177333	-0.419586	1.260565				
H	-4.395085	-3.650857	2.779041				
H	-6.221149	-2.508067	-0.914924				
H	-3.449273	3.809967	1.372152				
H	-2.399221	3.560879	-2.764718				
				82			
				[10H]			
C	1.204442	-3.507573	1.620917	C	1.204442	-3.507573	1.620917
C	1.042689	-2.142543	2.328494	C	1.042689	-2.142543	2.328494
C	0.605198	-1.045285	1.338999	C	0.605198	-1.045285	1.338999
C	-0.806055	-1.535088	0.851248	C	-0.806055	-1.535088	0.851248
C	-0.260960	-3.939848	1.312795	C	-0.260960	-3.939848	1.312795
C	-1.075814	-2.731591	1.800340	C	-1.075814	-2.731591	1.800340
C	-0.292735	-2.350325	3.070376	C	-0.292735	-2.350325	3.070376
P	1.650841	-0.491617	-0.110255	P	1.650841	-0.491617	-0.110255
C	2.282975	1.229673	0.178911	C	2.282975	1.229673	0.178911
C	3.178596	-1.550634	-0.278816	C	3.178596	-1.550634	-0.278816
C	3.114174	-2.504497	-1.326888	C	3.114174	-2.504497	-1.326888
C	4.227714	-3.284916	-1.630304	C	4.227714	-3.284916	-1.630304
C	5.428348	-3.153734	-0.935324	C	5.428348	-3.153734	-0.935324
C	5.480290	-2.228042	0.098568	C	5.480290	-2.228042	0.098568
C	4.382188	-1.432281	0.444432	C	4.382188	-1.432281	0.444432
C	2.656292	1.878736	-1.028983	C	2.656292	1.878736	-1.028983
C	2.913541	3.247177	-1.042170	C	2.913541	3.247177	-1.042170
C	2.794179	4.026681	0.104917	C	2.794179	4.026681	0.104917
C	2.495611	3.377240	1.294422	C	2.495611	3.377240	1.294422
C	2.244386	2.002446	1.361238	C	2.244386	2.002446	1.361238
C	4.543035	-0.500255	1.616390	C	4.543035	-0.500255	1.616390
C	6.628791	-3.986749	-1.305174	C	6.628791	-3.986749	-1.305174
C	1.847632	-2.733698	-2.119456	C	1.847632	-2.733698	-2.119456
C	1.920662	1.476331	2.742031	C	1.920662	1.476331	2.742031
C	2.900183	5.526434	0.043349	C	2.900183	5.526434	0.043349
C	2.726238	1.142323	-2.347367	C	2.726238	1.142323	-2.347367
H	1.689586	-4.219327	2.297765	H	1.689586	-4.219327	2.297765
H	1.828838	-3.445825	0.728290	H	1.828838	-3.445825	0.728290
H	1.902923	-1.872773	2.951327	H	1.902923	-1.872773	2.951327
H	0.427615	-0.132001	1.909001	H	0.427615	-0.132001	1.909001

H	-0.733131	-1.903394	-0.179380	H	-2.081737	-0.081600	2.154457
H	-0.434705	-4.136294	0.250110				
H	-0.522185	-4.850550	1.865420	81			
H	-2.138971	-2.941557	1.947061	10			
H	-0.250168	-3.161945	3.807667	C	-1.037698	-3.828424	0.195880
H	-0.664163	-1.438513	3.545973	C	-0.427582	-2.871409	-0.851455
H	4.154486	-4.016563	-2.432904	C	-0.297662	-1.435491	-0.301342
H	6.401279	-2.122724	0.669123	C	0.721669	-1.653587	0.912248
H	3.161185	3.725460	-1.987599	C	0.116379	-4.040500	1.220468
H	2.418197	3.961182	2.210007	C	1.213855	-3.102722	0.689671
H	5.507472	-0.664512	2.103595	C	1.051001	-3.302983	-0.828878
H	4.477925	0.549278	1.318912	P	-1.784990	-0.440967	0.285124
H	3.757833	-0.675797	2.355215	B	1.719346	-0.469438	0.734078
H	7.397255	-3.939699	-0.529590	C	1.231458	1.003811	0.992692
H	7.077231	-3.636483	-2.241112	C	3.188231	-0.708818	0.185068
H	6.352976	-5.035504	-1.449338	C	-1.881502	1.166105	-0.645761
H	1.528333	-1.826646	-2.640114	C	-3.344905	-1.374748	-0.097951
H	1.997605	-3.532474	-2.850377	C	-4.003751	-1.902835	1.041331
H	1.014949	-3.019745	-1.467730	C	-5.221686	-2.564430	0.890886
H	2.491927	2.038556	3.486620	C	-5.828194	-2.717879	-0.353138
H	0.857628	1.615354	2.968528	C	-5.171036	-2.200792	-1.463933
H	2.153413	0.420189	2.863268	C	-3.945703	-1.537160	-1.363251
H	3.556403	5.850444	-0.768914	C	-2.650986	2.135981	0.054249
H	3.276905	5.941708	0.982048	C	-2.665194	3.462404	-0.370173
H	1.906901	5.950936	-0.136774	C	-1.923080	3.892570	-1.467739
H	3.375691	0.262663	-2.295798	C	-1.219497	2.930686	-2.180192
H	3.108740	1.805319	-3.127418	C	-1.187395	1.581852	-1.805372
B	-1.912904	-0.338506	0.976021	C	1.502449	2.024194	0.079441
C	-1.369848	1.030734	0.238210	C	0.950889	3.293813	0.173839
C	-3.390079	-0.696490	0.347427	C	0.107291	3.583487	1.234700
C	-1.095234	2.213952	0.914640	C	-0.163350	2.612674	2.191255
C	-0.589274	3.356646	0.300889	C	0.387126	1.348667	2.053705
C	-0.335647	3.341037	-1.058974	C	4.193388	-0.888235	1.124881
C	-0.595512	2.186401	-1.783409	C	5.517696	-1.119122	0.780522
C	-1.103977	1.072889	-1.128689	C	5.859605	-1.175909	-0.564500
C	-3.755926	-1.848369	-0.340330	C	4.881095	-1.007320	-1.536565
C	-5.036856	-2.080536	-0.835414	C	3.569486	-0.776851	-1.145788
C	-6.022702	-1.124995	-0.658551	C	-3.315588	-1.044933	-2.638512
C	-5.712044	0.046280	0.017139	C	-7.163551	-3.401795	-0.484515
C	-4.422001	0.230007	0.495599	C	-3.429935	-1.801570	2.438134
F	-1.318796	-0.017159	-1.884554	C	-0.371061	0.687262	-2.711761
F	-0.320480	2.154577	-3.096565	C	-1.844764	5.350674	-1.830825
F	0.172818	4.421810	-1.664983	C	-3.442237	1.794653	1.296197
F	-0.319094	4.463045	1.009346	F	0.088635	0.457069	2.999942
F	-1.284177	2.308439	2.244003	F	-0.980327	2.893922	3.204346
F	-4.191698	1.385195	1.140489	F	-0.450145	4.782798	1.328481
F	-2.874523	-2.841557	-0.561848	F	1.192228	4.216265	-0.753947
F	-5.327095	-3.216623	-1.485064	F	2.273161	1.785098	-0.988812
F	-7.260009	-1.328753	-1.129184	F	2.649192	-0.635763	-2.112643
F	-6.659445	0.977586	0.195426	F	3.870043	-0.841062	2.426113
H	1.731166	0.795343	-2.646106	F	6.450114	-1.285185	1.713705

F	7.119375	-1.396734	-0.922027	C	2.02976	-0.42148	1.33061
F	5.208265	-1.068088	-2.824072	C	-1.73281	-1.45082	-0.03078
H	-1.314085	-4.770618	-0.285522	C	-2.97635	-2.05774	-0.13729
H	-1.944974	-3.429100	0.649658	C	-4.12386	-1.30305	0.05647
H	-0.921841	-2.910738	-1.825430	C	-4.01128	0.04666	0.35728
H	0.206297	-0.851381	-1.073960	C	-2.75244	0.62123	0.45352
H	0.170210	-1.565238	1.853297	F	-2.75040	1.91833	0.76581
H	-0.175583	-3.790605	2.244918	F	-5.31674	-1.86660	-0.03913
H	0.458614	-5.079773	1.218301	F	-0.69442	-2.26485	-0.20901
H	2.209674	-3.301640	1.095432	F	0.76773	-0.91305	-1.99764
H	1.194812	-4.345922	-1.129474	F	1.70342	0.17358	2.48594
H	1.686953	-2.661364	-1.443927	F	4.71866	-2.43147	0.01183
H	-5.711054	-2.970932	1.773114	F	-3.07496	-3.35342	-0.41453
H	-5.620944	-2.319146	-2.447146	F	-5.10505	0.77490	0.55644
H	-3.246495	4.187040	0.195617	F	3.09209	-2.26244	-2.15677
H	-0.656343	3.234020	-3.060528	F	4.01315	-1.22051	2.34270
H	-3.961631	-1.260753	-3.491870	H	2.61855	2.18294	-1.40772
H	-3.129088	0.031056	-2.611878	H	2.26518	3.64685	-2.32743
H	-2.358903	-1.544156	-2.815726	H	2.43253	4.50297	-0.00650
H	-7.259013	-4.223252	0.229870	H	1.45359	3.21278	1.88101
H	-7.979444	-2.698561	-0.287622	H	2.25345	1.99468	0.89609
H	-7.306924	-3.801840	-1.490771	H	-0.65497	2.45093	1.38902
H	-3.311276	-0.761346	2.752484	H	-1.45800	2.90738	-0.87967
H	-4.086192	-2.307404	3.149582	H	0.09662	2.91396	-2.80886
H	-2.438679	-2.261737	2.507599	H	0.44250	1.37182	-2.04417
H	-0.408220	1.076317	-3.732305	H	-0.17064	4.79068	0.47226
H	0.683238	0.670667	-2.416423	H	0.14380	4.98337	-1.27667
H	-0.733447	-0.338494	-2.738774				
H	-2.787311	5.864408	-1.626862	42			
H	-1.063821	5.837619	-1.237551	[10BH] <sup>-</sup>			
H	-1.596044	5.486570	-2.885752	C	-1.40019	4.05905	-1.43641
H	-4.138887	0.967794	1.124636	C	-0.60530	4.43981	-0.16745
H	-2.778082	1.496088	2.114811	C	0.47155	3.36439	0.06509
H	-4.019839	2.661299	1.624097	C	-0.34963	2.10396	0.49183
				C	-1.80495	2.64574	0.47944
41				C	-2.29157	2.87437	-0.96228
10B				C	-1.61228	4.10069	0.94622
C	1.88874	2.98865	-1.53953	B	-0.07414	0.79617	-0.44313
C	1.65886	3.76398	-0.22519	C	-1.14596	-0.39727	-0.08104
C	1.44918	2.73380	0.89767	C	1.43489	0.14930	-0.29624
C	0.03495	2.13820	0.59778	C	1.79957	-0.88120	-1.16305
C	-0.38413	2.92610	-0.69346	C	3.03793	-1.50867	-1.15574
C	0.46804	2.45420	-1.88806	C	3.99335	-1.10906	-0.23273
C	0.23465	4.30578	-0.42107	C	3.68428	-0.09459	0.65678
B	-0.13275	0.58746	0.37641	C	2.42615	0.50151	0.61304
C	-1.55455	-0.08607	0.25487	C	-2.11545	-0.86717	-0.95985
C	1.16940	-0.30609	0.24612	C	-3.03739	-1.85623	-0.63046
C	1.55939	-0.95684	-0.91820	C	-3.00446	-2.42691	0.63194
C	2.74917	-1.66198	-1.02092	C	-2.05294	-1.99791	1.54543
C	3.58160	-1.75120	0.08887	C	-1.15649	-1.00484	1.17123
C	3.22163	-1.13099	1.27792	F	-0.25598	-0.63762	2.10100

F	-3.88252	-3.38181	0.96742	H	1.64728	4.59669	-1.76170
F	-2.21765	-0.36978	-2.20304	H	0.50569	5.27238	0.33672
F	0.92241	-1.32420	-2.07856	H	-0.16130	3.59058	2.02028
F	2.22803	1.47076	1.52394	H	1.43366	3.02721	1.55511
F	5.19716	-1.69681	-0.20374	H	-1.31141	2.01326	0.91704
F	-3.95515	-2.27022	-1.51624	H	-1.10196	1.73643	-1.49495
F	-2.01434	-2.54793	2.76766	H	0.88163	2.59473	-2.69017
F	3.32511	-2.49240	-2.02071	H	1.62928	1.64081	-1.41760
F	4.59984	0.29713	1.55521	H	-1.74683	3.96323	-0.22728
H	-0.72858	3.76640	-2.24985	H	-0.89075	4.36744	-1.74033
H	-2.00835	4.89981	-1.78994	H	4.73325	-0.64687	-0.12027
H	-0.22471	5.46650	-0.17958	H	2.15062	-4.03941	-0.15618
H	1.16993	3.67347	0.85045	H	-4.74192	-1.12742	1.24667
H	1.05895	3.18458	-0.84405	H	-2.83659	-1.54506	-2.55439
H	-0.11549	1.87836	1.53946	H	0.08303	-1.77340	-1.95682
H	-2.49353	2.03925	1.07660	H	-0.74969	-0.56028	-2.93899
H	-3.34878	3.16701	-0.95978	H	0.35629	-0.07103	-1.64472
H	-2.18765	1.98725	-1.58846	H	-5.92769	-1.02895	-1.48265
H	-1.17676	4.17562	1.94891	H	-5.08558	-2.36077	-2.28178
H	-2.52876	4.70312	0.89978	H	-5.74683	-2.57394	-0.65257
H	-0.19441	1.08383	-1.61876	H	-2.43440	0.83073	2.82277
				H	-3.66257	-0.41450	3.08469
				H	-1.93487	-0.80314	3.20870
				H	2.62237	1.88086	0.28926
				H	4.12816	1.25103	0.95356
				H	2.66024	1.27223	1.94158
				H	0.26885	-3.99022	1.08817
				H	-0.48550	-2.52685	1.72611
				H	-0.76799	-2.99818	0.05592
				H	5.64123	-2.91540	-0.54212
				H	4.55891	-4.31729	-0.57971
				H	4.66272	-3.24045	-1.97376
59							
<b>10P</b>							
C	1.54119	3.82864	-0.98944				
C	0.44315	4.23183	0.01055				
C	0.42867	3.21714	1.17813				
C	-0.27642	1.97273	0.54652				
C	-0.39834	2.36242	-0.94471				
C	0.98725	2.50635	-1.60476				
C	-0.81297	3.83922	-0.78425				
P	-0.00432	0.22642	1.24155				
C	-1.50967	-0.46131	0.38553				
C	1.40078	-0.80116	0.58359				
C	2.70554	-0.27961	0.45854	60			
C	3.74215	-1.08309	-0.01454	<b>[10PH]<sup>+</sup></b>			
C	3.55168	-2.42742	-0.31644	C	-0.64229	3.18474	-1.91273
C	2.30260	-2.96881	-0.03260	C	0.42663	3.75230	-0.96247
C	1.23518	-2.20050	0.43903	C	1.13373	2.57722	-0.26428
C	-2.67211	-0.57650	1.18315	C	0.06159	2.08625	0.77874
C	-3.85836	-1.03913	0.61791	C	-1.15898	2.98205	0.45372
C	-3.94293	-1.39376	-0.72717	C	-1.71893	2.62009	-0.93592
C	-2.79609	-1.27193	-1.50160	C	-0.43924	4.31421	0.16885
C	-1.58186	-0.81389	-0.97711	P	-0.00774	0.21763	1.03993
C	-0.40670	-0.79332	-1.92700	C	-1.41043	-0.85701	0.56728
C	-5.24414	-1.86857	-1.31972	C	1.56700	-0.40361	0.41319
C	-2.67743	-0.22308	2.65368	C	1.72429	-0.58437	-0.97546
C	3.04560	1.10851	0.92841	C	2.95322	-1.03649	-1.45075
C	-0.00987	-2.96254	0.84329	C	4.01666	-1.31711	-0.59459
C	4.66446	-3.27159	-0.87904	C	3.83230	-1.12081	0.77509
H	2.51939	3.71549	-0.51339	C	2.63035	-0.65956	1.30534
				C	-2.73141	-0.38823	0.73028

C	-3.78606	-1.12887	0.19952	C	-3.580166	-0.377013	-2.696412
C	-3.58184	-2.34693	-0.43804	C	-2.430396	-0.949212	-3.557440
C	-2.28838	-2.86989	-0.42456	C	-4.328030	0.485717	-3.726965
C	-1.19331	-2.17943	0.08958	B	-1.906293	0.160647	-0.629444
C	0.09034	-2.97841	0.21049	C	-2.250099	-1.405714	-0.271416
C	-4.71849	-3.10732	-1.06079	C	-1.847010	1.086415	0.750576
C	-3.10613	0.81549	1.55823	C	-1.802733	0.620978	2.065858
C	0.61349	-0.35872	-1.97452	C	-1.738425	1.429466	3.198394
C	2.52783	-0.47344	2.80184	C	-1.705714	2.806737	3.054251
C	5.34125	-1.78610	-1.13016	C	-1.730763	3.332824	1.771900
H	-0.23600	2.42726	-2.58849	C	-1.802758	2.479867	0.677499
H	-1.06324	3.97978	-2.53272	C	-1.484218	-2.488346	-0.669123
H	1.12199	4.44700	-1.43531	C	-1.817085	-3.819228	-0.438732
H	2.03050	2.90070	0.27016	C	-2.998603	-4.110607	0.221116
H	1.44815	1.82100	-0.98090	C	-3.814124	-3.065156	0.640773
H	0.41674	2.36342	1.77944	C	-3.426574	-1.758525	0.386656
H	-1.89279	3.03838	1.25234	F	-4.243037	-0.789498	0.828479
H	-2.68354	3.11139	-1.08984	F	-3.347475	-5.375445	0.459285
H	-1.88977	1.54443	-1.05442	F	-0.297877	-2.301350	-1.309259
H	0.13506	4.68740	1.02211	F	-1.750070	-0.701543	2.342355
H	-1.13647	5.08955	-0.16034	F	-1.782919	3.093906	-0.513753
H	0.08447	0.12270	2.43248	F	-1.609464	3.605442	4.117438
H	3.07909	-1.17835	-2.52126	F	-1.004317	-4.805149	-0.835050
H	4.65543	-1.32963	1.45312	F	-4.951188	-3.336425	1.284128
H	-4.79792	-0.75055	0.32248	F	-1.667782	0.879840	4.415715
H	-2.12783	-3.87897	-0.79548	F	-1.637759	4.656704	1.594653
H	-0.17552	-4.03469	0.27541	H	-1.081602	0.532488	-4.524605
H	0.76349	-2.86193	-0.64177	H	-2.338848	-0.104005	-5.590598
H	0.65547	-2.73011	1.11001	H	-3.236174	2.099123	-4.847656
H	-5.67617	-2.82134	-0.62239	H	-3.080387	2.773990	-2.483099
H	-4.76729	-2.89855	-2.13424	H	-1.524746	1.986685	-2.727290
H	-4.58730	-4.18464	-0.94029	H	-3.900776	1.060753	-1.154003
H	-3.49204	1.63161	0.94281	H	-4.179952	-1.149905	-2.208714
H	-3.89950	0.52457	2.25101	H	-2.753464	-1.852570	-4.085365
H	-2.28209	1.19467	2.16650	H	-1.557653	-1.216267	-2.957305
H	0.07389	-1.28905	-2.18138	H	-5.126303	1.084419	-3.276798
H	1.02661	0.00359	-2.91881	H	-4.733895	-0.086608	-4.569470
H	-0.13062	0.36966	-1.64033	H	-0.788641	0.205334	-1.126662
H	1.78560	-1.14298	3.24958	C	2.948848	-2.860522	2.817708
H	3.48675	-0.69425	3.27126	C	1.434389	-2.612436	2.895431
H	2.26530	0.55405	3.07420	C	0.970222	-2.086302	1.523962
H	5.23078	-2.25637	-2.10874	C	1.417892	-0.583261	1.559253
H	6.02556	-0.93908	-1.24148	C	2.280792	-0.514984	2.840562
H	5.81010	-2.50124	-0.45109	C	3.528908	-1.418405	2.734413
				C	1.372804	-1.348826	3.769059
102				P	1.947733	-0.002282	-0.098945
<b>10PHBH</b>				C	1.581951	1.729721	-0.520907
C	-2.125633	0.201969	-4.560719	C	3.606886	-0.523509	-0.639358
C	-3.087670	1.310230	-4.104686	C	4.743834	0.204072	-0.223962
C	-2.609167	1.818534	-2.729649	C	5.998922	-0.193899	-0.670463
C	-3.029863	0.695349	-1.718442	C	6.164422	-1.287207	-1.520441

C	5.030750	-1.989387	-1.916007	C	-0.283745	0.971418	1.414522
C	3.744832	-1.636615	-1.499591	C	1.032087	1.425484	0.734829
C	1.396740	2.773211	0.414574	C	1.853034	1.728372	1.997249
C	1.007353	4.023944	-0.056195	C	0.881256	2.458010	2.946996
C	0.769112	4.274678	-1.404583	P	-1.577385	0.732894	0.147816
C	0.980990	3.242017	-2.309637	B	1.667922	0.431641	-0.445510
C	1.373300	1.969515	-1.899447	C	0.999739	-1.076443	-0.448936
C	1.480430	0.895313	-2.951603	C	3.296844	0.428815	-0.353340
C	0.212103	5.599964	-1.839738	C	-2.601127	2.208684	-0.102017
C	1.550760	2.628083	1.906371	C	-2.515469	-0.825769	0.198698
C	4.646178	1.376556	0.716147	C	-3.066119	-1.250139	-1.035179
C	2.592234	-2.465057	-2.017615	C	-3.678355	-2.497863	-1.105383
C	7.532758	-1.677862	-2.009800	C	-3.760061	-3.343110	-0.000947
H	3.220967	-3.471166	1.951769	C	-3.233238	-2.895045	1.205977
H	3.306336	-3.376458	3.713043	C	-2.607513	-1.654289	1.336927
H	0.853655	-3.467956	3.243250	C	-3.693587	2.480497	0.746876
H	-0.113002	-2.126760	1.406823	C	-4.452836	3.623800	0.514088
H	1.422004	-2.661111	0.710430	C	-4.157560	4.502815	-0.526548
H	0.513513	0.016147	1.706967	C	-3.071208	4.213649	-1.349054
H	2.491159	0.496217	3.186477	C	-2.275396	3.082830	-1.164617
H	4.194386	-1.212128	3.577472	C	0.926275	-1.909463	0.663715
H	4.106117	-1.257172	1.822146	C	0.241542	-3.115288	0.697539
H	0.365592	-0.933534	3.872735	C	-0.406338	-3.560180	-0.446708
H	1.814046	-1.492679	4.759764	C	-0.352589	-2.785336	-1.592596
H	1.075002	-0.718585	-0.916691	C	0.344725	-1.581303	-1.569527
H	6.872682	0.363758	-0.342764	C	4.138773	-0.654085	-0.130387
H	5.143838	-2.846406	-2.574424	C	5.526925	-0.551437	-0.083411
H	0.826105	4.814857	0.666612	C	6.129612	0.682927	-0.259837
H	0.794688	3.411300	-3.366831	C	5.333355	1.799639	-0.477484
H	1.404992	1.338262	-3.945746	C	3.956250	1.644887	-0.518897
H	2.427592	0.349358	-2.902962	C	-2.044514	-1.330143	2.699981
H	0.648754	0.183855	-2.848125	C	-4.354691	-4.718209	-0.123952
H	0.707127	6.429334	-1.328692	C	-2.962966	-0.441366	-2.305582
H	0.306148	5.743497	-2.917647	C	-1.125842	2.855814	-2.120779
H	-0.851258	5.635906	-1.580577	C	-4.973182	5.750166	-0.737071
H	2.568396	2.352020	2.191338	C	-4.060597	1.582207	1.900324
H	1.318626	3.576935	2.393802	F	0.276927	-0.861662	-2.707834
H	0.861639	1.885574	2.315621	F	-1.028982	-3.159754	-2.682954
H	4.086193	2.205987	0.274095	F	-1.104055	-4.697849	-0.427267
H	5.640902	1.739062	0.979535	F	0.139006	-3.816256	1.831477
H	4.147325	1.086561	1.647359	F	1.499561	-1.521884	1.820671
H	1.892820	-1.873079	-2.615625	F	3.231348	2.763764	-0.709856
H	2.973521	-3.262745	-2.656312	F	3.646352	-1.891162	0.055035
H	2.007732	-2.932971	-1.223699	F	6.281681	-1.631785	0.132349
H	7.851304	-1.016057	-2.821408	F	7.457293	0.800303	-0.214717
H	8.273799	-1.597830	-1.210837	F	5.899174	2.998805	-0.639572
H	7.541921	-2.701278	-2.389309	H	-1.137549	2.835899	2.165514
				H	-1.088386	1.557613	3.382569
				H	-0.103640	-0.011538	1.849831
				H	0.829124	2.406539	0.273377
				H	2.199291	0.787237	2.439261
79							
<b><sup>11</sup>H<sub>2</sub></b>							
C	-0.545092	1.993376	2.538400				

H	2.734582	2.331745	1.770118	C	-0.387187	2.175980	1.367203
H	0.965224	3.540217	2.817089	C	0.413011	3.268276	1.059939
H	1.086683	2.243067	3.998334	C	0.639944	3.586803	-0.272516
H	-0.874030	0.635028	-1.051562	C	0.073680	2.808471	-1.276274
H	1.380597	0.916583	-1.522734	C	-0.729595	1.736750	-0.922205
H	-4.082960	-2.826009	-2.059050	C	-4.001899	0.925315	-0.237662
H	-3.290361	-3.538076	2.080751	C	-5.308062	0.783588	-0.679030
H	-5.297618	3.833432	1.165323	C	-5.902692	-0.472917	-0.651335
H	-2.830084	4.890754	-2.164331	C	-5.187889	-1.569754	-0.181554
H	-2.038627	-0.264244	2.922500	C	-3.888074	-1.388892	0.260097
H	-1.019656	-1.707881	2.795042	C	2.910403	1.095234	2.431938
H	-2.642894	-1.825464	3.467214	C	4.631036	4.283485	-0.996556
H	-4.757250	-5.065261	0.829911	C	2.110534	0.279313	-2.610833
H	-3.577372	-5.421579	-0.437456	C	0.147525	-2.852304	-1.879937
H	-5.151829	-4.742325	-0.870092	C	3.888335	-6.155718	-1.617218
H	-3.625989	-0.857984	-3.064963	C	4.195234	-2.003296	1.189478
H	-1.943995	-0.480685	-2.707523	F	-1.210489	0.958140	-1.907368
H	-3.241111	0.606797	-2.160596	F	0.356780	3.054998	-2.549447
H	-1.030463	3.711128	-2.790895	F	1.427217	4.603923	-0.587524
H	-0.166182	2.721726	-1.613655	F	1.007762	3.962261	2.022507
H	-1.283578	1.967692	-2.743538	F	-0.549225	1.868455	2.665546
H	-4.978801	6.046497	-1.788096	F	-3.261201	-2.487598	0.691499
H	-4.554578	6.581320	-0.160487	F	-3.498611	2.156034	-0.288381
H	-6.005756	5.607834	-0.411096	F	-5.989028	1.827963	-1.124862
H	-4.329094	0.576207	1.565140	F	-7.141660	-0.625678	-1.070204
H	-4.908641	1.994824	2.448958	F	-5.751009	-2.768953	-0.160080
H	-3.228964	1.491075	2.606244	H	1.322941	-2.895024	2.211345
				H	1.690864	-1.677596	3.433407
				H	0.664273	0.065844	2.215019
				H	-1.094461	-2.050564	0.907182
				H	-1.492465	-0.485807	3.484038
				H	-2.470528	-1.847641	2.912842
				H	-0.682719	-3.406654	3.238424
				H	-0.305789	-2.292282	4.546969
				H	0.466660	-0.637809	-0.797932
				H	3.515047	2.523018	-2.732758
				H	4.149126	3.175319	1.445742
				H	4.921715	-4.354446	0.152431
				H	1.542256	-5.047280	-2.374215
				H	2.819833	0.030280	2.643172
				H	2.040388	1.609554	2.858069
				H	3.789075	1.460021	2.966917
				H	5.177385	4.662809	-0.131833
				H	3.906748	5.044436	-1.301805
				H	5.334642	4.145423	-1.820777
				H	2.537088	0.653332	-3.541953
				H	1.024426	0.420382	-2.678532
				H	2.319549	-0.793829	-2.560958
				H	-0.193153	-3.660956	-2.527050
				H	-0.629394	-2.697925	-1.124610
				H	0.201254	-1.947453	-2.495238
78							
[11H] <sup>+</sup>							
C	0.923483	-2.020884	2.734857				
C	0.536126	-0.904795	1.737367				
C	-0.972330	-1.115316	1.470971				
C	-1.468690	-1.415948	2.905936				
C	-0.402077	-2.374837	3.463271				
P	1.469477	-0.828159	0.153221				
B	-1.764554	0.038831	0.727836				
C	-0.980731	1.377372	0.398373				
C	-3.233162	-0.145450	0.253409				
C	2.188482	-2.407661	-0.344347				
C	2.509744	0.636500	-0.089799				
C	2.688394	1.037478	-1.439520				
C	3.386206	2.211200	-1.699693				
C	3.916435	3.000997	-0.677331				
C	3.739272	2.577164	0.636132				
C	3.048240	1.407828	0.961000				
C	3.431816	-2.819545	0.178355				
C	3.963252	-4.035017	-0.246916				
C	3.302273	-4.846799	-1.165346				
C	2.068914	-4.418644	-1.660991				
C	1.486562	-3.215458	-1.274556				

H 4.023612 -6.162779 -2.702301  
H 3.219880 -6.983965 -1.365946  
H 4.856078 -6.342929 -1.150074  
H 4.433662 -1.003425 0.815065  
H 5.133697 -2.495972 1.446094  
H 3.625037 -1.894901 2.118382

78

[11H]<sup>-</sup>

C -0.926882 0.686318 2.460478  
C -0.586940 0.160873 1.062121  
C 0.764827 0.841661 0.706766  
C 1.444748 1.062877 2.093895  
C 0.432393 0.606709 3.163046  
P -1.741330 0.341215 -0.405202  
B 1.645598 0.070462 -0.473499  
C 1.389558 -1.553474 -0.458487  
C 3.228005 0.497238 -0.336754  
C -2.261668 2.118289 -0.177786  
C -3.329818 -0.598791 -0.160730  
C -4.451447 -0.188352 -0.922090  
C -5.663521 -0.872716 -0.805027  
C -5.811124 -1.986633 0.011957  
C -4.673654 -2.449712 0.665528  
C -3.441790 -1.799760 0.578460  
C -3.198873 2.582015 0.771141  
C -3.495001 3.947758 0.837649  
C -2.900199 4.878074 -0.005495  
C -1.992327 4.408873 -0.949903  
C -1.665337 3.056449 -1.055598  
C 1.613017 -2.353691 0.658588  
C 1.329831 -3.709990 0.723871  
C 0.780916 -4.336262 -0.387321  
C 0.528257 -3.590015 -1.525994  
C 0.832956 -2.228807 -1.541305  
C 4.332569 -0.322323 -0.129119  
C 5.639786 0.148474 -0.024817  
C 5.891224 1.505187 -0.128428  
C 4.826817 2.370200 -0.337832  
C 3.543567 1.852599 -0.436650  
C -2.265746 -2.477816 1.241811  
C -7.138826 -2.682886 0.163431  
C -4.411199 0.956552 -1.910487  
C -0.686525 2.656022 -2.134900  
C -3.207882 6.349024 0.110149  
C -3.978663 1.688079 1.708399  
F 0.558144 -1.596074 -2.688841  
F 0.005604 -4.189206 -2.603939  
F 0.502560 -5.645149 -0.356547  
F 1.575388 -4.422258 1.831984  
F 2.130793 -1.803840 1.772919

F 2.564685 2.753971 -0.641154  
F 4.204349 -1.657085 -0.025577  
F 6.658900 -0.698710 0.174196  
F 7.140800 1.977018 -0.030577  
F 5.054825 3.686577 -0.444172  
H -1.262583 1.729274 2.401078  
H -1.702271 0.109233 2.977940  
H -0.387236 -0.906568 1.150226  
H 0.525165 1.844217 0.328887  
H 2.382777 0.510173 2.186327  
H 1.687708 2.123907 2.223633  
H 0.473095 1.198452 4.083485  
H 0.633230 -0.437152 3.431378  
H 1.294936 0.460686 -1.566134  
H -6.513564 -0.526018 -1.390719  
H -4.735859 -3.364403 1.252492  
H -4.218827 4.287788 1.576768  
H -1.522877 5.114835 -1.632260  
H -1.909734 -1.936675 2.122823  
H -1.422828 -2.574150 0.549175  
H -2.548193 -3.484223 1.559770  
H -7.675143 -2.324272 1.049121  
H -7.009328 -3.762974 0.275427  
H -7.780217 -2.504512 -0.703844  
H -5.201429 0.823208 -2.654134  
H -3.452403 0.999778 -2.436166  
H -4.555869 1.929240 -1.430395  
H -0.501928 3.501118 -2.803300  
H 0.272812 2.334063 -1.719515  
H -1.057694 1.813240 -2.724127  
H -3.243522 6.824183 -0.874216  
H -2.437978 6.864957 0.693965  
H -4.167466 6.515931 0.606389  
H -4.921659 1.373581 1.245826  
H -4.217931 2.232433 2.626552  
H -3.441941 0.780670 1.973053

77

11

C -0.986264 2.212331 2.406687  
C -0.558957 1.036408 1.520951  
C 0.960027 1.259009 1.378399  
C 1.380682 1.595799 2.832700  
C 0.166874 2.363496 3.426641  
P -1.361492 0.816146 -0.160812  
B 1.801186 0.131023 0.672362  
C 1.119753 -1.275659 0.420996  
C 3.279491 0.375539 0.185975  
C -2.534788 2.238430 -0.396350  
C -2.331945 -0.759601 -0.155477  
C -2.504743 -1.307039 -1.453952



C	-3.129643	-2.541934	-1.614472	H	-3.430166	-5.394418	-0.852698
C	-3.588377	-3.282107	-0.526508	H	-4.847515	-4.659028	-1.608078
C	-3.421759	-2.735883	0.740128	H	-2.317062	-1.158223	-3.587791
C	-2.815257	-1.492617	0.949418	H	-0.918278	-0.527248	-2.698326
C	-3.939525	2.229239	-0.219747	H	-2.403213	0.414033	-2.778216
C	-4.678303	3.368210	-0.546794	H	-0.225751	4.409311	-1.756165
C	-4.092335	4.530074	-1.038385	H	0.083262	3.717827	-0.167552
C	-2.712711	4.533654	-1.200914	H	-0.011432	2.654797	-1.571916
C	-1.930600	3.417375	-0.901380	H	-5.300989	5.641671	-2.431616
C	0.558115	-2.026678	1.443407	H	-4.347354	6.650999	-1.341546
C	-0.151863	-3.197865	1.218940	H	-5.795781	5.821248	-0.747760
C	-0.326006	-3.641884	-0.083100	H	-4.728780	0.209467	-0.369510
C	0.207286	-2.912795	-1.139428	H	-5.757043	1.357090	0.498483
C	0.929049	-1.762540	-0.868377	H	-4.311762	0.699461	1.266152
C	4.089858	-0.651585	-0.325049				
C	5.385867	-0.451296	-0.777671				
C	5.933789	0.822901	-0.734719	37			
C	5.181029	1.876872	-0.237082	<b>11B</b>			
C	3.890076	1.639103	0.211951	C	-1.456483	-1.599133	2.944786
C	-2.747972	-1.037736	2.389849	C	-1.380304	-2.838378	2.047267
C	-4.210429	-4.638692	-0.720317	C	-0.043770	-2.659272	1.319288
C	-2.010490	-0.604244	-2.698177	C	0.081341	-1.139415	1.059517
C	-0.440444	3.551117	-1.115778	C	-0.979090	-0.466424	2.019822
C	-4.928184	5.727921	-1.405636	B	-0.283144	0.807014	2.593557
C	-4.722226	1.056998	0.320613	C	0.539430	0.814252	3.940942
F	1.429919	-1.078998	-1.905928	C	-0.296408	2.138762	1.747202
F	-0.007486	-3.305843	-2.391973	C	0.493088	1.917978	4.795823
F	-1.012700	-4.753455	-0.321862	C	1.182352	1.975648	5.998040
F	-0.707137	-3.859743	2.231879	C	1.982021	0.903554	6.372410
F	0.681167	-1.612904	2.717731	C	2.075061	-0.209075	5.547438
F	3.247004	2.711061	0.679429	C	1.354770	-0.235302	4.361559
F	3.652430	-1.907848	-0.390041	C	0.858862	2.904924	1.580850
F	6.105627	-1.465627	-1.245886	C	0.897202	4.059323	0.813331
F	7.169100	1.030936	-1.161147	C	-0.265878	4.497475	0.192837
F	5.701740	3.099081	-0.188964	C	-1.443928	3.777931	0.342289
H	-1.082910	3.116922	1.795912	C	-1.438369	2.617307	1.103888
H	-1.959365	2.055019	2.881989	F	-0.261003	2.976288	4.483015
H	-0.697351	0.112294	2.081559	F	2.655623	0.943256	7.513096
H	1.104234	2.171678	0.787730	F	1.089867	3.041294	6.787032
H	1.547249	0.671063	3.393888	F	2.850583	-1.231182	5.895709
H	2.305315	2.175452	2.865704	F	1.503831	-1.323811	3.597179
H	0.407143	3.416326	3.594889	F	-2.607282	1.982334	1.234833
H	-0.111523	1.940947	4.395550	F	-2.560346	4.205559	-0.239410
H	-3.250245	-2.941951	-2.618636	F	-0.251629	5.602711	-0.538519
H	-3.782459	-3.288312	1.605431	F	2.026104	4.745868	0.666681
H	-5.756184	3.344704	-0.401486	F	2.003996	2.521536	2.154119
H	-2.223408	5.428504	-1.579252	H	-2.461291	-1.409578	3.332008
H	-2.736894	0.047492	2.492085	H	-0.789385	-1.725409	3.803175
H	-1.857179	-1.435744	2.890998	H	-1.441838	-3.779442	2.599897
H	-3.616548	-1.418036	2.933292	H	-2.207073	-2.819035	1.327162
H	-4.812970	-4.926508	0.144036	H	0.019960	-3.236792	0.393575
				H	0.770943	-2.988266	1.970001

H -0.151902 -0.877489 0.024759  
H 1.108262 -0.804343 1.244151  
H -1.821971 -0.171762 1.389109

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[11BH]<sup>-</sup>

C -1.563912 -0.785761 2.554266  
C -2.092840 -2.189509 2.222589  
C -0.823865 -3.022384 1.902773  
C 0.322463 -1.988208 1.765854  
C -0.355541 -0.613641 1.622150  
B 0.669703 0.635586 1.865509  
C 1.122264 0.687254 3.446706  
C 0.107731 2.125358 1.436927  
C 0.342052 1.277252 4.436564  
C 0.694956 1.325740 5.779861  
C 1.890103 0.752359 6.185979  
C 2.700370 0.139779 5.243169  
C 2.304629 0.119157 3.909667  
C 0.938754 3.231509 1.618836  
C 0.604489 4.531633 1.265698  
C -0.631826 4.780747 0.688565  
C -1.497411 3.721228 0.480782  
C -1.116525 2.434803 0.854727  
F -0.838722 1.838467 4.118245  
F 2.252756 0.782039 7.475737  
F -0.099826 1.910985 6.687514  
F 3.853795 -0.423690 5.632324  
F 3.140327 -0.506375 3.065251  
F -2.036008 1.483014 0.604960  
F -2.695234 3.946925 -0.079256  
F -0.979710 6.025832 0.335203  
F 1.455955 5.547517 1.469008  
F 2.156154 3.069980 2.164636  
H -2.317549 -0.003104 2.438460  
H -1.222147 -0.763568 3.599228  
H -2.695587 -2.630256 3.024301  
H -2.733718 -2.131394 1.334918  
H -0.957761 -3.595555 0.979030  
H -0.614928 -3.750720 2.693774  
H 0.997767 -2.207212 0.932959  
H 0.938068 -1.994719 2.675108  
H -0.749945 -0.553294 0.595373  
H 1.673937 0.463834 1.199848

55

11P

C 0.197362 4.513203 -0.393738  
C 0.849157 3.781043 -1.576448  
C 0.441243 2.295092 -1.416009  
C -0.120796 2.178377 0.027464

C 0.272905 3.487091 0.740687  
P -0.010098 0.600580 1.064029  
C 1.421076 -0.463879 0.562727  
C -1.505867 -0.216933 0.304969  
C 2.697917 0.085246 0.315202  
C 3.747381 -0.746177 -0.077789  
C 3.599445 -2.125492 -0.179283  
C 2.381398 -2.665577 0.221403  
C 1.301970 -1.872883 0.615071  
C -2.676537 -0.178362 1.100441  
C -3.868575 -0.703938 0.608104  
C -3.952986 -1.272194 -0.661704  
C -2.800244 -1.298148 -1.435137  
C -1.579197 -0.782604 -0.983256  
C -2.690339 0.423469 2.488463  
C -0.404549 -0.946571 -1.919841  
C -5.259254 -1.819573 -1.175309  
C 0.084456 -2.596995 1.149210  
C 3.017725 1.534684 0.588103  
C 4.726888 -3.002695 -0.655966  
H 0.689074 5.460083 -0.156054  
H -0.852905 4.731246 -0.620835  
H 0.554275 4.192351 -2.544871  
H 1.938236 3.881533 -1.506379  
H 1.293284 1.632404 -1.590133  
H -0.328380 2.009547 -2.138429  
H -1.213398 2.230653 -0.062530  
H -0.401131 3.707529 1.573179  
H 1.288375 3.451953 1.143702  
H 4.718568 -0.298835 -0.279421  
H 2.266895 -3.747496 0.253478  
H -4.757719 -0.669100 1.234300  
H -2.840303 -1.737261 -2.430233  
H -2.438447 1.488552 2.472087  
H -3.681561 0.317891 2.934897  
H -1.959350 -0.056673 3.144505  
H -0.739420 -0.851853 -2.956368  
H 0.390526 -0.227608 -1.744625  
H 0.040977 -1.941635 -1.804798  
H -5.717005 -2.494042 -0.446152  
H -5.119245 -2.370010 -2.108135  
H -5.973459 -1.012100 -1.365416  
H 0.391487 -3.569206 1.542200  
H -0.394330 -2.043730 1.961997  
H -0.679929 -2.768548 0.385961  
H 2.628310 2.221023 -0.165582  
H 2.604510 1.838033 1.556117  
H 4.099909 1.675460 0.632038  
H 5.698734 -2.555404 -0.433007  
H 4.687540 -3.988785 -0.186491  
H 4.673871 -3.151791 -1.739622

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[11PH]<sup>+</sup>

C	0.996916	4.424491	0.451769
C	0.408422	4.152628	-0.938219
C	-0.558163	2.964573	-0.737551
C	-0.094198	2.298155	0.591821
C	1.193104	3.022522	1.043273
P	-0.040190	0.469480	0.712430
C	1.451441	-0.468684	0.290966
C	-1.588291	-0.261092	0.132100
C	2.396238	-0.097485	-0.681727
C	3.514376	-0.912449	-0.869895
C	3.713768	-2.080319	-0.144274
C	2.745455	-2.442754	0.796268
C	1.618978	-1.667509	1.037188
C	-2.673937	-0.328124	1.038537
C	-3.869538	-0.882379	0.592479
C	-4.023517	-1.370966	-0.705691
C	-2.936959	-1.291388	-1.573905
C	-1.713897	-0.748678	-1.185108
C	-2.598777	0.150239	2.470579
C	-0.587081	-0.731198	-2.187879
C	-5.323601	-1.986653	-1.143296
C	0.636004	-2.147888	2.081242
C	2.285355	1.107910	-1.579190
C	4.932417	-2.935711	-0.352112
H	1.925574	4.997059	0.418672
H	0.281533	4.984624	1.063556
H	-0.098566	5.021251	-1.361443
H	1.212023	3.878484	-1.629221
H	-0.567801	2.285409	-1.594195
H	-1.586456	3.310616	-0.615435
H	-0.869302	2.500731	1.342609
H	1.305830	3.018935	2.130029
H	2.083761	2.551768	0.615494
H	-0.084245	0.304217	2.097343
H	4.244400	-0.620684	-1.620953
H	2.875040	-3.362682	1.360251
H	-4.709847	-0.933194	1.279666
H	-3.041926	-1.662959	-2.589553
H	-2.274683	1.191921	2.556530
H	-3.582084	0.083548	2.936661
H	-1.916026	-0.465730	3.067325
H	-0.971004	-0.948237	-3.185437
H	-0.088936	0.240682	-2.237070
H	0.173344	-1.480653	-1.947047
H	-6.175543	-1.457967	-0.710586
H	-5.422961	-1.976238	-2.229948
H	-5.378847	-3.028412	-0.811926
H	0.875211	-3.172018	2.368554

H	0.683977	-1.539901	2.992255
H	-0.397761	-2.144213	1.720275
H	1.379791	1.685987	-1.416303
H	3.140527	1.775204	-1.434721
H	2.293025	0.792756	-2.627074
H	5.477937	-2.642620	-1.250259
H	5.610717	-2.843337	0.501533
H	4.659048	-3.989982	-0.440291

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11PHBH

C	2.345989	-1.766972	3.294185
C	2.323940	-1.731852	4.843131
C	1.796493	-0.323852	5.216636
C	1.240849	0.239889	3.901531
C	2.191747	-0.307134	2.825923
B	1.670376	-0.199610	1.292233
C	2.509012	-1.191632	0.294357
C	1.658105	1.301504	0.601374
C	3.850168	-0.968338	-0.000766
C	4.591836	-1.759371	-0.869977
C	3.980283	-2.837262	-1.496930
C	2.645574	-3.103458	-1.233208
C	1.957038	-2.294333	-0.339093
C	1.245051	1.454518	-0.719497
C	1.209420	2.652627	-1.414436
C	1.577577	3.815926	-0.757717
C	1.993109	3.737397	0.561284
C	2.048190	2.498400	1.197949
F	4.482690	0.074050	0.557052
F	4.664709	-3.602172	-2.347857
F	5.875207	-1.494953	-1.119216
F	2.031478	-4.120576	-1.856380
F	0.648807	-2.622716	-0.150222
F	2.505103	2.530201	2.457411
F	2.354317	4.850031	1.204114
F	1.514562	4.995314	-1.384232
F	0.814617	2.699372	-2.694021
F	0.804488	0.374615	-1.416536
H	3.246800	-2.244671	2.896523
H	1.490822	-2.350065	2.919641
H	1.681718	-2.519609	5.249238
H	3.321929	-1.897292	5.259043
H	2.623865	0.309002	5.555150
H	1.058939	-0.348255	6.024849
H	1.154541	1.329659	3.903511
H	0.234169	-0.173485	3.727943
H	3.162667	0.193653	2.956214
H	0.517937	-0.613839	1.285832
C	-0.705937	-3.061680	-3.521851
C	-1.208136	-3.961534	-2.387174

C	-2.104908	-3.061453	-1.505988	H	-0.634223	5.947571	-0.879700
C	-1.870001	-1.606322	-2.027673	H	-2.206361	6.104093	-1.671424
C	-0.573558	-1.689717	-2.855756	H	-2.097145	6.119314	0.100104
P	-1.918792	-0.459219	-0.584055				
C	-1.915202	1.357973	-0.761475				
C	-3.366100	-0.966041	0.395146				
C	-1.799167	2.076939	0.456649				
C	-1.750500	3.467003	0.408588	82			
C	-1.819845	4.174538	-0.789484	<b>12H<sub>2</sub></b>			
C	-1.947348	3.446559	-1.966371	C	-0.606422	-0.470216	-1.431379
C	-1.976696	2.050934	-1.984853	C	0.725187	-0.258193	-1.282460
C	-4.653923	-0.592400	-0.037963	B	1.556017	-0.051095	0.096014
C	-5.759154	-1.029325	0.691094	P	-1.526298	-0.464950	0.103580
C	-5.624098	-1.815768	1.831349	Si	-1.377702	-0.478883	-3.161240
C	-4.339350	-2.168297	2.240285	C	3.120482	-0.434284	-0.136627
C	-3.197164	-1.760416	1.552615	C	-3.204931	0.173453	-0.182147
C	-4.898817	0.289955	-1.239127	C	-1.526660	-1.922739	1.181191
C	-1.853819	-2.151926	2.123934	C	-1.915108	-1.700957	2.520364
C	-6.827964	-2.257554	2.619740	C	-1.967559	-2.793237	3.384504
C	-1.962241	1.397743	-3.341627	C	-1.631189	-4.078851	2.967971
C	-1.693527	1.421474	1.810807	C	-1.231075	-4.261301	1.645888
C	-1.691415	5.672865	-0.810233	C	-1.163057	-3.207843	0.736277
H	0.241382	-3.407414	-3.941016	C	-3.312475	1.571538	-0.346838
H	-1.439848	-3.013083	-4.335119	C	-4.573834	2.122048	-0.577916
H	-1.742914	-4.841844	-2.749683	C	-5.718502	1.333765	-0.645500
H	-0.352735	-4.301408	-1.800787	C	-5.582687	-0.044965	-0.481678
H	-1.826964	-3.173422	-0.456423	C	-4.348680	-0.649189	-0.251225
H	-3.166255	-3.309700	-1.577529	C	4.214003	0.265653	0.362429
H	-2.704668	-1.347356	-2.684784	C	5.533062	-0.124617	0.154500
H	-0.465198	-0.871740	-3.566742	C	5.801658	-1.269473	-0.579771
H	0.294581	-1.684769	-2.196422	C	4.745440	-2.008418	-1.093521
H	-0.775118	-0.766366	0.174303	C	3.447670	-1.577477	-0.859598
H	-1.640554	4.012570	1.342167	C	-2.117011	2.493697	-0.289984
H	-1.980949	3.974880	-2.915574	C	-7.071397	1.940019	-0.907537
H	-6.752982	-0.744775	0.354772	C	-4.307338	-2.152439	-0.109288
H	-4.217358	-2.782236	3.129118	C	-2.254094	-0.333229	3.065491
H	-4.300893	-0.000111	-2.107542	C	-1.663463	-5.236711	3.929267
H	-5.947555	0.236508	-1.535917	C	-0.688430	-3.503652	-0.663861
H	-4.659227	1.334422	-1.017360	F	4.041804	1.378662	1.092147
H	-1.987495	-2.909372	2.897867	F	6.541564	0.590078	0.656127
H	-1.147664	-2.548418	1.391013	F	7.059065	-1.657966	-0.788172
H	-1.360529	-1.291691	2.588587	F	4.986619	-3.115699	-1.798996
H	-7.739615	-2.193554	2.022445	F	2.464175	-2.344459	-1.380430
H	-6.713942	-3.286828	2.968064	C	-0.040121	-1.124457	-4.315968
H	-6.960865	-1.624526	3.502764	C	-2.913013	-1.558991	-3.338345
H	-0.932976	1.123043	-3.587301	C	-1.840525	1.280584	-3.644614
H	-2.588876	0.508864	-3.414131	F	1.266058	4.870672	-0.862507
H	-2.304343	2.104118	-4.099702	F	0.636342	5.449580	1.722387
H	-0.864108	0.708143	1.843442	F	0.437853	3.435485	3.547254
H	-1.487686	2.175993	2.571579	F	0.859964	0.904282	2.816604
H	-2.617180	0.904222	2.089360	F	1.684928	2.332998	-1.614844
				C	1.323611	1.500514	0.568093
				C	1.405593	2.566803	-0.320427

C	1.181393	3.890172	0.037491	C	0.986058	2.069189	3.245857
C	0.858290	4.189156	1.354652	C	1.262726	0.705210	3.234945
C	0.758719	3.160815	2.281628	C	0.523121	-0.191186	2.464500
C	0.999099	1.853369	1.873187	C	-3.864220	-0.024437	-0.577860
H	1.284451	-0.186101	-2.221101	C	-5.240210	0.215049	-0.591324
H	1.098817	-0.789546	0.947909	C	-6.039279	0.038855	0.533049
H	-0.961213	0.513668	0.923192	C	-5.429059	-0.387021	1.716179
H	-2.274545	-2.629890	4.414431	C	-4.068589	-0.658381	1.788775
H	-0.957962	-5.257682	1.307638	C	3.952643	0.129240	-0.754312
H	-4.657829	3.197657	-0.709725	C	5.248389	-0.246762	-0.433419
H	-6.467414	-0.674500	-0.542610	C	5.487232	-1.528016	0.050237
H	-1.306642	2.154825	-0.943902	C	4.432552	-2.423128	0.197649
H	-2.400237	3.499085	-0.605825	C	3.153989	-2.016234	-0.143008
H	-1.707186	2.568702	0.725439	C	-3.105689	0.296190	-1.841612
H	-7.026807	3.030503	-0.899334	C	-7.520760	0.291537	0.488176
H	-7.454013	1.623429	-1.882505	C	-3.497230	-1.114231	3.112367
H	-7.794899	1.620193	-0.152718	C	-1.913163	2.307743	0.807153
H	-5.245398	-2.581561	-0.466689	C	1.830382	3.033909	4.028390
H	-3.496842	-2.597240	-0.692862	C	0.845418	-1.662917	2.567431
H	-4.164927	-2.458035	0.931674	F	3.806861	1.347795	-1.263266
H	-1.357453	0.294791	3.112184	F	6.257094	0.594705	-0.599309
H	-3.007417	0.185222	2.463868	F	6.712777	-1.899126	0.359321
H	-2.646177	-0.422943	4.079576	F	4.659848	-3.651485	0.641031
H	-2.385435	-5.067231	4.730961	F	2.190806	-2.937576	-0.012769
H	-1.922914	-6.167239	3.419368	C	-0.514285	-4.484669	-1.960069
H	-0.680577	-5.375451	4.390794	C	-2.490255	-4.140970	0.398614
H	-0.640314	-4.582978	-0.818984	C	-3.180879	-2.993753	-2.371362
H	-1.349978	-3.081970	-1.425688	F	-1.274076	2.953281	-3.540245
H	0.306920	-3.083622	-0.834251	F	-0.530432	4.976709	-1.876101
H	-0.472127	-1.374719	-5.289744	F	1.171249	4.494006	0.181471
H	0.744122	-0.381306	-4.484148	F	2.159827	2.035289	0.556665
H	0.433482	-2.023520	-3.909184	F	-0.303755	0.484946	-3.157802
H	-3.212490	-1.536134	-4.392087	C	0.964200	1.161228	-1.280653
H	-3.755940	-1.180595	-2.753603	C	0.083455	1.454923	-2.322341
H	-2.744087	-2.607621	-3.076935	C	-0.415364	2.729685	-2.552738
H	-0.995633	1.957785	-3.481725	C	-0.033759	3.764430	-1.706616
H	-2.109690	1.325217	-4.704892	C	0.850855	3.517782	-0.660331
H	-2.694607	1.648115	-3.066539	C	1.345182	2.237397	-0.477481
				H	0.661706	-2.154644	-1.989667
81				H	-1.581850	-1.955804	1.708995
[12H] <sup>+</sup>				H	-0.285650	3.603572	2.449122
C	-0.853165	-1.762417	-0.656122	H	2.077286	0.321933	3.843478
C	0.334392	-1.454856	-1.210811	H	-5.692587	0.567217	-1.515079
B	1.393906	-0.312436	-0.978716	H	-6.035642	-0.511631	2.609368
P	-1.532720	-0.909815	0.785409	H	-2.105379	-0.130829	-1.876160
Si	-1.793938	-3.367982	-1.168084	H	-3.651882	-0.074176	-2.712336
C	2.846824	-0.723730	-0.599423	H	-3.016770	1.382035	-1.964520
C	-3.282678	-0.488425	0.618720	H	-7.806926	0.829435	-0.416813
C	-0.524881	0.314904	1.660140	H	-8.068096	-0.655891	0.506119
C	-0.830788	1.695678	1.658846	H	-7.844582	0.872762	1.354903
C	-0.069228	2.538250	2.460204	H	-4.235940	-0.975100	3.902202

H	-3.238768	-2.179875	3.095859	C	-0.977948	-3.396503	-0.686052
H	-2.602256	-0.551584	3.398594	F	4.197987	1.415874	0.967151
H	-1.861706	1.940469	-0.221923	F	6.664741	0.662908	0.357202
H	-2.913282	2.087198	1.191364	F	7.125183	-1.678307	-0.959051
H	-1.794404	3.392968	0.779627	F	5.018314	-3.261369	-1.661061
H	0.135836	-2.169769	3.233410	F	2.522029	-2.529390	-1.065479
H	0.831028	-2.177207	1.603825	C	-0.148499	-1.842736	-3.916651
H	1.839864	-1.799842	2.995771	C	-2.975465	-0.947856	-3.304580
H	-0.943652	-5.480914	-2.103581	C	-0.844128	1.150633	-3.847890
H	-0.207178	-4.122476	-2.945737	F	1.641537	4.793015	-0.402592
H	0.378186	-4.589190	-1.336804	F	0.539726	5.256202	2.047714
H	-2.951499	-5.101517	0.149128	F	-0.020250	3.158108	3.695875
H	-3.271923	-3.520056	0.851023	F	0.521107	0.662714	2.941262
H	-1.715194	-4.338109	1.146748	F	2.171011	2.274718	-1.187252
H	-2.820602	-2.437222	-3.241128	C	1.391238	1.349055	0.840272
H	-3.597645	-3.939993	-2.731356	C	1.641772	2.455235	0.036884
H	-3.992465	-2.429297	-1.903555	C	1.371143	3.763925	0.411833
H	2.484278	3.583710	3.343263	C	0.808910	4.004087	1.658115
H	2.457249	2.520831	4.759114	C	0.530008	2.933934	2.494501
H	1.211404	3.766867	4.550895	C	0.830395	1.641256	2.076673
				H	1.371505	-0.353265	-2.009441
81				H	1.253440	-0.966341	1.127293
[12H] <sup>-</sup>				H	-2.905772	-2.710518	4.290739
C	-0.555967	-0.431623	-1.231359	H	-1.398351	-5.219611	1.176549
C	0.784968	-0.331642	-1.079198	H	-4.184214	3.370915	-1.615017
B	1.640211	-0.172493	0.295463	H	-6.446643	-0.202060	-1.004340
P	-1.530455	-0.232983	0.314288	H	-1.022914	2.160551	-1.199178
Si	-1.158460	-0.517990	-3.014093	H	-2.040818	3.589905	-0.950908
C	3.211993	-0.512359	-0.023615	H	-1.514274	2.591733	0.425040
C	-3.159492	0.376162	-0.329665	H	-6.445840	2.971389	-2.783961
C	-1.819396	-1.843425	1.174046	H	-7.449526	1.624861	-2.221043
C	-2.323970	-1.706223	2.489432	H	-7.141209	3.006223	-1.163725
C	-2.500531	-2.835247	3.288121	H	-5.535769	-2.122808	-0.399732
C	-2.161993	-4.109499	2.842197	H	-3.787775	-2.392530	-0.505674
C	-1.656979	-4.231200	1.552184	H	-4.501640	-1.936106	1.026812
C	-1.481185	-3.130761	0.709520	H	-1.843718	0.305190	3.093420
C	-3.111506	1.732870	-0.745770	H	-3.473774	0.133733	2.442697
C	-4.248400	2.336780	-1.280962	H	-3.112280	-0.476037	4.066221
C	-5.464031	1.662921	-1.375441	H	-3.166193	-5.201452	4.411570
C	-5.509893	0.347498	-0.929246	H	-2.453712	-6.225905	3.153207
C	-4.386561	-0.314086	-0.421636	H	-1.420489	-5.453585	4.357919
C	4.325965	0.250776	0.309734	H	-0.959425	-4.472395	-0.880203
C	5.633981	-0.117830	0.007707	H	-1.627079	-2.926359	-1.432541
C	5.874296	-1.306209	-0.661188	H	0.026109	-2.993366	-0.839727
C	4.799617	-2.107801	-1.016353	H	-0.307656	-1.780267	-4.998835
C	3.513517	-1.697387	-0.693194	H	0.923141	-1.748516	-3.721598
C	-1.856023	2.565976	-0.615861	H	-0.453058	-2.842498	-3.590268
C	-6.690898	2.350815	-1.917347	H	-3.104729	-1.203520	-4.362936
C	-4.561641	-1.768122	-0.052656	H	-3.632108	-0.104455	-3.072773
C	-2.711674	-0.360423	3.055876	H	-3.311558	-1.805419	-2.713376
C	-2.312274	-5.312631	3.737441	H	0.150660	1.529444	-3.591388

H -0.917393 1.074572 -4.937991  
H -1.581285 1.887141 -3.510282

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**12**

C 1.058458 -1.400833 0.636508  
C -0.254319 -1.510098 0.983477  
B -1.416061 -0.485939 0.873999  
P 1.684265 0.203937 0.019017  
Si 2.152081 -2.954287 0.921534  
C -2.879389 -1.019007 0.598753  
C 3.489085 -0.009208 -0.243165  
C 0.798747 0.623066 -1.537302  
C 0.731759 2.012407 -1.811822  
C -0.136765 2.482043 -2.791406  
C -0.949640 1.617364 -3.525161  
C -0.814826 0.253223 -3.301484  
C 0.053683 -0.267620 -2.335361  
C 4.238575 0.108444 0.950857  
C 5.622097 -0.078808 0.913601  
C 6.298276 -0.314091 -0.279277  
C 5.552449 -0.350303 -1.456689  
C 4.165055 -0.209909 -1.466639  
C -4.032531 -0.272892 0.884898  
C -5.320107 -0.730266 0.645030  
C -5.505377 -1.988636 0.089975  
C -4.401442 -2.772558 -0.211678  
C -3.129336 -2.285432 0.052442  
C 3.605031 0.480340 2.275849  
C 7.791799 -0.507790 -0.311993  
C 3.461927 -0.296478 -2.798381  
C 1.603335 3.001574 -1.077729  
C -1.951602 2.155562 -4.510593  
C 0.167278 -1.771848 -2.267971  
F -3.949866 0.935680 1.440696  
F -6.374498 0.020696 0.947460  
F -6.727867 -2.438639 -0.148236  
F -4.569083 -3.980107 -0.743021  
F -2.127367 -3.111668 -0.268383  
C 0.981524 -4.433993 0.980204  
C 3.425291 -3.264884 -0.431675  
C 3.062359 -2.875933 2.570274  
F 0.567047 3.319212 3.369708  
F -0.481319 5.111237 1.614296  
F -1.967301 4.247187 -0.494164  
F -2.475375 1.627067 -0.788974  
F 0.148331 0.696664 3.020896  
C -1.197940 1.058995 1.110839  
C -0.422174 1.544060 2.161072

C -0.186959 2.896542 2.355933  
C -0.720650 3.814471 1.458928  
C -1.486366 3.372722 0.387968  
C -1.724324 2.014349 0.246121  
H -0.566600 -2.493303 1.339205  
H -0.193402 3.552713 -2.975228  
H -1.394810 -0.442254 -3.905210  
H 6.186373 -0.012083 1.841061  
H 6.066762 -0.512995 -2.401641  
H 2.784874 -0.179158 2.568538  
H 4.355377 0.455244 3.069672  
H 3.184604 1.491062 2.229053  
H 8.226996 -0.405273 0.684175  
H 8.048826 -1.500547 -0.693620  
H 8.267596 0.226630 -0.968474  
H 4.178640 -0.543963 -3.584197  
H 2.684341 -1.063947 -2.795795  
H 2.973897 0.645103 -3.065621  
H 1.509263 2.888274 0.006572  
H 2.661894 2.845948 -1.317011  
H 1.339022 4.026729 -1.347700  
H -1.548238 3.007287 -5.064092  
H -2.257195 1.390472 -5.227757  
H -2.848245 2.499638 -3.984316  
H 0.133117 -2.181383 -3.281581  
H 1.098852 -2.092394 -1.800146  
H -0.647077 -2.222339 -1.695588  
H 1.569690 -5.357262 0.971311  
H 0.371340 -4.445001 1.888147  
H 0.305270 -4.454780 0.120177  
H 3.712325 -4.321414 -0.393020  
H 4.324303 -2.662649 -0.276014  
H 3.055434 -3.062848 -1.440979  
H 2.419013 -2.517851 3.379197  
H 3.397014 -3.886032 2.829989  
H 3.945754 -2.234361 2.515255

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**12B**

C -2.17527 -1.51515 0.16769  
C -0.92252 -1.51796 -0.33197  
B 0.03100 -0.30300 -0.21555  
Si -3.32529 -3.00916 0.17594  
C -0.57066 1.14559 -0.06258  
C 1.58921 -0.51435 -0.20863  
C -0.04892 2.06523 0.84846  
C -0.57843 3.33226 1.03342  
C -1.66901 3.72619 0.26738  
C -2.21111 2.85383 -0.66600  
C -1.66308 1.58571 -0.81234  
C 2.49745 0.48592 -0.57547

C	3.87093	0.29871	-0.58343	F	1.31519	1.98294	1.09891
C	4.39086	-0.93003	-0.19627	F	-0.39471	-0.50439	1.90755
C	3.53476	-1.95233	0.18827	F	-2.07158	-2.33047	2.93514
C	2.16437	-1.73251	0.17119	F	-3.36860	-4.07622	1.29111
F	1.00632	1.73226	1.59727	F	-2.95838	-3.96025	-1.39551
F	-0.05803	4.16945	1.92584	F	-1.29106	-2.15927	-2.43694
F	-2.18691	4.93646	0.42429	C	5.38588	-2.33683	-0.76205
F	-3.24508	3.23782	-1.40947	C	5.74713	0.68544	-0.81538
F	-2.20964	0.80282	-1.74426	C	4.46099	-0.64503	1.62217
F	2.06371	1.68595	-0.96408	H	2.80602	-0.41376	-2.10580
F	4.69091	1.27664	-0.95527	H	1.87183	-0.43789	0.79011
F	5.70090	-1.12430	-0.19269	H	0.31825	-0.18398	-2.11319
F	4.03128	-3.12588	0.56804	H	6.38978	-2.43601	-0.33500
F	1.40171	-2.75249	0.56960	H	4.78400	-3.18333	-0.41847
C	-3.76268	-3.42129	1.95901	H	5.47455	-2.41354	-1.85040
C	-4.88510	-2.56211	-0.77627	H	6.75086	0.55556	-0.39637
C	-2.44211	-4.45544	-0.63548	H	5.36595	1.65905	-0.49361
H	-2.53422	-0.58398	0.61765	H	5.83869	0.70876	-1.90602
H	-0.54752	-2.45085	-0.75337	H	3.85935	-1.47449	2.00559
H	-4.45364	-4.26886	2.00060	H	5.45443	-0.70632	2.07870
H	-2.87058	-3.68514	2.53363	H	3.98738	0.28487	1.95149
H	-4.24475	-2.57333	2.45428				
H	-5.58750	-3.40122	-0.78347	58			
H	-4.65351	-2.30549	-1.81360	12P			
H	-5.39248	-1.70534	-0.32339	C	-0.50115	1.91148	0.83768
H	-1.51936	-4.70758	-0.10423	C	-0.07478	2.88243	1.66252
H	-3.08152	-5.34321	-0.63338	P	0.20767	0.25116	1.21712
H	-2.18467	-4.23384	-1.67549	Si	-1.89920	2.32888	-0.38016
				C	-0.90296	-0.94034	0.33387
41				C	1.88968	0.05632	0.47719
[12BH] <sup>-</sup>				C	2.54787	-1.12897	0.89060
C	2.89882	-0.48609	-1.01774	C	3.85858	-1.37307	0.48442
C	1.76790	-0.36361	-0.29847	C	4.56555	-0.47077	-0.30490
B	0.29317	-0.11630	-0.90429	C	3.90850	0.68792	-0.70382
Si	4.57774	-0.69766	-0.26078	C	2.58961	0.96989	-0.33910
C	-0.33627	1.34957	-0.49612	C	-0.70754	-1.49496	-0.94969
C	-0.74571	-1.24499	-0.31315	C	-1.62681	-2.43060	-1.43430
C	-1.52472	1.76040	-1.09647	C	-2.73719	-2.83646	-0.70138
C	-2.14734	2.97438	-0.83857	C	-2.92296	-2.27709	0.56037
C	-1.57780	3.84470	0.07930	C	-2.02489	-1.35308	1.09249
C	-0.40275	3.47996	0.71501	C	1.86118	-2.17833	1.73255
C	0.18490	2.25161	0.42444	C	5.99589	-0.73343	-0.69729
C	-1.00133	-1.34663	1.05068	C	1.98882	2.23633	-0.89769
C	-1.86609	-2.27756	1.61149	C	-2.29642	-0.81029	2.47701
C	-2.52966	-3.16631	0.77850	C	-3.69635	-3.86352	-1.24359
C	-2.31522	-3.10333	-0.58927	C	0.43419	-1.11911	-1.86358
C	-1.43899	-2.15296	-1.10527	C	-1.97991	4.20983	-0.51930
F	-2.13568	0.95779	-1.98282	C	-1.69295	1.63682	-2.11948
F	-3.28817	3.31622	-1.45466	C	-3.54964	1.71386	0.28734
F	-2.15828	5.02196	0.34770	H	-0.41648	3.91184	1.57360
F	0.14973	4.31318	1.60848	H	0.65152	2.69211	2.45363



H	4.33969	-2.29697	0.79851	C	6.05594	-0.74835	-0.58785
H	4.43261	1.39825	-1.33991	C	1.95722	2.05483	-1.17942
H	-1.47123	-2.84410	-2.42857	C	-2.22968	-0.75282	2.45593
H	-3.78819	-2.57010	1.15120	C	-3.86862	-3.85485	-1.12763
H	1.44507	-1.74439	2.64750	C	0.32027	-1.24831	-1.98831
H	1.02853	-2.64459	1.19439	C	-1.82359	4.33295	-0.35791
H	2.56644	-2.96444	2.00953	C	-1.78885	1.75775	-2.05251
H	6.68321	-0.39088	0.08337	C	-3.50292	1.87695	0.47497
H	6.17557	-1.80102	-0.84708	H	-0.19548	3.79816	1.73064
H	6.25633	-0.20895	-1.61973	H	0.91287	2.47518	2.37202
H	2.59791	2.60042	-1.72817	H	0.26128	-0.05658	2.25630
H	0.97226	2.07449	-1.26268	H	4.42759	-2.20412	1.02637
H	1.92551	3.02828	-0.14629	H	4.44788	1.24273	-1.50505
H	-3.24584	-1.19581	2.85530	H	-1.68254	-2.93094	-2.44439
H	-1.50103	-1.09323	3.17308	H	-3.82019	-2.51288	1.23777
H	-2.34820	0.28299	2.48565	H	1.73426	-1.62779	2.87354
H	-4.71869	-3.66307	-0.91366	H	0.95412	-2.45005	1.51003
H	-3.68423	-3.87920	-2.33587	H	2.55074	-2.95384	2.05708
H	-3.42889	-4.86649	-0.89487	H	6.69529	-0.32832	0.19507
H	0.21210	-1.44156	-2.88371	H	6.26793	-1.81791	-0.64746
H	0.60102	-0.04060	-1.87730	H	6.33857	-0.28367	-1.53397
H	1.37557	-1.58452	-1.55521	H	2.49303	2.29321	-2.09972
H	-2.72597	4.48736	-1.27076	H	0.90949	1.88807	-1.43673
H	-2.27083	4.68446	0.42226	H	1.99214	2.93586	-0.53130
H	-1.01913	4.63179	-0.83078	H	-3.22870	-0.98423	2.82740
H	-2.50829	2.03970	-2.73109	H	-1.51093	-1.18047	3.16499
H	-1.77590	0.54736	-2.13531	H	-2.11959	0.33617	2.47672
H	-0.75421	1.92500	-2.60023	H	-4.84510	-3.68813	-0.66923
H	-3.61328	0.62220	0.26422	H	-3.98253	-3.82374	-2.21290
H	-3.71680	2.05071	1.31477	H	-3.54233	-4.86422	-0.85739
H	-4.36059	2.11207	-0.33188	H	0.10095	-1.65016	-2.97847

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**[12PH]<sup>+</sup>**

C	-0.43765	1.91146	0.80078
C	0.12053	2.75871	1.67806
P	0.20839	0.22266	0.88650
Si	-1.90519	2.46101	-0.31607
C	-0.95825	-0.98880	0.23411
C	1.92667	-0.00226	0.38000
C	2.58677	-1.12068	0.94492
C	3.91695	-1.34274	0.60415
C	4.60917	-0.49787	-0.26436
C	3.92761	0.58699	-0.81197
C	2.59343	0.85914	-0.51383
C	-0.81288	-1.57021	-1.04411
C	-1.77860	-2.48514	-1.45799
C	-2.86251	-2.84222	-0.65542
C	-2.97785	-2.25166	0.60276
C	-2.04402	-1.33197	1.07262
C	1.91267	-2.08504	1.89328

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**12PHBH**

C	1.020139	2.746889	-1.121308
C	2.052616	2.026594	-0.642745
B	1.964651	0.481203	-0.201100
Si	1.039128	4.601794	-1.288908
C	1.905333	0.306132	1.432098
C	3.187196	-0.452376	-0.746989

C	1.460430	-0.900894	1.963891	C	-1.797738	-2.336986	2.115503
C	1.299052	-1.144024	3.321224	C	-2.419096	-6.772953	-0.106369
C	1.606772	-0.137181	4.226739	C	-2.641914	-2.697200	-2.972056
C	2.071420	1.079849	3.751056	C	-1.228984	1.525791	1.678649
C	2.219567	1.274968	2.379508	C	-6.013499	2.369022	2.899829
C	4.515454	-0.113624	-0.509724	C	-5.012660	-1.234098	-0.439585
C	5.594069	-0.879852	-0.930726	C	-1.915983	2.279900	-4.140817
C	5.354821	-2.063531	-1.616237	C	-4.523373	1.075504	-3.041939
C	4.047900	-2.456130	-1.861111	C	-2.885779	2.983084	-1.306954
C	3.002962	-1.652848	-1.418625	H	-0.330235	0.325316	-3.614112
F	1.100549	-1.903474	1.131430	H	0.094240	-0.962861	-2.370794
F	0.844661	-2.322849	3.765281	H	-0.650651	-0.511221	0.194898
F	1.460408	-0.341526	5.535997	H	-1.980616	-4.962729	1.878041
F	2.372053	2.050703	4.615376	H	-2.748757	-5.230800	-2.317474
F	2.665712	2.483131	2.010450	H	-6.469592	0.390136	1.086467
F	4.798651	1.006391	0.175442	H	-3.313570	2.647687	2.890063
F	6.849833	-0.502549	-0.681346	H	-1.072838	-1.525213	2.026715
F	6.373060	-2.818368	-2.031379	H	-2.744642	-1.900839	2.451832
F	3.808433	-3.598829	-2.512099	H	-1.424733	-3.000756	2.895220
F	1.760407	-2.116424	-1.680960	H	-1.419329	-7.204595	-0.217352
C	0.133982	5.169702	-2.849031	H	-2.807190	-7.084126	0.865933
C	0.151559	5.355117	0.201981	H	-3.053310	-7.198653	-0.886836
C	2.810649	5.235903	-1.310634	H	-3.194061	-3.426453	-3.567635
H	0.082593	2.205546	-1.295621	H	-3.198089	-1.758481	-2.982623
H	2.991032	2.565640	-0.481012	H	-1.689985	-2.504957	-3.475503
H	0.922238	0.022481	-0.626555	H	-1.142494	2.451697	2.250327
H	0.132903	6.261530	-2.928101	H	-0.707932	0.743008	2.243567
H	0.602362	4.767639	-3.752829	H	-0.674568	1.672875	0.744434
H	-0.910761	4.838977	-2.836091	H	-5.715531	3.413321	3.016986
H	0.177094	6.449389	0.175906	H	-7.003418	2.339829	2.440187
H	0.636115	5.024077	1.126195	H	-6.096848	1.935827	3.901672
H	-0.899167	5.048186	0.244823	H	-6.082524	-1.102492	-0.613731
H	3.383735	4.788934	-2.127992	H	-4.522334	-1.252077	-1.416315
H	2.832361	6.323081	-1.434410	H	-4.858579	-2.215590	0.020416
H	3.321929	4.995230	-0.373864	H	-2.450222	3.163410	-4.504822
C	-1.708011	0.157541	-2.017908	H	-0.888345	2.586211	-3.920882
C	-0.599103	-0.188647	-2.693973	H	-1.897529	1.545872	-4.951943
P	-1.893959	-0.681429	-0.433290	H	-5.009359	1.878078	-3.606892
Si	-2.776566	1.628540	-2.604647	H	-5.127036	0.896876	-2.147688
C	-3.122470	0.168516	0.586450	H	-4.543316	0.177119	-3.666336
C	-2.136846	-2.481481	-0.435534	H	-3.636993	2.757354	-0.544761
C	-1.991503	-3.101456	0.828647	H	-1.925944	3.157615	-0.810478
C	-2.098136	-4.487640	0.907630	H	-3.175482	3.917526	-1.800404
C	-2.352109	-5.273619	-0.212827				
C	-2.527006	-4.633660	-1.436575				
C	-2.425662	-3.250252	-1.582776				
C	-4.492823	-0.130819	0.450539				
C	-5.410099	0.607464	1.196802				
C	-5.006631	1.606247	2.081453				
C	-3.643369	1.867588	2.208792				
C	-2.681837	1.172836	1.477032				
				90			
				<b><sup>13</sup>H<sub>2</sub></b>			
				P	1.86949	-0.63907	0.36662
				C	0.34068	-1.01192	-0.52512
				C	-0.77238	-0.33575	-0.13731
				B	-0.86770	0.91914	0.92834

C	-2.06920	-0.93113	-0.58061	F	-5.42464	0.05817	2.68514
C	-2.97358	-0.26173	-1.39977	F	-0.37330	2.11155	-1.73533
C	-4.23005	-0.77623	-1.68535	F	1.62952	3.75940	-2.37161
C	-4.61511	-1.99073	-1.13211	F	3.32606	4.67001	-0.44691
C	-3.73855	-2.68093	-0.30686	F	3.01857	3.82567	2.12407
C	-2.48473	-2.14745	-0.04469	F	1.04614	2.16383	2.77489
F	-1.67587	-2.83208	0.76970	H	1.43118	-0.01520	1.53333
F	-4.10295	-3.84427	0.22624	H	-0.53023	0.44221	1.99414
F	-5.81458	-2.49439	-1.40043	H	-0.34874	-0.83524	-3.08452
F	-5.06401	-0.11768	-2.48552	H	-0.47317	-2.63205	-4.78777
F	-2.63656	0.90667	-1.94455	H	0.11534	-4.96662	-4.17097
C	2.60183	-2.18768	0.96374	H	0.77374	-5.49087	-1.83725
C	3.14259	0.49401	-0.26627	H	0.86301	-3.71087	-0.13945
C	0.32232	-2.13514	-1.51162	H	2.22965	-4.31532	3.57886
C	-0.08129	-1.85692	-2.82570	H	4.84519	-4.61131	0.20662
C	-0.15676	-2.86705	-3.77686	H	5.70201	2.30211	1.04026
C	0.17019	-4.17627	-3.42951	H	4.29875	2.13386	-2.99627
C	0.54707	-4.46876	-2.12262	H	2.25630	-0.64330	-2.78037
C	0.61492	-3.45967	-1.16461	H	1.26156	0.77822	-2.46973
C	2.09140	-2.70676	2.17494	H	2.57409	0.86158	-3.64624
C	2.62091	-3.90487	2.65153	H	7.04096	3.29938	-0.78783
C	3.62276	-4.59414	1.97012	H	6.47211	3.21212	-2.46654
C	4.08592	-4.06949	0.76489	H	5.72566	4.34680	-1.33476
C	3.59204	-2.87760	0.23831	H	3.06276	1.11264	2.62975
C	4.03901	1.00069	0.70363	H	3.92564	-0.41418	2.35780
C	5.02076	1.90151	0.29425	H	4.81974	1.06904	2.69690
C	5.13458	2.32008	-1.02936	H	0.09196	-1.86437	2.33468
C	4.23639	1.80623	-1.96198	H	0.67897	-2.67789	3.78668
C	3.23523	0.90168	-1.61112	H	1.28798	-1.07673	3.36917
C	2.28103	0.44491	-2.68131	H	4.70829	-1.50907	-1.02351
C	6.15831	3.34624	-1.42916	H	4.70281	-3.19456	-1.56604
C	3.95261	0.66392	2.17386	H	3.26463	-2.20238	-1.78266
C	0.97910	-2.04265	2.95233	H	5.01962	-5.64947	3.21427
C	4.09802	-2.41268	-1.10375	H	3.44176	-6.42930	3.08714
C	4.19501	-5.86938	2.52855	H	4.58570	-6.50969	1.73490
C	0.20385	2.08945	0.55607				
C	-2.40672	1.40545	1.10186	89			
C	1.09440	2.59316	1.49871	[13H] <sup>+</sup>			
C	2.13422	3.46224	1.19140	P	1.54464	-0.70217	0.52500
C	2.30279	3.88003	-0.11903	C	0.11132	-1.20445	-0.51142
C	1.42834	3.42514	-1.09531	C	-0.97079	-0.38053	-0.53156
C	0.40510	2.55889	-0.73814	B	-1.00414	1.11993	-0.00220
C	-3.28243	0.59921	1.82637	C	-2.25668	-0.82036	-1.13076
C	-4.63241	0.87424	1.98748	C	-2.99972	0.08476	-1.88866
C	-5.15888	2.02092	1.40684	C	-4.22020	-0.23767	-2.45937
C	-4.33030	2.85499	0.67221	C	-4.75198	-1.50254	-2.23454
C	-2.98381	2.53271	0.53056	C	-4.06854	-2.41233	-1.43426
F	-6.45016	2.31255	1.55043	C	-2.84769	-2.06102	-0.87735
F	-4.83167	3.95286	0.10513	F	-2.26846	-2.92350	-0.05005
F	-2.25306	3.37222	-0.21604	F	-4.60263	-3.59786	-1.18009
F	-2.83151	-0.54266	2.37715	F	-5.91779	-1.83181	-2.76043

F	-4.88095	0.64665	-3.19150	H	0.35385	-5.79913	-3.28171
F	-2.52515	1.32789	-2.05648	H	0.81071	-5.82140	-0.84434
C	2.02955	-1.99539	1.69349	H	0.66834	-3.74380	0.46607
C	2.98138	0.14829	-0.18368	H	1.11984	-3.11982	4.76219
C	0.18599	-2.50302	-1.23530	H	4.28621	-4.46496	2.22031
C	-0.09873	-2.50472	-2.60905	H	5.39282	2.23371	0.98396
C	-0.03719	-3.68291	-3.34117	H	4.80745	0.73103	-2.97713
C	0.30426	-4.87849	-2.71034	H	2.54227	-1.77249	-2.33128
C	0.56946	-4.88965	-1.34439	H	1.60996	-0.32805	-2.70721
C	0.50776	-3.71112	-0.60574	H	3.13027	-0.63317	-3.54117
C	1.29478	-2.08650	2.89866	H	7.14399	2.53397	-0.71944
C	1.68325	-3.03896	3.83659	H	6.94762	1.84509	-2.34260
C	2.76414	-3.89341	3.61955	H	6.09792	3.32934	-1.90080
C	3.45647	-3.79032	2.41326	H	2.42049	1.70590	2.30048
C	3.11609	-2.85854	1.43564	H	3.17190	0.14916	2.70533
C	3.71407	0.93267	0.74166	H	4.12304	1.63125	2.72425
C	4.83265	1.62485	0.27962	H	-0.63915	-1.23536	2.40498
C	5.24720	1.56533	-1.04977	H	-0.38619	-1.55363	4.11665
C	4.50487	0.78350	-1.93488	H	0.39910	-0.16550	3.37129
C	3.37677	0.07026	-1.53508	H	4.56711	-1.98557	0.08149
C	2.62473	-0.71083	-2.57780	H	4.50948	-3.75231	0.07956
C	6.43209	2.35642	-1.52744	H	3.23732	-2.84089	-0.72172
C	3.33022	1.10326	2.19387	H	3.88655	-4.43218	5.36356
C	0.10514	-1.20998	3.20571	H	2.32100	-5.23774	5.24451
C	3.90045	-2.84996	0.14832	H	3.66999	-5.75599	4.21637
C	3.17895	-4.89072	4.66541				
C	0.14038	2.05437	-0.51979	89			
C	-2.07912	1.57645	1.01822	<b>[13H]</b>			
C	0.87724	2.86037	0.35000	P	1.87428	-0.50142	0.57507
C	2.03227	3.52075	-0.03168	C	0.38503	-1.01312	-0.40693
C	2.46515	3.41524	-1.34964	C	-0.76031	-0.36588	-0.06896
C	1.74894	2.64850	-2.25939	B	-0.89854	0.89623	0.99437
C	0.61155	1.97988	-1.83145	C	-2.04246	-0.97466	-0.54608
C	-2.85675	0.67264	1.75871	C	-2.92467	-0.33335	-1.41142
C	-3.84094	1.06877	2.64834	C	-4.16172	-0.86643	-1.74618
C	-4.09686	2.42656	2.81235	C	-4.55741	-2.07723	-1.19703
C	-3.36385	3.36633	2.09511	C	-3.70801	-2.74245	-0.32601
C	-2.37822	2.93345	1.22228	C	-2.47443	-2.18835	-0.01343
F	-5.03295	2.82154	3.65022	F	-1.70318	-2.86012	0.84422
F	-3.61556	4.65671	2.24788	F	-4.08600	-3.90681	0.20717
F	-1.72449	3.87535	0.54988	F	-5.74306	-2.60256	-1.51244
F	-2.65578	-0.64567	1.64816	F	-4.97083	-0.22733	-2.59510
F	-4.53589	0.17424	3.33593	F	-2.58780	0.83298	-1.96438
F	-0.01621	1.21113	-2.72865	C	2.70823	-2.11065	0.94501
F	2.19906	2.49391	-3.49744	C	3.12380	0.52413	-0.32952
F	3.58488	4.01091	-1.72436	C	0.36423	-2.16869	-1.35761
F	2.76227	4.18402	0.85511	C	-0.07520	-1.96448	-2.67601
F	0.53138	2.91876	1.64383	C	-0.14076	-3.01088	-3.58849
H	0.98971	0.27571	1.35294	C	0.22705	-4.29776	-3.20238
H	-0.35385	-1.56810	-3.09793	C	0.63510	-4.52407	-1.89190
H	-0.25108	-3.66791	-4.40440	C	0.69536	-3.47618	-0.97594

C	2.27616	-2.70930	2.15361	H	6.89948	3.46072	-1.23285
C	2.84627	-3.91251	2.56858	H	6.13437	3.41101	-2.83229
C	3.84538	-4.54418	1.83109	H	5.50449	4.49015	-1.58096
C	4.24966	-3.95358	0.63822	H	3.25278	1.01262	2.50967
C	3.69522	-2.75739	0.17441	H	4.31318	-0.35449	2.17149
C	4.11271	1.06296	0.53267	H	5.01077	1.24765	2.47411
C	5.03498	1.98672	0.04124	H	0.23066	-2.04430	2.41648
C	5.00145	2.43150	-1.27668	H	0.98455	-2.71785	3.87299
C	4.02367	1.90329	-2.11206	H	1.40166	-1.08481	3.29305
C	3.08897	0.96445	-1.66834	H	4.74883	-1.34747	-1.09760
C	2.06159	0.48746	-2.65807	H	4.71526	-3.01907	-1.69379
C	5.94246	3.50293	-1.75993	H	3.26738	-2.00537	-1.79050
C	4.17901	0.71872	2.00302	H	5.28730	-5.61641	3.02558
C	1.16610	-2.10776	2.98459	H	3.74537	-6.45226	2.83581
C	4.13731	-2.25057	-1.17424	H	4.89786	-6.39810	1.49099
C	4.47566	-5.82337	2.31942				
C	0.16247	2.09227	0.65054	88			
C	-2.46279	1.37281	1.10894	<b>13PB</b>			
C	1.08770	2.54741	1.58808	P	-1.04066	1.10150	-0.05766
C	2.11757	3.43000	1.28608	C	0.40265	1.12028	-1.18448
C	2.24648	3.91812	-0.00466	C	0.92120	-0.07891	-0.82735
C	1.34347	3.50957	-0.97156	B	0.08471	-0.63745	0.44870
C	0.33363	2.62180	-0.62359	C	2.21561	-0.64846	-1.26264
C	-3.35685	0.53823	1.78083	C	2.38437	-2.03306	-1.36884
C	-4.71522	0.79132	1.90904	C	3.59251	-2.61638	-1.72271
C	-5.24052	1.94968	1.35422	C	4.70349	-1.81316	-1.93704
C	-4.39757	2.81719	0.68045	C	4.59378	-0.43906	-1.77890
C	-3.04243	2.51538	0.56894	C	3.37391	0.12191	-1.42564
F	-6.54401	2.22419	1.47044	F	3.36161	1.43225	-1.19764
F	-4.89588	3.93718	0.14313	F	5.66632	0.33235	-1.93274
F	-2.31032	3.41233	-0.10706	F	5.86755	-2.35657	-2.26892
F	-2.91914	-0.61061	2.32495	F	3.69459	-3.93701	-1.83708
F	-5.52053	-0.05624	2.56065	F	1.36950	-2.85479	-1.10692
F	-0.47591	2.23157	-1.62254	C	-1.41401	2.71638	0.74555
F	1.49012	3.92386	-2.23616	C	-2.60329	0.50779	-0.83379
F	3.24754	4.74984	-0.31655	C	0.92722	2.15188	-2.09936
F	3.02312	3.77041	2.21351	C	1.30706	1.83136	-3.40733
F	1.07653	2.08455	2.84898	C	1.86525	2.79982	-4.23513
H	-0.60328	0.44414	2.07725	C	2.05169	4.09764	-3.76632
H	-0.37583	-0.96294	-2.97299	C	1.68376	4.42220	-2.46251
H	-0.48299	-2.81988	-4.60125	C	1.12853	3.45621	-1.63123
H	0.18132	-5.11780	-3.91267	C	-1.23686	2.90764	2.12938
H	0.89907	-5.52664	-1.56872	C	-1.49480	4.16927	2.67736
H	0.97801	-3.68254	0.04938	C	-1.93443	5.23738	1.91080
H	2.49626	-4.36917	3.49244	C	-2.15434	5.01449	0.55051
H	5.00599	-4.44879	0.03186	C	-1.91804	3.78158	-0.04731
H	5.77831	2.39521	0.72291	C	-3.61041	0.12089	0.08459
H	3.96580	2.24503	-3.14344	C	-4.70197	-0.61450	-0.36978
H	2.09858	-0.59720	-2.78630	C	-4.83048	-0.99946	-1.70215
H	1.04838	0.73968	-2.33682	C	-3.86600	-0.55554	-2.59902
H	2.23094	0.95127	-3.63297	C	-2.75442	0.19179	-2.20053

C	-1.77018	0.57111	-3.27669	H	-1.38080	3.29957	-2.08787
C	-5.93249	-1.92823	-2.13294	H	-2.18660	6.54835	3.60528
C	-3.55098	0.44794	1.55698	H	-1.38713	7.29398	2.21638
C	-0.83891	1.83986	3.11864	H	-3.12720	7.01213	2.17668
C	-2.24292	3.64331	-1.51324				
C	-2.17489	6.59506	2.51462	88			
C	-0.97625	-1.83711	0.35489	<b>13</b>			
C	1.09302	-0.60541	1.70607	P	-1.07413	0.97656	0.29291
C	-1.68854	-2.24449	1.47981	C	0.17222	1.22769	-1.03075
C	-2.78196	-3.09707	1.43488	C	0.97258	0.17345	-0.73703
C	-3.20718	-3.58148	0.20588	B	0.23894	-0.75157	0.36457
C	-2.52885	-3.21178	-0.94496	C	2.33340	-0.09052	-1.24052
C	-1.43459	-2.36285	-0.85004	C	2.81821	-1.40311	-1.30365
C	1.77392	0.55312	2.07774	C	4.10935	-1.70701	-1.70790
C	2.73515	0.59866	3.07574	C	4.98982	-0.67860	-2.01314
C	3.09409	-0.57591	3.72256	C	4.56726	0.63854	-1.90487
C	2.47415	-1.76364	3.36555	C	3.26899	0.91857	-1.50108
C	1.50285	-1.76057	2.37005	F	2.95667	2.19946	-1.33731
F	4.01823	-0.55985	4.67717	F	5.41976	1.62876	-2.15393
F	2.82088	-2.89833	3.96902	F	6.23151	-0.95268	-2.39171
F	0.97527	-2.94972	2.06288	F	4.51415	-2.97172	-1.77809
F	1.46757	1.72616	1.49553	F	2.03684	-2.42885	-0.96125
F	3.30687	1.75267	3.41716	C	-1.25320	2.54382	1.25057
F	-0.85949	-2.01061	-2.00892	C	-2.78772	0.47966	-0.16974
F	-2.96794	-3.63023	-2.13285	C	0.36203	2.24953	-2.07973
F	-4.28381	-4.36084	0.12341	C	0.62135	1.82411	-3.38897
F	-3.44572	-3.41861	2.54513	C	0.85929	2.75000	-4.39890
F	-1.36768	-1.74380	2.68616	C	0.84336	4.11285	-4.11345
H	1.16464	0.81789	-3.77126	C	0.59636	4.54383	-2.81206
H	2.15437	2.53997	-5.24829	C	0.36046	3.62051	-1.79962
H	2.48679	4.85229	-4.41324	C	-0.73968	2.68868	2.55189
H	1.83919	5.42856	-2.08759	C	-0.85750	3.92451	3.19601
H	0.86457	3.70090	-0.60597	C	-1.48446	5.01198	2.60547
H	-1.34934	4.30428	3.74700	C	-2.04393	4.83070	1.34010
H	-2.53164	5.82743	-0.06534	C	-1.95715	3.62230	0.65506
H	-5.45480	-0.92859	0.35004	C	-3.65756	0.19619	0.91039
H	-3.95781	-0.82291	-3.64876	C	-4.85643	-0.47109	0.65864
H	-1.45988	1.61424	-3.21511	C	-5.22678	-0.87293	-0.62029
H	-0.87413	-0.04935	-3.21318	C	-4.38786	-0.52742	-1.67570
H	-2.21978	0.41360	-4.25908	C	-3.17480	0.13513	-1.48332
H	-6.86019	-1.72747	-1.59183	C	-2.35068	0.43364	-2.71116
H	-6.12802	-1.84784	-3.20426	C	-6.44788	-1.72163	-0.84767
H	-5.63935	-2.96242	-1.92206	C	-3.35549	0.55287	2.34767
H	-2.59919	0.15417	2.00809	C	-0.12347	1.57588	3.36050
H	-3.68433	1.51930	1.73741	C	-2.67601	3.52667	-0.66912
H	-4.33687	-0.09060	2.09080	C	-1.56620	6.34494	3.30001
H	0.09818	2.11446	3.61252	C	-0.76333	-1.86474	-0.22487
H	-1.60836	1.76199	3.89315	C	1.15010	-1.11904	1.62879
H	-0.71056	0.85331	2.68055	C	-1.80161	-2.35014	0.56808
H	-3.06231	2.93667	-1.67296	C	-2.84617	-3.11821	0.08486
H	-2.54136	4.61014	-1.92232	C	-2.86425	-3.45738	-1.26211

C	-1.84477	-3.02035	-2.09127	C	1.64801	0.46090	1.54575
C	-0.82293	-2.23808	-1.56280	C	2.72986	1.14533	2.08006
C	2.07738	-0.19182	2.10708	C	3.92364	1.17486	1.37164
C	2.95640	-0.43998	3.14911	C	4.01789	0.53094	0.14322
C	2.96337	-1.69616	3.73959	C	2.91749	-0.14105	-0.36964
C	2.08623	-2.66696	3.28065	F	3.03399	-0.71400	-1.56277
C	1.20880	-2.37070	2.24256	F	5.15709	0.58125	-0.54033
F	3.79841	-1.96337	4.73722	F	4.97241	1.82337	1.86309
F	2.09599	-3.87867	3.83162	F	2.63133	1.77028	3.24961
F	0.42231	-3.37443	1.84819	F	0.49478	0.46268	2.22693
F	2.10916	1.04639	1.58692	C	1.60411	-3.10443	-0.77153
F	3.77569	0.51401	3.58994	C	1.66678	-3.96179	-1.87663
F	0.08052	-1.78542	-2.45138	C	2.69462	-4.88915	-1.99737
F	-1.87270	-3.30905	-3.39239	C	3.65803	-4.99224	-0.99729
F	-3.88222	-4.15877	-1.75609	C	3.58528	-4.16836	0.12454
F	-3.85555	-3.48941	0.87223	C	2.56817	-3.22908	0.23822
F	-1.84980	-1.98945	1.85942	C	-0.76318	1.49474	-0.41641
H	0.63309	0.75839	-3.60371	C	-2.20647	-0.77214	-0.00615
H	1.05597	2.40643	-5.40928	C	-1.63695	2.37224	0.22849
H	1.02845	4.83617	-4.90084	C	-1.57541	3.74811	0.06981
H	0.59920	5.60421	-2.58098	C	-0.61869	4.28958	-0.78039
H	0.19860	3.95926	-0.78073	C	0.26177	3.45568	-1.45728
H	-0.45126	4.02289	4.20038	C	0.17758	2.08414	-1.26376
H	-2.57688	5.65568	0.87285	C	-3.35115	-0.36211	-0.69542
H	-5.50187	-0.71420	1.49899	C	-4.58517	-0.97280	-0.54114
H	-4.66646	-0.81306	-2.68779	C	-4.70974	-2.02664	0.35673
H	-2.20078	1.50749	-2.85685	C	-3.60649	-2.45594	1.08160
H	-1.36154	-0.02425	-2.67136	C	-2.38080	-1.83154	0.88965
H	-2.85663	0.04767	-3.59869	F	-5.88310	-2.61823	0.52272
H	-7.20397	-1.55018	-0.07841	F	-3.73319	-3.45253	1.95192
H	-6.89403	-1.52788	-1.82583	F	-1.36745	-2.26564	1.63833
H	-6.16669	-2.77958	-0.81202	F	-3.28069	0.64992	-1.56289
H	-2.35171	0.24351	2.64690	F	-5.64336	-0.56366	-1.23346
H	-3.44101	1.62992	2.52013	F	1.02727	1.32418	-1.96023
H	-4.05967	0.04294	3.00737	F	1.16508	3.97437	-2.28302
H	0.93420	1.77645	3.55324	F	-0.55082	5.60173	-0.94956
H	-0.63042	1.51066	4.32791	F	-2.41660	4.54923	0.71526
H	-0.20247	0.60464	2.87587	F	-2.57380	1.89800	1.05193
H	-3.64909	3.04110	-0.54323	H	-0.44586	-2.50335	-1.10060
H	-2.83960	4.52609	-1.07796	H	0.90875	-3.88580	-2.65124
H	-2.11833	2.95777	-1.41239	H	2.73964	-5.53643	-2.86685
H	-1.39620	6.24388	4.37383	H	4.45676	-5.72144	-1.08455
H	-0.80975	7.03064	2.90511	H	4.32020	-4.26371	0.91702
H	-2.54303	6.81045	3.14680	H	2.50028	-2.60758	1.12516

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**13B**

C	0.49573	-2.14284	-0.68481
C	0.49454	-0.88557	-0.18658
B	-0.82306	-0.05860	-0.19634
C	1.71373	-0.21702	0.33051

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**[13BH]<sup>-</sup>**

C	-1.01269	1.99942	-1.42103
C	-0.59137	0.87356	-0.82032
B	0.85205	0.21455	-1.20910
C	-1.45356	0.18290	0.17296

C	-0.93836	-0.34135	1.36179	C	-2.42503	0.39241	0.39120
C	-1.70179	-1.09081	2.24660	C	-3.29123	0.09950	-0.66401
C	-3.02649	-1.36819	1.94623	C	-4.67001	0.11918	-0.50698
C	-3.56775	-0.89394	0.76116	C	-5.21941	0.46288	0.72153
C	-2.78384	-0.14745	-0.10792	C	-4.38615	0.78346	1.78507
F	-3.35762	0.24532	-1.24442	C	-3.01122	0.75081	1.60440
F	-4.83821	-1.17559	0.45688	F	-2.22942	1.05764	2.64224
F	-3.77340	-2.08547	2.78942	F	-4.90850	1.11379	2.96360
F	-1.16955	-1.55252	3.38132	F	-6.53858	0.48855	0.87738
F	0.33956	-0.14074	1.69127	F	-5.46999	-0.16566	-1.53123
C	-2.19406	2.81978	-1.08752	F	-2.80775	-0.19305	-1.86973
C	-2.97296	3.38539	-2.10505	C	2.81377	-1.01451	0.01068
C	-4.08406	4.16642	-1.80755	C	1.65488	1.61645	-0.58349
C	-4.43309	4.41005	-0.48096	C	-0.79979	-1.85944	-0.76009
C	-3.65327	3.87460	0.54166	C	-0.54628	-2.40196	-2.02507
C	-2.54177	3.09390	0.24212	C	-1.11300	-3.61657	-2.40023
C	0.83054	-1.40363	-0.94159	C	-1.93213	-4.31281	-1.51724
C	2.09883	0.99043	-0.48034	C	-2.18112	-3.78891	-0.24984
C	1.68798	-2.14703	-0.13756	C	-1.61956	-2.57488	0.12468
C	1.58060	-3.52458	0.03538	C	2.67491	-1.89289	1.10600
C	0.56775	-4.22008	-0.60297	C	3.81963	-2.42913	1.69712
C	-0.32615	-3.52499	-1.40409	C	5.10334	-2.13576	1.24677
C	-0.17474	-2.15320	-1.55162	C	5.22457	-1.28021	0.15738
C	3.39572	0.71746	-0.91163	C	4.11189	-0.72563	-0.47566
C	4.52806	1.36396	-0.44206	C	2.11369	2.16286	0.63242
C	4.38949	2.35144	0.52358	C	2.28760	3.54662	0.73020
C	3.12568	2.65696	0.99607	C	2.00286	4.40804	-0.32403
C	2.01640	1.97756	0.49577	C	1.49836	3.85684	-1.50070
F	5.46547	2.99506	0.99334	C	1.31886	2.48365	-1.64884
F	2.98190	3.60380	1.93352	C	0.73096	1.96506	-2.94066
F	0.84049	2.34746	1.03414	C	2.23080	5.89193	-0.20189
F	3.59463	-0.24279	-1.82827	C	2.38987	1.33436	1.86377
F	5.74822	1.05285	-0.90057	C	1.34687	-2.29944	1.69165
F	-1.08622	-1.53782	-2.32377	C	4.35959	0.19152	-1.65109
F	-1.31668	-4.18375	-2.01918	C	6.31499	-2.75085	1.89648
F	0.44966	-5.54371	-0.44628	H	-0.47121	1.31366	0.60197
F	2.44218	-4.18560	0.81887	H	0.08315	-1.85596	-2.72031
F	2.68381	-1.56293	0.54617	H	-0.91443	-4.01745	-3.38889
H	-0.39532	2.38050	-2.23517	H	-2.37037	-5.26110	-1.81073
H	1.00759	0.37558	-2.40429	H	-2.80771	-4.33115	0.45096
H	-2.70371	3.19110	-3.13984	H	-1.79541	-2.17718	1.12047
H	-4.68112	4.58544	-2.61250	H	3.69873	-3.09581	2.54825
H	-5.29979	5.02065	-0.24627	H	6.21500	-1.03569	-0.22016
H	-3.90455	4.07664	1.57886	H	2.64259	3.96124	1.67126
H	-1.91223	2.70367	1.03603	H	1.23310	4.51460	-2.32550
				H	1.42662	1.30012	-3.46092
				H	-0.18488	1.39116	-2.75808
				H	0.48233	2.79531	-3.60493
				H	2.24122	6.20671	0.84400
				H	3.19243	6.17374	-0.64324
				H	1.45321	6.45573	-0.72335
66							
<b>13P</b>							
P	1.47796	-0.18393	-0.95639				
C	-0.21983	-0.55399	-0.34541				
C	-0.95791	0.41242	0.23786				



H	1.63199	0.55798	1.99842	C	3.57708	0.31737	-1.64735
H	3.36108	0.83272	1.81331	C	5.72360	-3.85816	0.09013
H	2.38154	1.97373	2.74932	H	1.32292	0.54839	2.11822
H	0.82452	-2.99830	1.03269	H	-1.07759	1.41737	1.29306
H	1.49744	-2.79645	2.65228	H	1.07103	-1.35154	-1.81887
H	0.68231	-1.44660	1.85051	H	0.79281	-3.60137	-2.76490
H	4.15285	1.23701	-1.39986	H	-0.81964	-5.19362	-1.75583
H	5.40119	0.12053	-1.97039	H	-2.14957	-4.51426	0.22633
H	3.72107	-0.06703	-2.50208	H	-1.87797	-2.25080	1.18353
H	6.54225	-3.72516	1.45136	H	3.77081	-3.68650	1.97070
H	6.15346	-2.90779	2.96581	H	5.26489	-1.72070	-1.52171
H	7.19610	-2.11712	1.77143	H	3.54499	4.71271	1.02727

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[13PH]<sup>+</sup>

P	1.37095	0.36839	0.73154
C	-0.28489	-0.28375	0.33274
C	-1.29799	0.51130	0.72683
C	-2.72337	0.30973	0.43985
C	-3.20371	-0.12238	-0.79998
C	-4.56181	-0.25938	-1.04421
C	-5.47684	0.05525	-0.04421
C	-5.03157	0.51178	1.19201
C	-3.66941	0.64244	1.41205
F	-3.24922	1.08475	2.59632
F	-5.90191	0.81676	2.14207
F	-6.77076	-0.07193	-0.27302
F	-4.99145	-0.66562	-2.22978
F	-2.35840	-0.37761	-1.79614
C	2.67750	-0.84303	0.47668
C	1.67271	2.03298	0.11283
C	-0.40705	-1.63321	-0.26500
C	0.35677	-2.03415	-1.36675
C	0.20335	-3.30720	-1.90352
C	-0.70312	-4.19973	-1.33760
C	-1.45310	-3.81755	-0.22744
C	-1.30518	-2.54417	0.30833
C	2.73561	-1.90087	1.41457
C	3.72365	-2.86717	1.25853
C	4.64771	-2.81544	0.21520
C	4.55888	-1.76441	-0.69696
C	3.59139	-0.76713	-0.59652
C	2.58131	2.81114	0.87100
C	2.84391	4.11158	0.45464
C	2.24030	4.66017	-0.67786
C	1.36910	3.86029	-1.41462
C	1.06755	2.54802	-1.05290
C	0.12481	1.78363	-1.95264
C	2.51871	6.08035	-1.08493
C	3.28722	2.28702	2.10028
C	1.77864	-2.02029	2.57639

C	3.57708	0.31737	-1.64735
C	5.72360	-3.85816	0.09013
H	1.32292	0.54839	2.11822
H	-1.07759	1.41737	1.29306
H	1.07103	-1.35154	-1.81887
H	0.79281	-3.60137	-2.76490
H	-0.81964	-5.19362	-1.75583
H	-2.14957	-4.51426	0.22633
H	-1.87797	-2.25080	1.18353
H	3.77081	-3.68650	1.97070
H	5.26489	-1.72070	-1.52171
H	3.54499	4.71271	1.02727
H	0.91336	4.26608	-2.31403
H	0.20870	2.16392	-2.97233
H	0.31445	0.70933	-1.98351
H	-0.91556	1.90837	-1.63686
H	2.35874	6.22619	-2.15463
H	1.84924	6.76264	-0.55148
H	3.54384	6.36765	-0.84268
H	3.75693	1.31237	1.93011
H	4.07414	2.97916	2.40108
H	2.60176	2.19047	2.95015
H	0.73154	-1.96423	2.26122
H	1.91428	-2.98034	3.07491
H	1.95412	-1.23883	3.32499
H	3.88292	1.28537	-1.23975
H	4.26714	0.05825	-2.45114
H	2.58811	0.45254	-2.09576
H	6.58186	-3.59111	0.71493
H	5.36667	-4.83568	0.42067
H	6.07585	-3.94497	-0.93920

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13PHBH

C	-2.442217	-0.616218	2.047188
C	-2.324450	-0.923390	0.746068
B	-0.910936	-1.443777	0.130440
C	-3.470803	-0.729766	-0.178896
C	-3.817403	-1.696181	-1.125066
C	-4.807972	-1.497266	-2.076387
C	-5.478103	-0.283189	-2.121369
C	-5.140468	0.716169	-1.219929
C	-4.143946	0.491608	-0.279707
F	-3.831131	1.510178	0.523519
F	-5.760153	1.895203	-1.278561
F	-6.430053	-0.075097	-3.028599
F	-5.111939	-2.456690	-2.950163
F	-3.167291	-2.864232	-1.155440
C	-3.670448	-0.240241	2.776685
C	-3.656828	0.826506	3.683136
C	-4.807654	1.189235	4.373443
C	-5.991996	0.481893	4.178352

C	-6.013435	-0.594071	3.294362	C	1.766458	3.012427	-3.453244
C	-4.861751	-0.955016	2.602653	C	1.478287	2.574121	-2.167988
C	-0.812544	-1.075020	-1.463570	C	3.923050	-0.835879	-1.728484
C	-0.593845	-3.013628	0.472841	C	4.928504	-1.306922	-2.574221
C	-0.580978	-1.944818	-2.525480	C	6.242319	-1.448849	-2.151838
C	-0.516193	-1.538144	-3.856229	C	6.547776	-1.114559	-0.831221
C	-0.710690	-0.204597	-4.180298	C	5.594277	-0.641476	0.064220
C	-0.982322	0.697152	-3.162432	C	2.866987	-0.838789	3.208021
C	-1.010830	0.248645	-1.849966	C	3.056788	-0.725062	4.584161
C	0.680770	-3.519340	0.244028	C	3.564387	0.434095	5.167474
C	1.116442	-4.781145	0.607814	C	3.909240	1.499764	4.336405
C	0.218580	-5.643231	1.222817	C	3.744569	1.443435	2.955271
C	-1.077004	-5.209709	1.451590	C	4.181361	2.637183	2.138484
C	-1.459738	-3.921861	1.077558	C	3.723038	0.537338	6.660181
F	0.600524	-6.866782	1.588744	C	2.302761	-2.123973	2.653269
F	-1.950360	-6.030632	2.036761	C	2.542113	-0.736006	-2.328940
F	-2.732360	-3.608411	1.349596	C	6.064687	-0.354114	1.471970
F	1.608023	-2.729344	-0.358369	C	7.306670	-1.983464	-3.070897
F	2.380093	-5.161914	0.390375	H	1.867832	-0.811315	0.514674
F	-1.246914	1.192515	-0.912395	H	0.846719	1.432575	1.677418
F	-1.178461	1.991044	-3.451762	H	4.655867	2.143666	-1.025471
F	-0.646561	0.206159	-5.445927	H	5.158154	2.954234	-3.287500
F	-0.251027	-2.419567	-4.821852	H	3.320848	3.481253	-4.869124
F	-0.373926	-3.251847	-2.320058	H	0.950246	3.224264	-4.135498
H	-1.531883	-0.654075	2.649995	H	0.447629	2.454229	-1.854341
H	-0.032198	-0.787645	0.697203	H	4.659810	-1.570990	-3.594130
H	-2.735675	1.384329	3.826072	H	7.569791	-1.236142	-0.481862
H	-4.782968	2.026886	5.063818	H	2.799975	-1.570508	5.216879
H	-6.890750	0.763052	4.717999	H	4.330441	2.400785	4.775533
H	-6.927953	-1.161088	3.150492	H	4.981118	3.168007	2.659502
H	-4.865772	-1.810044	1.933054	H	4.560550	2.357563	1.151552
P	2.902296	0.125686	0.622927	H	3.359978	3.339616	1.970336
C	2.138750	1.682553	0.039432	H	2.792156	0.888736	7.116540
C	1.120405	2.066717	0.834328	H	3.960220	-0.433345	7.100672
C	0.276422	3.258826	0.713483	H	4.511627	1.243482	6.928084
C	0.713674	4.508412	0.269243	H	2.876944	-2.514766	1.805944
C	-0.147332	5.592304	0.192182	H	2.292589	-2.893873	3.426259
C	-1.471506	5.452779	0.594053	H	1.269134	-1.984253	2.313332
C	-1.929160	4.234499	1.082443	H	1.748622	-0.464388	-1.632343
C	-1.047587	3.167505	1.154074	H	2.541807	0.008307	-3.132915
F	-1.477272	2.020402	1.661751	H	2.264383	-1.704797	-2.753441
F	-3.180783	4.108576	1.496918	H	5.522658	-0.940777	2.217216
F	-2.290439	6.492137	0.529098	H	7.122933	-0.606137	1.553346
F	0.293645	6.772154	-0.233444	H	5.957660	0.698308	1.743846
F	1.990872	4.699834	-0.060630	H	7.496120	-3.040306	-2.858222
C	4.263637	-0.486239	-0.402835	H	7.005578	-1.901571	-4.116818
C	3.209650	0.264326	2.396605	H	8.248993	-1.446784	-2.936709
C	2.509537	2.252781	-1.274957				
C	3.836866	2.397780	-1.691297				
C	4.124200	2.847698	-2.976781				
C	3.092776	3.147068	-3.862395				

<b>14H<sub>2</sub></b>				F	0.36611	1.40073	-1.86456
P	2.24060	-0.67931	0.80464	F	2.27262	3.07674	-2.65722
C	0.77339	-1.21411	-0.06911	F	3.64652	4.56099	-0.83557
C	-0.36507	-0.50014	0.11881	F	3.02964	4.36541	1.80564
B	-0.49069	0.90846	0.95940	F	1.11793	2.69185	2.62361
C	-1.61546	-1.13668	-0.38368	H	1.84872	0.14813	1.86210
C	-2.46010	-0.52900	-1.30993	H	-0.19365	0.62575	2.10396
C	-3.68298	-1.08043	-1.66427	H	0.40694	-1.17471	-2.68011
C	-4.09682	-2.26733	-1.07354	H	0.54714	-3.05232	-4.30409
C	-3.28086	-2.89544	-0.14322	H	1.11587	-5.33532	-3.50632
C	-2.05811	-2.32903	0.18752	H	1.51217	-5.73262	-1.09153
F	-1.30899	-2.95744	1.09606	H	1.34938	-3.87287	0.52020
F	-3.67392	-4.03270	0.42493	H	1.54812	-2.21702	3.12484
F	-5.26480	-2.80490	-1.40593	H	2.54398	-4.23797	4.15468
F	-4.45663	-0.48379	-2.56675	H	4.57823	-5.25703	3.17014
F	-2.09456	0.60750	-1.90059	H	5.63884	-4.24648	1.17322
C	3.05399	-2.09075	1.57711	H	4.66114	-2.21101	0.14459
C	3.44103	0.23084	-0.17993	H	4.32744	1.17338	1.55457
C	0.89956	-2.39069	-0.98059	H	5.92131	2.51145	0.21809
C	0.66266	-2.17819	-2.34696	H	5.91732	2.34123	-2.25364
C	0.73871	-3.23101	-3.25113	H	4.33151	0.81905	-3.39729
C	1.05594	-4.51157	-2.80262	H	2.72304	-0.52169	-2.07320
C	1.28374	-4.73341	-1.44770				
C	1.20464	-3.68211	-0.53779				
C	2.45203	-2.65510	2.70761	71			
C	3.00513	-3.79498	3.27874	<b>[14H]<sup>+</sup></b>			
C	4.15010	-4.36597	2.72295	P	-1.78994	0.59063	1.09536
C	4.74803	-3.79920	1.60057	C	-0.52000	1.32644	0.04136
C	4.20214	-2.65666	1.02232	C	0.53514	0.54771	-0.30184
C	4.34251	1.07813	0.47151	B	0.61968	-1.02614	-0.06876
C	5.23930	1.83080	-0.27982	C	1.71504	1.11211	-0.99370
C	5.23262	1.73545	-1.66978	C	2.35112	0.35119	-1.97573
C	4.34211	0.87947	-2.31485	C	3.48187	0.78364	-2.64609
C	3.43932	0.12388	-1.57407	C	4.03361	2.01383	-2.30096
C	0.60256	1.99590	0.41757	C	3.45676	2.77924	-1.29312
C	-2.02632	1.43251	0.98251	C	2.32087	2.32074	-0.63983
C	1.32739	2.79173	1.30277	F	1.83964	3.04966	0.35975
C	2.33193	3.66729	0.90662	F	4.00912	3.93052	-0.94187
C	2.64418	3.77708	-0.44031	F	5.11629	2.44682	-2.91938
C	1.94654	3.01513	-1.36401	F	4.04209	0.03875	-3.58632
C	0.95236	2.15284	-0.92059	F	1.84994	-0.85802	-2.27024
C	-2.95961	0.73830	1.74873	C	-2.17407	1.62663	2.50658
C	-4.30706	1.06358	1.80698	C	-3.25803	0.07688	0.20052
C	-4.77080	2.14266	1.06596	C	-0.78110	2.70445	-0.45904
C	-3.88413	2.85918	0.27673	C	-0.79429	2.88861	-1.85055
C	-2.54303	2.49032	0.24471	C	-1.05109	4.14253	-2.39163
F	-6.05854	2.47948	1.10601	C	-1.29693	5.22676	-1.55129
F	-4.32620	3.88668	-0.44973	C	-1.28030	5.05237	-0.17027
F	-1.75490	3.20373	-0.57182	C	-1.02605	3.79929	0.37870
F	-2.56753	-0.33934	2.45092	C	-1.16309	1.84394	3.45228
F	-5.15592	0.35701	2.55593	C	-1.41552	2.68463	4.52804

C	-2.66346	3.29823	4.65467	C	-0.24820	-0.40557	0.19125
C	-3.66376	3.07465	3.71247	B	-0.58270	0.96395	1.04904
C	-3.42458	2.23470	2.62802	C	-1.42801	-1.16284	-0.33429
C	-4.02935	-0.96164	0.73686	C	-2.24495	-0.69751	-1.36142
C	-5.12794	-1.43180	0.02452	C	-3.40520	-1.35456	-1.74641
C	-5.44884	-0.86923	-1.21047	C	-3.78404	-2.51713	-1.09089
C	-4.68524	0.17328	-1.73360	C	-2.99556	-3.00985	-0.06253
C	-3.58249	0.65227	-1.03366	C	-1.83923	-2.33286	0.30175
C	-0.54542	-1.89063	-0.64840	F	-1.12215	-2.84055	1.30546
C	1.78014	-1.59467	0.78410	F	-3.35665	-4.12910	0.57051
C	-1.07618	-2.98536	0.04506	F	-4.89485	-3.16175	-1.45462
C	-2.21415	-3.65758	-0.36970	F	-4.15613	-0.88164	-2.74440
C	-2.85712	-3.24533	-1.53344	F	-1.92434	0.41923	-2.01771
C	-2.35521	-2.17993	-2.26928	C	3.13173	-1.83077	1.61650
C	-1.22404	-1.51936	-1.81393	C	3.62155	0.16306	-0.37940
C	2.46311	-0.80386	1.71763	C	1.13272	-2.17563	-0.86980
C	3.52637	-1.27464	2.46885	C	0.98542	-2.01534	-2.25519
C	3.95450	-2.58588	2.28123	C	1.11069	-3.09606	-3.12162
C	3.31401	-3.41000	1.36014	C	1.38095	-4.36592	-2.61792
C	2.24340	-2.90895	0.63678	C	1.50436	-4.54472	-1.24291
F	4.96885	-3.04938	2.98237	C	1.37872	-3.46331	-0.37500
F	3.73244	-4.65313	1.18456	C	2.60313	-2.25517	2.84205
F	1.66772	-3.72122	-0.24367	C	3.00505	-3.45858	3.41487
F	2.07353	0.45875	1.94070	C	3.96269	-4.24608	2.77943
F	4.13177	-0.49844	3.35632	C	4.50874	-3.82547	1.56914
F	-0.80990	-0.47133	-2.53141	C	4.09105	-2.63124	0.98766
F	-2.98526	-1.77233	-3.36314	C	4.97914	0.28056	-0.04717
F	-3.97144	-3.84169	-1.91547	C	5.90145	0.76091	-0.96984
F	-2.72115	-4.65029	0.34748	C	5.48138	1.15821	-2.23819
F	-0.53326	-3.36199	1.20406	C	4.13464	1.06664	-2.57287
H	-1.23031	-0.57573	1.63748	C	3.21409	0.56599	-1.65438
H	-0.61293	2.03534	-2.49834	C	0.39755	2.19596	0.61164
H	-1.06115	4.27253	-3.46846	C	-2.17734	1.31942	0.92382
H	-1.49581	6.20622	-1.97270	C	0.98746	3.02932	1.55865
H	-1.45477	5.89791	0.48616	C	1.92477	4.00596	1.24357
H	-0.97736	3.68783	1.45612	C	2.31110	4.18514	-0.07634
H	-0.18614	1.37931	3.33713	C	1.73839	3.39495	-1.05940
H	-0.64277	2.86236	5.26753	C	0.79350	2.44363	-0.69791
H	-2.85520	3.95408	5.49719	C	-3.09641	0.57180	1.65862
H	-4.63063	3.55343	3.81951	C	-4.47226	0.74086	1.58424
H	-4.19821	2.05745	1.88683	C	-4.98870	1.70837	0.73423
H	-3.77049	-1.41088	1.69288	C	-4.12041	2.47251	-0.02784
H	-5.72209	-2.24595	0.42520	C	-2.74822	2.26150	0.07548
H	-6.29725	-1.24902	-1.76958	F	-6.30979	1.89653	0.64889
H	-4.93808	0.60374	-2.69592	F	-4.61210	3.39998	-0.85804
H	-2.97568	1.45088	-1.44924	F	-1.98577	3.02000	-0.72567
				F	-2.66536	-0.40949	2.46836
				F	-5.30464	-0.01087	2.31502
71				F	0.27738	1.72126	-1.70820
<b>[14H]<sup>-</sup></b>				F	2.10793	3.54357	-2.33777
P	2.40598	-0.27199	0.93483	F	3.21797	5.11491	-0.39484
C	0.96135	-0.98308	0.01424				

F	2.46636	4.77428	2.19808	C	-5.58385	0.69533	0.68365
F	0.68571	2.90542	2.85814	C	-4.67805	1.54137	0.04669
H	-0.36546	0.71373	2.21251	C	-3.31703	1.42406	0.30530
H	0.73725	-1.02925	-2.63968	C	-1.23968	-0.53573	-1.42060
H	0.99016	-2.94622	-4.19040	C	0.81721	-1.85822	-0.09239
H	1.48047	-5.21214	-3.29119	C	-2.29996	-1.42848	-1.27448
H	1.69256	-5.53437	-0.83698	C	-3.45589	-1.38611	-2.03342
H	1.44828	-3.62097	0.69583	C	-3.57899	-0.40143	-3.00758
H	1.85440	-1.64000	3.33599	C	-2.55718	0.51768	-3.18644
H	2.57360	-3.77893	4.35837	C	-1.41612	0.44117	-2.39220
H	4.28201	-5.18309	3.22597	C	1.80925	-1.87898	0.88947
H	5.24916	-4.43919	1.06436	C	2.61289	-2.97933	1.15206
H	4.49478	-2.32977	0.02580	C	2.45141	-4.12899	0.39212
H	5.31483	-0.00986	0.94576	C	1.49299	-4.15423	-0.61015
H	6.94916	0.83740	-0.69379	C	0.70695	-3.03054	-0.83904
H	6.19877	1.54649	-2.95466	F	3.21025	-5.19601	0.62143
H	3.78929	1.39276	-3.54887	F	1.34053	-5.25030	-1.35103
H	2.16383	0.51893	-1.92056	F	-0.17398	-3.12957	-1.83929
				F	2.02402	-0.79219	1.64896
				F	3.53600	-2.93865	2.11164
				F	-0.50049	1.40525	-2.57624
				F	-2.68069	1.47513	-4.10557
				F	-4.67808	-0.33453	-3.75375
				F	-4.44817	-2.25101	-1.83220
				F	-2.24090	-2.34048	-0.28733
				H	0.78761	3.76168	-0.57687
				H	0.48217	6.13468	0.03418
				H	-0.76177	6.74267	2.09443
				H	-1.71784	4.95516	3.52728
				H	-1.41229	2.58514	2.92018
				H	0.24967	1.29494	3.72911
				H	0.89784	0.21426	5.85783
				H	0.42929	-2.19053	6.22653
				H	-0.67024	-3.52926	4.45291
				H	-1.30366	-2.45913	2.30676
				H	-3.41942	-1.13356	2.55632
				H	-5.83677	-0.91544	2.08866
				H	-6.64471	0.78085	0.47278
				H	-5.02972	2.28902	-0.65652
				H	-2.60782	2.07677	-0.19793
				70			
				14			
P	-1.06922	0.17946	1.29589	P	-1.12743	0.52270	1.23011
C	-0.09488	1.59610	0.77867	C	-0.16756	1.63883	0.19283
C	0.67215	0.89945	-0.11423	C	0.64972	0.68999	-0.34109
B	-0.06746	-0.53819	-0.31457	B	-0.04682	-0.74594	-0.04119
C	1.94337	1.27783	-0.74010	C	1.92673	0.87925	-1.03884
C	2.34975	0.66807	-1.93429	C	2.36674	-0.05915	-1.97830
C	3.58468	0.91867	-2.51271	C	3.60634	0.03387	-2.59347
C	4.48282	1.76253	-1.87198	C	4.46990	1.06205	-2.23889
C	4.13439	2.35160	-0.66396				
C	2.89097	2.09049	-0.10715				
F	2.62037	2.64090	1.07281				
F	5.00222	3.13960	-0.03594				
F	5.67023	2.00314	-2.41121				
F	3.92283	0.34053	-3.66065				
F	1.54362	-0.18515	-2.56331				
C	-0.62276	-0.50087	2.91035				
C	-2.85921	0.45617	1.20800				
C	-0.23276	3.00424	1.16259				
C	0.27073	4.02413	0.34153				
C	0.08521	5.35737	0.67881				
C	-0.61793	5.69946	1.83354				
C	-1.15091	4.69762	2.63881				
C	-0.96783	3.36092	2.30064				
C	0.01988	0.24747	3.89939				
C	0.39378	-0.36465	5.09130				
C	0.13303	-1.71765	5.29599				
C	-0.48789	-2.47056	4.30233				
C	-0.85579	-1.86845	3.10320				
C	-3.77009	-0.38273	1.85468				
C	-5.13075	-0.25953	1.59058				

C	4.08517	1.98800	-1.27735	H	-1.05854	3.49050	1.97936
C	2.83762	1.87866	-0.68192	H	1.15285	1.81318	2.47931
F	2.53143	2.75665	0.27245	H	1.73405	2.31548	4.82173
F	4.92260	2.95631	-0.91781	H	0.16740	1.72402	6.65432
F	5.66195	1.15710	-2.81280	H	-2.00019	0.64001	6.12071
F	3.98013	-0.86199	-3.50116	H	-2.59689	0.14554	3.78990
F	1.58591	-1.08463	-2.31606	H	-3.39611	-1.07729	2.21534
C	-0.74946	0.91593	2.97394	H	-5.76821	-1.14229	1.56909
C	-2.92397	0.61884	0.95623	H	-6.63948	0.43576	-0.13570
C	-0.26226	3.09309	0.01511	H	-5.12464	2.11168	-1.15904
C	0.08751	3.66032	-1.21872	H	-2.75031	2.21648	-0.48537
C	-0.02642	5.02966	-1.42013				
C	-0.50373	5.85063	-0.39944				
C	-0.87763	5.29221	0.81977	48			
C	-0.76429	3.92121	1.02628	<b>14B</b>			
C	0.46766	1.54103	3.27617	C	-1.572798	2.284216	0.698517
C	0.79144	1.82783	4.59724	C	-2.216388	1.335740	-0.019225
C	-0.08924	1.49797	5.62462	B	-2.377573	-0.094467	0.571188
C	-1.30371	0.88796	5.32674	C	-2.741510	1.570586	-1.386657
C	-1.63638	0.59827	4.00673	C	-4.030464	1.143166	-1.697483
C	-3.78046	-0.33536	1.52238	C	-4.582046	1.287824	-2.962066
C	-5.11557	-0.39070	1.13824	C	-3.817610	1.864593	-3.967462
C	-5.60175	0.49187	0.17586	C	-2.518048	2.279463	-3.699938
C	-4.75174	1.43203	-0.40003	C	-1.990224	2.116770	-2.426989
C	-3.41459	1.49612	-0.01643	F	-0.732840	2.491864	-2.217983
C	-1.21788	-1.09487	-1.09350	F	-1.783731	2.811061	-4.672419
C	0.86276	-1.91837	0.55473	F	-4.324269	2.013462	-5.185297
C	-2.26549	-1.92290	-0.69849	F	-5.821211	0.878158	-3.216540
C	-3.44528	-2.06687	-1.40769	F	-4.769380	0.561211	-0.743924
C	-3.59721	-1.37699	-2.60403	C	-1.311439	3.689122	0.354225
C	-2.57327	-0.55888	-3.05601	C	-0.110588	4.273204	0.775008
C	-1.41423	-0.42630	-2.29813	C	0.176095	5.599556	0.475607
C	1.88061	-1.62289	1.45990	C	-0.749844	6.369466	-0.223537
C	2.74598	-2.56790	1.99016	C	-1.963867	5.808655	-0.616240
C	2.61838	-3.89207	1.59484	C	-2.244375	4.478026	-0.332666
C	1.63500	-4.23809	0.68015	C	-2.340565	-1.338350	-0.386030
C	0.78969	-3.25766	0.17269	C	-2.557791	-0.297002	2.115744
F	3.43427	-4.81877	2.08557	C	-3.132135	-2.467971	-0.169712
F	1.51686	-5.50392	0.28478	C	-3.134818	-3.560153	-1.023561
F	-0.10344	-3.67147	-0.73022	C	-2.303653	-3.551024	-2.137329
F	2.06113	-0.35410	1.86538	C	-1.485204	-2.456754	-2.385201
F	3.69347	-2.21826	2.85873	C	-1.518817	-1.376669	-1.514585
F	-0.49445	0.42680	-2.77689	C	-1.986041	-1.378633	2.791515
F	-2.71438	0.10709	-4.20174	C	-2.134244	-1.581888	4.153973
F	-4.72099	-1.49409	-3.30508	C	-2.906092	-0.690297	4.889874
F	-4.44013	-2.82019	-0.94072	C	-3.513130	0.387433	4.259846
F	-2.18370	-2.54062	0.49098	C	-3.329661	0.569985	2.895284
H	0.42407	3.01121	-2.02218	F	-3.064878	-0.872260	6.192177
H	0.24590	5.45705	-2.37964	F	-4.264585	1.228178	4.963547
H	-0.59434	6.92002	-0.55895	F	-3.964610	1.602580	2.341727
H	-1.26080	5.92499	1.61360	F	-1.242308	-2.264025	2.124696
				F	-1.554582	-2.613097	4.759841

F -0.691438 -0.362221 -1.780902  
F -0.678511 -2.457065 -3.441670  
F -2.288042 -4.589648 -2.959517  
F -3.916028 -4.609374 -0.789385  
F -3.943582 -2.523138 0.888186  
H -1.169451 1.975307 1.663576  
H 0.606392 3.673112 1.328400  
H 1.117433 6.034649 0.794312  
H -0.532574 7.407887 -0.451108  
H -2.697567 6.413234 -1.139132  
H -3.201251 4.052708 -0.617322

F -0.192647 -0.476155 -1.692617  
F -0.614268 -2.246066 -3.651372  
F -2.573148 -4.128699 -3.402417  
F -4.101934 -4.185535 -1.149705  
F -3.715092 -2.434683 0.798697  
H -0.161685 2.010656 1.414097  
H -0.386236 -0.415995 1.137636  
H 1.209711 3.948190 0.333109  
H 1.152424 6.352617 -0.256699  
H -1.023173 7.482009 -0.659895  
H -3.133844 6.192309 -0.434793  
H -3.062806 3.791504 0.181749

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**14BH**

C -0.867918 2.265023 0.623076  
C -1.606987 1.258056 0.127343  
B -1.538623 -0.230470 0.796944  
C -2.462466 1.470703 -1.068449  
C -3.757581 0.951944 -1.152942  
C -4.529258 1.039075 -2.303769  
C -4.004001 1.636334 -3.439272  
C -2.710797 2.135272 -3.407704  
C -1.958580 2.035403 -2.245270  
F -0.712031 2.502942 -2.296798  
F -2.192104 2.693587 -4.505529  
F -4.735909 1.729485 -4.552357  
F -5.770585 0.546605 -2.328709  
F -4.307494 0.332719 -0.106031  
C -0.921095 3.695232 0.260467  
C 0.258322 4.444206 0.160369  
C 0.224797 5.793631 -0.172773  
C -0.994520 6.427944 -0.400668  
C -2.177192 5.701710 -0.280325  
C -2.141721 4.351915 0.053532  
C -1.898870 -1.375664 -0.320751  
C -2.438170 -0.332000 2.163723  
C -2.894730 -2.344574 -0.259234  
C -3.130646 -3.271734 -1.271056  
C -2.358526 -3.245846 -2.420075  
C -1.361702 -2.288902 -2.540986  
C -1.159340 -1.390058 -1.502905  
C -2.276247 -1.445818 2.985682  
C -2.908433 -1.614313 4.207396  
C -3.766619 -0.623985 4.665181  
C -3.973094 0.499799 3.885258  
C -3.317203 0.623648 2.661783  
F -4.388568 -0.758278 5.843231  
F -4.805223 1.458392 4.314970  
F -3.600692 1.749994 1.983233  
F -1.475794 -2.446421 2.585757  
F -2.707870 -2.711718 4.949899

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**14P**

P -1.87515 0.56732 -1.48660  
C -0.29609 -0.01218 -0.70920  
C 0.81298 0.56311 -1.21087  
C 2.18036 0.41700 -0.67835  
C 2.48464 0.49735 0.68200  
C 3.78600 0.38403 1.15061  
C 4.82945 0.20675 0.25125  
C 4.56495 0.14649 -1.11070  
C 3.25540 0.25893 -1.55337  
F 3.02534 0.19726 -2.86591  
F 5.56155 -0.02037 -1.97534  
F 6.07708 0.10171 0.69252  
F 4.04289 0.46697 2.45273  
F 1.52398 0.71437 1.57974  
C -3.04192 -0.76538 -0.97906  
C -2.35156 1.96379 -0.38231  
C -0.26502 -1.06854 0.33104  
C -1.09224 -1.01779 1.45928  
C -1.05455 -2.03392 2.40582  
C -0.20319 -3.12354 2.23392  
C 0.61024 -3.19282 1.10679  
C 0.57734 -2.17342 0.16082  
C -2.83472 -2.02376 -1.55670  
C -3.64910 -3.09998 -1.22483  
C -4.70051 -2.92721 -0.32726  
C -4.92553 -1.67591 0.23750  
C -4.09867 -0.60072 -0.08118  
C -3.52733 2.65195 -0.71241  
C -3.95067 3.74035 0.04235  
C -3.19021 4.17425 1.12621  
C -2.00944 3.51254 1.44822  
C -1.59041 2.41288 0.70136  
H 0.72297 1.21497 -2.07805  
H -1.76570 -0.17641 1.59196  
H -1.69723 -1.97825 3.27832

H	-0.18161	-3.91943	2.97123
H	1.26502	-4.04539	0.95773
H	1.19609	-2.23376	-0.73010
H	-2.01847	-2.16441	-2.26214
H	-3.46665	-4.07249	-1.67066
H	-5.34191	-3.76442	-0.07163
H	-5.74264	-1.53448	0.93804
H	-4.27191	0.36523	0.38386
H	-4.11637	2.32872	-1.56783
H	-4.86768	4.25682	-0.22280
H	-3.51343	5.02895	1.71149
H	-1.40825	3.84977	2.28663
H	-0.66370	1.90990	0.96358

H	-1.23536	2.98188	3.05231
H	-0.03462	1.62795	4.74676
H	1.09173	-0.47778	4.07655
H	1.00195	-1.23638	1.72311
H	-0.82998	-2.46066	0.72702
H	-1.93576	-4.38307	1.82179
H	-4.36544	-4.75597	1.51664
H	-5.70060	-3.20996	0.11404
H	-4.61751	-1.27622	-0.97689
H	-2.17374	1.61077	-3.09829
H	-3.58200	3.63664	-3.22094
H	-5.12349	4.19203	-1.36266
H	-5.26791	2.72102	0.62536
H	-3.86226	0.68797	0.77077

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**[14PH]<sup>+</sup>**

P	-1.84640	-0.39653	-1.04819
C	-0.22428	-0.04360	-0.34396
C	0.83722	-0.36413	-1.11216
C	2.25084	-0.16795	-0.77572
C	2.75734	0.95799	-0.11871
C	4.11341	1.09524	0.13972
C	5.00016	0.10718	-0.27538
C	4.53079	-1.01375	-0.95320
C	3.17346	-1.12865	-1.20288
F	2.73019	-2.20216	-1.85597
F	5.37368	-1.95313	-1.35229
F	6.29003	0.23689	-0.03145
F	4.56875	2.17337	0.75922
F	1.95186	1.95058	0.23944
C	-2.65408	-1.74904	-0.18965
C	-2.93370	1.02394	-1.15580
C	-0.18771	0.43556	1.06148
C	-0.81672	1.62598	1.44253
C	-0.75896	2.05049	2.76615
C	-0.07850	1.29353	3.71597
C	0.55541	0.11088	3.34021
C	0.50180	-0.31793	2.01942
C	-1.89453	-2.62340	0.59430
C	-2.51739	-3.70430	1.20838
C	-3.88378	-3.91158	1.03531
C	-4.63779	-3.04245	0.24771
C	-4.02874	-1.95621	-0.36822
C	-2.84763	1.85226	-2.28070
C	-3.63874	2.99340	-2.35010
C	-4.50570	3.30233	-1.30377
C	-4.58916	2.47561	-0.18377
C	-3.80377	1.33199	-0.10204
H	-1.57998	-0.75926	-2.37657
H	0.67506	-0.84421	-2.07597
H	-1.31035	2.24309	0.69870

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**14PHBH**

P	1.827080	-2.099052	-0.120720
C	2.827820	-0.627977	0.162033
C	2.163133	0.522650	0.344397
C	2.853019	1.812558	0.547393
C	3.681286	2.346043	-0.436748
C	4.258088	3.600401	-0.295687
C	4.021367	4.335809	0.860320
C	3.215238	3.818088	1.867830
C	2.640715	2.567006	1.697967
F	1.879543	2.071391	2.672706
F	3.011084	4.513611	2.977995
F	4.578645	5.529073	1.007030
F	5.038109	4.097005	-1.248545
F	3.919645	1.656277	-1.552728
C	1.957856	-2.616813	-1.838700
C	2.301005	-3.423749	0.988928
C	4.298185	-0.803524	0.302462
C	4.886054	-0.537060	1.544130
C	6.253051	-0.715253	1.724819
C	7.043489	-1.165455	0.669832
C	6.463934	-1.433173	-0.567456
C	5.095852	-1.255606	-0.753837
C	2.267591	-1.670752	-2.821998
C	2.338206	-2.069590	-4.151208
C	2.076901	-3.393438	-4.497016
C	1.747896	-4.328153	-3.518109
C	1.694098	-3.946610	-2.182009
C	1.467407	-3.684319	2.081883
C	1.826771	-4.680430	2.985769
C	3.003231	-5.399855	2.798439
C	3.832765	-5.132974	1.708441
C	3.486964	-4.143630	0.797250
H	0.515196	-1.757990	0.240441
H	1.073072	0.559634	0.316549



H	4.259252	-0.197044	2.363857	F	-2.754778	-2.820822	4.902943
H	6.699800	-0.506609	2.691110	F	-0.170985	-0.466388	-1.632923
H	8.110038	-1.304954	0.811445	F	-0.610921	-2.183083	-3.641207
H	7.078135	-1.774134	-1.394204	F	-2.579443	-4.060130	-3.437681
H	4.651846	-1.452515	-1.724605	F	-4.119051	-4.149026	-1.197152
H	2.451711	-0.634913	-2.549011	F	-3.732986	-2.446928	0.788127
H	2.581377	-1.342211	-4.917678	H	-0.210101	2.052178	1.527859
H	2.121913	-3.697215	-5.537549	H	1.177482	3.886061	-0.154235
H	1.536047	-5.355485	-3.792973	H	1.040558	6.270606	-0.783672
H	1.450797	-4.675181	-1.413867	H	-1.152069	7.435892	-0.771179
H	0.548470	-3.122248	2.227084	H	-3.198608	6.197084	-0.108488
H	1.181981	-4.891986	3.831518	H	-3.042919	3.809786	0.559226
H	3.277982	-6.176492	3.504670	H	-0.416900	-0.452916	1.221571
H	4.748418	-5.697257	1.569622				
H	4.129058	-3.931139	-0.053173				
C	-0.855425	2.266048	0.673029	71			
C	-1.579002	1.249766	0.171813	<b>15H<sub>2</sub></b>			
B	-1.567406	-0.237703	0.839743	P	-2.20856	-0.96086	-0.52733
C	-2.392761	1.470010	-1.053245	C	-0.74633	-1.35496	0.43744
C	-3.709107	1.016229	-1.153675	C	0.37470	-0.64141	0.16328
C	-4.450898	1.121618	-2.321870	B	0.48133	0.64772	-0.86655
C	-3.870017	1.675454	-3.454087	C	1.66496	-1.19727	0.66405
C	-2.552569	2.107105	-3.404466	C	2.53586	-0.47765	1.48074
C	-1.833368	1.990303	-2.222837	C	3.80632	-0.94144	1.79210
F	-0.553311	2.367419	-2.251716	C	4.24291	-2.15266	1.27080
F	-1.979099	2.609503	-4.498397	C	3.40221	-2.89374	0.45208
F	-4.568066	1.781024	-4.582363	C	2.13447	-2.41020	0.16239
F	-5.709719	0.688032	-2.367058	F	1.35692	-3.14751	-0.63828
F	-4.296943	0.430776	-0.106831	F	3.81230	-4.05742	-0.04581
C	-0.925187	3.687284	0.253060	F	5.45469	-2.60686	1.56621
C	0.220236	4.399057	-0.120793	F	4.60687	-0.23531	2.58459
C	0.141596	5.737469	-0.488561	F	2.16215	0.69435	1.98613
C	-1.088985	6.390505	-0.486612	C	-2.94869	-2.52553	-1.05766
C	-2.236703	5.694146	-0.117347	C	-3.47532	0.08032	0.22531
C	-2.155410	4.354395	0.250660	C	-0.84887	-2.60593	1.29185
C	-1.914447	-1.369457	-0.302376	C	-1.98954	-2.61054	2.31437
C	-2.459887	-0.362978	2.196110	C	-2.13144	-3.39126	-1.79520
C	-2.918497	-2.334672	-0.264761	C	-2.63724	-4.61216	-2.22391
C	-3.151109	-3.239156	-1.298162	C	-3.94976	-4.96939	-1.91587
C	-2.372830	-3.196142	-2.444825	C	-4.75775	-4.11009	-1.17746
C	-1.370648	-2.242255	-2.544280	C	-4.26045	-2.88287	-0.74485
C	-1.178446	-1.367186	-1.485323	C	-4.53538	0.53485	-0.57025
C	-2.316118	-1.499485	2.984239	C	-5.49587	1.37407	-0.01915
C	-2.944131	-1.699217	4.200984	C	-5.40152	1.75622	1.31974
C	-3.785249	-0.706899	4.687837	C	-4.34601	1.30803	2.10781
C	-3.974135	0.444447	3.941600	C	-3.37361	0.47400	1.56001
C	-3.318427	0.596124	2.721241	C	2.00873	1.19257	-0.97178
F	-4.404872	-0.865292	5.857464	C	-0.64484	1.77681	-0.52120
F	-4.784050	1.401161	4.398965	C	2.52101	2.33998	-0.37813
F	-3.571122	1.743475	2.073739	C	3.85716	2.71770	-0.47093
F	-1.529908	-2.508954	2.540844	C	4.74502	1.92206	-1.17834

C	4.28592	0.75792	-1.78013	F	4.52432	3.43917	-1.23111
C	2.94333	0.42700	-1.66697	F	5.53997	1.64883	-2.99633
C	-0.88198	2.25328	0.76582	F	4.18858	-0.64456	-3.54431
C	-1.90945	3.12811	1.08475	F	1.81832	-1.12512	-2.32306
C	-2.77763	3.55188	0.08907	C	-1.97927	2.49485	1.85453
C	-2.58588	3.11248	-1.21043	C	-3.27082	0.42970	0.13484
C	-1.52991	2.25053	-1.48627	C	-0.43867	2.94583	-0.92006
F	-3.81946	4.32488	0.39243	C	-1.76659	3.38429	-1.54833
F	-3.45111	3.46450	-2.16399	C	-0.85702	3.02202	2.50808
F	-1.46146	1.79836	-2.75012	C	-1.01637	4.11278	3.35269
F	-0.14931	1.80109	1.78995	C	-2.28163	4.67143	3.53872
F	-2.14217	3.48046	2.35168	C	-3.39172	4.14516	2.88391
F	2.56256	-0.73013	-2.23747	C	-3.24751	3.05002	2.03630
F	5.13400	-0.02293	-2.45225	C	-4.10607	-0.23275	1.04590
F	6.02762	2.26623	-1.27471	C	-5.29919	-0.78971	0.59980
F	4.29266	3.83145	0.11914	C	-5.65828	-0.68313	-0.74454
F	1.73456	3.14500	0.34918	C	-4.82571	-0.02686	-1.64801
C	-2.10209	-3.96078	3.01611	C	-3.62347	0.52540	-1.21376
H	-1.80119	-0.33004	-1.70974	C	1.61732	-1.39820	0.90105
H	0.21062	0.17676	-1.95318	C	-0.70707	-1.75078	-0.50045
H	-0.94913	-3.48695	0.64448	C	1.93391	-2.75821	1.02727
H	0.09761	-2.72659	1.82689	C	2.93328	-3.22038	1.86872
H	-1.81812	-1.81665	3.05036	C	3.64841	-2.30692	2.63778
H	-2.94728	-2.38239	1.82651	C	3.36401	-0.94654	2.55734
H	-1.10018	-3.11790	-2.01131	C	2.36880	-0.52055	1.69475
H	-2.00728	-5.28550	-2.79478	C	-1.32323	-1.58609	-1.74435
H	-4.34153	-5.92394	-2.25135	C	-2.50705	-2.22318	-2.08194
H	-5.77664	-4.39268	-0.93573	C	-3.13954	-3.02426	-1.14052
H	-4.88839	-2.21045	-0.16762	C	-2.56431	-3.21988	0.11168
H	-4.59864	0.25161	-1.61850	C	-1.36152	-2.59805	0.40228
H	-6.30709	1.74311	-0.63688	F	-4.31057	-3.56663	-1.41915
H	-6.14490	2.42370	1.74222	F	-3.19180	-3.95384	1.01902
H	-4.25503	1.63280	3.13812	F	-0.87520	-2.75356	1.63569
H	-2.51298	0.17154	2.15033	F	-0.80782	-0.75096	-2.64724
H	-2.89272	-3.95476	3.76972	F	-3.09217	-1.98889	-3.24971
H	-2.32776	-4.75134	2.29371	F	2.11643	0.79546	1.66671
H	-1.16341	-4.22086	3.51421	F	4.03648	-0.08157	3.30276
				F	4.59499	-2.73079	3.44942
				F	3.21204	-4.51136	1.94884
70				F	1.28112	-3.66315	0.30538
[15H] <sup>+</sup>				C	-1.74807	4.87555	-1.87401
P	-1.71946	1.08549	0.76909	H	-1.19938	0.06597	1.58175
C	-0.40458	1.52212	-0.40581	H	-0.18967	3.63164	-0.10136
C	0.58525	0.61512	-0.57937	H	0.35151	3.05621	-1.66767
B	0.52458	-0.89461	-0.07567	H	-1.94360	2.80670	-2.46227
C	1.86098	0.96380	-1.24773	H	-2.60757	3.17951	-0.87101
C	2.45076	0.03520	-2.10715	H	0.12988	2.59073	2.34887
C	3.67372	0.25195	-2.71836	H	-0.15556	4.52868	3.86414
C	4.36888	1.42359	-2.43183	H	-2.40030	5.52416	4.19856
C	3.84122	2.34633	-1.53539	H	-4.37150	4.58546	3.03137
C	2.60993	2.10183	-0.94202	H	-4.11039	2.63602	1.52277
F	2.17190	2.97151	-0.03318				

H	-3.82702	-0.32105	2.09355	C	-0.14999	3.21095	1.27993
H	-5.94386	-1.31143	1.29829	F	1.70130	5.91329	-0.26333
H	-6.58687	-1.12479	-1.08973	F	0.12080	5.48212	1.91901
H	-5.09638	0.03530	-2.69592	F	-0.91776	3.05827	2.36944
H	-2.94901	0.98782	-1.92711	F	1.12851	1.47811	-1.60518
H	-2.67671	5.18451	-2.35712	F	2.19978	3.85134	-1.98524
H	-1.62502	5.46824	-0.96301	F	-1.93185	-1.52984	2.00639
H	-0.92156	5.11728	-2.54790	F	-4.58116	-1.84017	2.23996
				F	-6.27246	0.10915	1.35743
				F	-5.24955	2.36854	0.23428
				F	-2.63153	2.69309	-0.02215
70				C	2.60688	-2.66377	-3.37648
<b>[15H]<sup>-</sup></b>				H	-0.08113	0.47788	2.03328
P	2.57095	-0.20928	0.97642	H	2.70908	-2.57103	-0.67073
C	1.30884	-1.03988	-0.09312	H	1.05533	-2.94362	-1.08124
C	0.04100	-0.58886	-0.02675	H	1.05764	-1.23236	-2.86505
B	-0.49680	0.65800	0.90663	H	2.67781	-0.72592	-2.42967
C	-1.00082	-1.27716	-0.84598	H	1.19621	-2.69389	1.81784
C	-1.76771	-0.55452	-1.76058	H	1.82101	-4.51670	3.36453
C	-2.84953	-1.10455	-2.43226	H	4.05239	-4.52696	4.45467
C	-3.20592	-2.42375	-2.18848	H	5.65226	-2.68207	3.99112
C	-2.47775	-3.17077	-1.27545	H	5.02640	-0.85701	2.45239
C	-1.40157	-2.59129	-0.61548	H	3.44955	1.92631	-0.67586
F	-0.75230	-3.35523	0.27069	H	5.14733	2.20951	-2.43240
F	-2.82021	-4.43917	-1.03472	H	6.71196	0.34684	-2.96804
F	-4.23852	-2.97115	-2.83291	H	6.55116	-1.78737	-1.70985
F	-3.55195	-0.38011	-3.30591	H	4.83311	-2.07548	0.03587
F	-1.48467	0.72950	-1.98794	H	3.58672	-2.97985	-3.00185
C	3.07268	-1.65431	2.01198	H	1.96342	-3.54942	-3.41911
C	3.99646	-0.10345	-0.20831	H	2.74195	-2.29480	-4.39723
C	1.78014	-2.12343	-1.04326				
C	2.01270	-1.59461	-2.46507				
C	2.17628	-2.69314	2.28851				
C	2.52949	-3.71861	3.16358	69			
C	3.77909	-3.72487	3.77565	<b>15PB</b>			
C	4.67599	-2.69029	3.51490	P	1.09908	-0.14443	1.32434
C	4.32165	-1.66218	2.64827	C	-0.61454	0.08633	1.80942
C	4.12275	1.10571	-0.90424	C	-1.12065	0.13210	0.55504
C	5.08616	1.26775	-1.89556	B	0.13736	-0.09142	-0.47813
C	5.95931	0.22533	-2.19472	C	-2.55417	0.37297	0.27783
C	5.86765	-0.97234	-1.48908	C	-3.31329	-0.50903	-0.48567
C	4.89507	-1.13536	-0.50537	C	-4.65279	-0.27570	-0.76798
C	-2.13222	0.60821	1.01471	C	-5.26110	0.87802	-0.29323
C	0.06773	2.12013	0.43922	C	-4.52851	1.78508	0.46262
C	-3.04187	1.56057	0.56901	C	-3.19476	1.52365	0.73536
C	-4.42278	1.41433	0.67869	F	-2.51450	2.42495	1.45102
C	-4.94880	0.26689	1.24772	F	-5.10783	2.89447	0.91256
C	-4.08473	-0.72120	1.69852	F	-6.54075	1.11333	-0.55737
C	-2.71677	-0.52448	1.57915	F	-5.35308	-1.14767	-1.48707
C	0.84061	2.41044	-0.67873	F	-2.76034	-1.62775	-0.95672
C	1.40462	3.66161	-0.92074	C	2.08145	1.33043	1.70611
C	1.16919	4.70508	-0.04419	C	1.96591	-1.57964	2.00080
C	0.36980	4.47841	1.06791	C	-1.27240	0.11229	3.15431

C	-1.76903	-1.28834	3.54679				
C	1.43667	2.57261	1.74334	69			
C	2.19082	3.73977	1.79951	<b>15</b>			
C	3.58298	3.67203	1.81237	P	1.63825	-0.75943	1.20294
C	4.22441	2.43590	1.78235	C	0.48776	-1.53296	-0.03112
C	3.47724	1.26322	1.72884	C	-0.50966	-0.69589	-0.38877
C	2.68006	-2.39779	1.11993	B	-0.43009	0.83484	0.02774
C	3.36458	-3.50702	1.61039	C	-1.73236	-1.06823	-1.13734
C	3.33210	-3.79940	2.97091	C	-2.29684	-0.16211	-2.03724
C	2.62525	-2.98065	3.85086	C	-3.48125	-0.40536	-2.71312
C	1.94554	-1.86762	3.36963	C	-4.17111	-1.58487	-2.46177
C	0.72749	1.23742	-1.17428	C	-3.67015	-2.49127	-1.53712
C	0.23244	-1.48495	-1.27729	C	-2.48182	-2.21540	-0.87333
C	0.03006	2.42186	-1.35765	F	-2.07061	-3.09650	0.03673
C	0.64361	3.61633	-1.72375	F	-4.34377	-3.60658	-1.27273
C	2.01611	3.64742	-1.91372	F	-5.30966	-1.83805	-3.09390
C	2.75956	2.48454	-1.74307	F	-3.96716	0.48090	-3.57588
C	2.09984	1.31780	-1.40071	F	-1.68457	1.01188	-2.24449
C	-0.13709	-2.68683	-0.66940	C	1.98504	-2.22144	2.26135
C	-0.03222	-3.92620	-1.28004	C	3.19852	-0.50958	0.26075
C	0.46040	-4.00152	-2.57636	C	0.72200	-2.96497	-0.45835
C	0.83930	-2.83877	-3.22773	C	0.44752	-3.26693	-1.93894
C	0.71969	-1.61448	-2.57657	C	0.91728	-2.71399	3.02350
F	0.57108	-5.17908	-3.18279	C	1.09633	-3.81243	3.85580
F	1.31246	-2.89965	-4.47114	C	2.34793	-4.41939	3.95112
F	1.10233	-0.54388	-3.28120	C	3.41428	-3.92768	3.20527
F	-0.60288	-2.68174	0.58986	C	3.23537	-2.83538	2.35790
F	-0.39408	-5.03735	-0.64065	C	4.16906	0.30869	0.85256
F	2.85369	0.22272	-1.18838	C	5.32740	0.65393	0.16064
F	4.08195	2.51036	-1.89746	C	5.52328	0.19539	-1.14002
F	2.62120	4.78277	-2.25035	C	4.56499	-0.61894	-1.73927
F	-0.07375	4.72806	-1.88150	C	3.40996	-0.96958	-1.04485
F	-1.29422	2.46962	-1.14509	C	-1.57176	1.44044	0.91153
C	-2.39836	-1.30410	4.93555	C	0.76682	1.69210	-0.51772
H	-2.11385	0.81392	3.14436	C	-1.92854	2.79141	0.86421
H	-0.56674	0.48511	3.90809	C	-2.95838	3.32480	1.62453
H	-2.49098	-1.62197	2.79261	C	-3.67344	2.49277	2.47700
H	-0.93398	-1.99722	3.49793	C	-3.35936	1.14230	2.55611
H	0.35077	2.62353	1.70419	C	-2.33080	0.64066	1.77201
H	1.69114	4.70264	1.82243	C	1.40723	1.38114	-1.71794
H	4.16869	4.58484	1.84308	C	2.59145	1.98624	-2.11846
H	5.30792	2.38430	1.79066	C	3.18661	2.92488	-1.29152
H	3.97618	0.29918	1.68526	C	2.57800	3.27717	-0.09106
H	2.69743	-2.16288	0.05882	C	1.38778	2.66873	0.26750
H	3.91834	-4.14375	0.92880	F	4.34196	3.47757	-1.63456
H	3.86111	-4.66777	3.34968	F	3.16101	4.16824	0.70696
H	2.60647	-3.20910	4.91120	F	0.87391	2.99267	1.45568
H	1.40237	-1.22196	4.05513	F	0.91562	0.44392	-2.53389
H	-2.76130	-2.30106	5.19581	F	3.17912	1.63546	-3.25947
H	-1.67322	-1.00049	5.69748	F	-2.07750	-0.66678	1.88841
H	-3.24463	-0.61253	4.98953	F	-4.04577	0.34839	3.37251

F	-4.65766	2.98739	3.21261	F	-1.40555	2.33536	1.28968
F	-3.27133	4.61391	1.54320	C	-2.16366	-0.05155	-0.12746
F	-1.29039	3.62866	0.04829	C	-3.04489	0.87304	-0.69206
C	1.17595	-4.53163	-2.38702	C	-4.41978	0.79754	-0.53490
H	0.14838	-3.64763	0.17902	C	-4.95647	-0.22490	0.23911
H	1.77305	-3.19979	-0.24652	C	-4.11853	-1.15461	0.84023
H	-0.62453	-3.38991	-2.11451	C	-2.74696	-1.05489	0.64926
H	0.76021	-2.41100	-2.55055	F	-1.98714	-1.95180	1.28197
H	-0.05852	-2.23715	2.95325	C	-1.08420	-4.98956	-0.06872
H	0.26103	-4.19196	4.43549	F	-4.63249	-2.12046	1.59506
H	2.48976	-5.27257	4.60649	F	-6.26794	-0.30931	0.40592
H	4.38977	-4.39846	3.27543	F	-5.22419	1.68695	-1.10755
H	4.06882	-2.46411	1.76871	F	-2.57145	1.87493	-1.43657
H	4.00438	0.69592	1.85582	H	-1.31781	-2.16384	-1.58806
H	6.06508	1.29742	0.62920	H	1.23448	-3.75063	-0.96588
H	6.41517	0.47990	-1.68857	H	0.74055	-3.49184	-2.63250
H	4.70556	-0.96542	-2.75786	H	-0.12873	-5.64619	-1.89251
H	2.65375	-1.57089	-1.54093	H	-1.47845	-4.55455	-2.15051
H	0.95133	-4.77439	-3.42841	H	-1.58621	-4.10800	0.33987
H	2.26007	-4.41072	-2.29401	H	-0.23302	-5.21285	0.58229
H	0.88419	-5.38746	-1.77071	H	-1.77845	-5.83137	-0.01431

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**15B**

C	-0.28778	-2.27265	-1.23982
C	0.23358	-1.23671	-0.55194
B	-0.61037	0.04897	-0.32401
C	1.61465	-1.25805	-0.01059
C	1.82223	-0.85938	1.30933
C	3.08064	-0.81701	1.88875
C	4.18717	-1.16869	1.12497
C	4.02207	-1.54634	-0.20120
C	2.74851	-1.57312	-0.75502
F	2.63570	-1.89004	-2.04435
F	5.08435	-1.85921	-0.93700
F	5.40106	-1.13547	1.66058
F	3.23713	-0.44325	3.15487
F	0.76802	-0.48941	2.04750
C	0.09217	1.45259	-0.31661
C	-0.34733	2.50155	0.49422
C	0.36243	-3.57135	-1.60524
C	-0.61552	-4.74746	-1.50112
C	0.28130	3.73660	0.53490
C	1.38690	3.96075	-0.27666
C	1.85093	2.95397	-1.11323
C	1.20374	1.72657	-1.11752
F	1.67241	0.80343	-1.96164
F	2.89840	3.17604	-1.90080
F	1.99504	5.13726	-0.25616
F	-0.15974	4.70237	1.33400

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**[15BH]<sup>-</sup>**

C	-0.16188	-2.47103	-1.63383
C	0.12832	-1.34790	-0.96180
B	-0.69591	0.04284	-1.22609
C	1.26808	-1.32588	-0.00981
C	1.16047	-0.72479	1.24853
C	2.23780	-0.58616	2.11154
C	3.49244	-1.03334	1.72262
C	3.65017	-1.60761	0.47189
C	2.55467	-1.73022	-0.37411
F	2.78776	-2.25014	-1.58228
F	4.85954	-2.02435	0.08217
F	4.53666	-0.91246	2.54658
F	2.08093	-0.02332	3.31274
F	-0.01042	-0.23682	1.66227
C	0.25494	1.33280	-0.86605
C	0.00204	2.34829	0.05003
C	0.44926	-3.84171	-1.51426
C	-0.61064	-4.94955	-1.48097
C	0.88379	3.39623	0.30284
C	2.09342	3.45286	-0.36806
C	2.40454	2.45583	-1.28104
C	1.49033	1.43590	-1.50530
F	1.86529	0.49003	-2.38307
F	3.57605	2.49264	-1.92938
F	2.95322	4.45195	-0.13614
F	0.57852	4.34828	1.19398

F	-1.12837	2.36973	0.77331	C	-2.84720	2.99144	1.76230
C	-2.16210	0.09858	-0.49589	C	-2.70825	1.76893	1.11193
C	-3.04600	1.11533	-0.85513	C	1.11837	-2.63162	-3.43716
C	-4.34280	1.22899	-0.37969	H	0.00627	1.54189	0.18993
C	-4.81853	0.28340	0.51846	H	-0.86140	-2.22609	-1.57420
C	-3.98143	-0.74242	0.91856	H	0.67942	-2.10021	-0.75075
C	-2.68254	-0.80983	0.41767	H	0.00745	-0.77477	-3.42914
F	-1.95235	-1.83887	0.88370	H	1.56199	-0.67785	-2.61587
C	-1.47270	-4.89526	-0.22286	H	-4.88297	-0.82482	-1.25958
F	-4.42676	-1.65851	1.78975	H	-6.16965	-2.42900	0.11495
F	-6.06858	0.36666	0.99154	H	-5.06556	-3.62221	1.98989
F	-5.14097	2.23342	-0.76757	H	-2.67630	-3.18668	2.49322
F	-2.63784	2.07310	-1.70273	H	-1.39787	-1.55710	1.14728
H	-0.97315	-2.40036	-2.36340	H	-2.12536	2.90093	-2.03628
H	-0.92022	0.09871	-2.42016	H	-2.34888	5.07488	-0.87308
H	1.06919	-3.90930	-0.61138	H	-2.82275	5.13457	1.56193
H	1.12184	-4.01375	-2.36539	H	-3.05801	3.01460	2.82682
H	-0.11774	-5.92689	-1.55312	H	-2.81087	0.84326	1.67092
H	-1.24817	-4.85738	-2.36997	H	1.61223	-2.44875	-4.39457
H	-1.96012	-3.92292	-0.12462	H	1.81471	-3.18455	-2.79903
H	-0.85461	-5.03554	0.67054	H	0.25360	-3.27598	-3.62230
H	-2.24142	-5.67393	-0.22631				

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**15P**

P	-2.19525	0.16629	-1.20753
C	-0.45132	-0.26305	-0.79957
C	0.36633	0.57172	-0.14445
C	1.78861	0.28669	0.15520
C	2.19890	-0.80525	0.91762
C	3.53420	-1.03721	1.22022
C	4.50195	-0.14716	0.77518
C	4.12769	0.96181	0.02739
C	2.78682	1.16527	-0.26501
F	2.45443	2.23763	-0.98392
F	5.05309	1.81482	-0.40254
F	5.78171	-0.35588	1.06211
F	3.88819	-2.09351	1.94752
F	1.30017	-1.67457	1.39170
C	-3.05708	-1.07051	-0.14546
C	-2.44188	1.72514	-0.26091
C	0.00213	-1.56599	-1.42360
C	0.69169	-1.32597	-2.77386
C	-4.40220	-1.33316	-0.42773
C	-5.12558	-2.23884	0.34220
C	-4.50570	-2.90840	1.39418
C	-3.16408	-2.66442	1.67623
C	-2.44286	-1.74774	0.91505
C	-2.32091	2.92679	-0.96733
C	-2.44902	4.14998	-0.31425
C	-2.71485	4.18274	1.05168

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**[15PH]<sup>+</sup>**

P	-2.04426	0.22102	-0.79741
C	-0.32589	-0.32236	-0.77745
C	0.56870	0.53085	-0.24711
C	1.98033	0.21998	0.01123
C	2.39297	-0.95684	0.63831
C	3.72775	-1.20252	0.92553
C	4.68385	-0.24734	0.59654
C	4.30227	0.94730	-0.00814
C	2.96180	1.17039	-0.27859
F	2.59993	2.31899	-0.84489
F	5.21353	1.85633	-0.31452
F	5.95598	-0.47125	0.86426
F	4.08893	-2.32614	1.52594
F	1.48915	-1.86325	1.01863
C	-3.01978	-0.92720	0.17087
C	-2.24325	1.91110	-0.23806
C	-0.04863	-1.70651	-1.32206
C	-0.80970	-2.04430	-2.61019
C	-4.37778	-1.10154	-0.12010
C	-5.13624	-1.95746	0.66912
C	-4.54297	-2.62845	1.73806
C	-3.19099	-2.45167	2.02502
C	-2.41858	-1.60075	1.24105
C	-1.93851	2.95848	-1.11744
C	-2.05362	4.27066	-0.67614
C	-2.47132	4.53182	0.62892

C	-2.77598	3.48740	1.49896	F	-1.587474	-1.764980	1.104163
C	-2.66426	2.16864	1.07038	C	-2.176790	2.454162	-0.085414
C	-0.34132	-3.37515	-3.19258	C	-1.283042	3.295483	0.566538
H	-2.53091	0.17814	-2.11015	C	-1.302046	4.681295	0.450304
H	0.26269	1.53976	0.02361	C	-2.262996	5.282886	-0.344498
H	1.02802	-1.77870	-1.51112	C	-3.183489	4.487376	-1.016313
H	-0.28150	-2.45892	-0.55906	C	-3.116549	3.107455	-0.882334
H	-1.88735	-2.10899	-2.40494	F	-3.995034	2.394722	-1.597210
H	-0.66670	-1.24397	-3.34662	C	-3.621898	0.272750	-4.600703
H	-4.83907	-0.57792	-0.95307	F	-4.102780	5.060026	-1.794971
H	-6.18780	-2.10365	0.44927	F	-2.299333	6.608603	-0.473534
H	-5.13922	-3.29718	2.34954	F	-0.376950	5.426046	1.065805
H	-2.73575	-2.98024	2.85501	F	-0.288914	2.798492	1.335317
H	-1.36048	-1.46751	1.45439	H	-1.351604	2.068480	-2.470467
H	-1.61497	2.75454	-2.13499	H	-0.997380	0.632383	0.577655
H	-1.82375	5.08842	-1.34984	H	-1.038227	-0.549484	-4.078140
H	-2.56381	5.55820	0.96750	H	-0.220242	0.982465	-4.381593
H	-3.10574	3.69858	2.50996	H	-2.029103	0.725443	-5.993895
H	-2.90989	1.35054	1.74130	H	-2.432781	2.047085	-4.905347
H	-0.89928	-3.62581	-4.09635	H	-3.927926	0.526456	-3.582534
H	0.71989	-3.33378	-3.45207	H	-3.517764	-0.817015	-4.659076
H	-0.48140	-4.18627	-2.47272	H	-4.423320	0.568800	-5.282352

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**15PHBH**

C	-1.414925	0.988201	-2.614454	C	1.423226	-0.654706	1.158011
C	-1.780899	0.246761	-1.559175	C	2.865592	0.100317	0.363225
B	-2.016906	0.838775	-0.046990	C	3.967305	-0.656549	0.244806
C	-1.879123	-1.228880	-1.742916	C	5.279907	-0.164453	-0.209076
C	-3.104081	-1.894480	-1.729454	C	6.022592	-0.896379	-1.135349
C	-3.202284	-3.278225	-1.817865	C	7.285355	-0.497423	-1.546223
C	-2.050645	-4.044243	-1.936928	C	7.844291	0.655307	-1.006138
C	-0.815505	-3.413928	-1.974596	C	7.141130	1.394397	-0.062827
C	-0.751189	-2.032548	-1.871693	C	5.878274	0.974174	0.330466
F	0.476226	-1.466234	-1.887218	F	5.248810	1.680412	1.272303
F	0.300999	-4.143368	-2.108328	F	7.685411	2.481999	0.468890
F	-2.127960	-5.369028	-2.029712	F	9.050486	1.046631	-1.387501
F	-4.390708	-3.874723	-1.795221	F	7.961189	-1.205711	-2.441864
F	-4.237062	-1.199545	-1.635730	F	5.504967	-2.009530	-1.650218
C	-3.152270	0.008088	0.790498	C	1.677434	-2.399103	1.509325
C	-2.840784	-1.259606	1.276011	C	1.120638	0.259135	2.673827
C	-1.158816	0.538632	-4.025600	C	2.702673	1.544584	-0.049535
C	-2.306591	0.958824	-4.959792	C	1.508163	1.791172	-0.981947
C	-3.720095	-2.084605	1.962891	C	1.654793	-3.303481	0.441581
C	-5.008524	-1.631870	2.203364	C	1.799029	-4.661966	0.693914
C	-5.372376	-0.368349	1.762164	C	1.973569	-5.111391	2.001967
C	-4.452730	0.416879	1.073897	C	2.002674	-4.207651	3.061276
F	-4.890753	1.623608	0.699109	C	1.849541	-2.845306	2.821892
F	-6.603529	0.081461	2.003933	C	2.183618	0.900591	3.319314
F	-5.878779	-2.394272	2.862987	C	1.945728	1.586333	4.505294
F	-3.340456	-3.290951	2.391743	C	0.658599	1.631637	5.036517
				C	-0.395530	0.988796	4.391558
				C	-0.171863	0.297196	3.206904
				C	1.419991	3.266631	-1.360530

H	0.294230	-0.526813	0.340903	C	3.70301	-3.07418	-3.18812
H	3.933597	-1.713285	0.501992	C	4.47617	-3.88023	-2.35544
H	3.621508	1.871414	-0.545626	C	4.69390	-3.52015	-1.02728
H	2.582987	2.167989	0.846395	C	4.13024	-2.35464	-0.52019
H	0.571999	1.501133	-0.495020	C	0.72562	2.45252	-0.54482
H	1.600908	1.163778	-1.875908	C	-1.86002	1.89107	-1.22249
H	1.524579	-2.952811	-0.576388	C	1.51889	3.22836	-1.38856
H	1.759849	-5.362927	-0.132395	C	2.46059	4.14425	-0.93431
H	2.080122	-6.173295	2.197414	C	2.63492	4.31744	0.43091
H	2.132737	-4.563191	4.077526	C	1.86541	3.57664	1.31372
H	1.849675	-2.138509	3.646081	C	0.94345	2.66735	0.81286
H	3.183266	0.879041	2.892158	C	-2.43391	2.84818	-0.39305
H	2.762408	2.093235	5.007317	C	-3.77554	3.21210	-0.45824
H	0.475126	2.177299	5.956213	C	-4.60673	2.59501	-1.37999
H	-1.397743	1.033283	4.802972	C	-4.08656	1.61877	-2.21924
H	-0.989809	-0.191700	2.689877	C	-2.74043	1.29606	-2.12425
H	2.323591	3.601000	-1.880282	F	-5.89420	2.92664	-1.45352
H	1.290915	3.884779	-0.466088	F	-4.88133	1.00497	-3.09760
H	0.564203	3.447005	-2.016314	F	-2.30440	0.31069	-2.92715
				F	-1.70871	3.46216	0.55265
				F	-4.26983	4.14044	0.36183
				F	0.28933	1.93160	1.72217
				F	2.06016	3.69901	2.62877
				F	3.57378	5.14439	0.88807
				F	3.22884	4.82199	-1.79028
				F	1.44463	3.06929	-2.71849
				C	0.93088	-3.83829	-1.02313
				C	1.06352	-5.08011	-1.64220
				C	1.44843	-6.19525	-0.90523
				C	1.70890	-6.06787	0.45848
				C	1.59635	-4.82679	1.07368
				C	-2.40701	-3.20638	2.97950
				C	-1.28724	-3.20533	2.15270
				H	2.12536	0.61886	-1.81118
				H	0.02300	1.07113	-2.27091
				H	0.20748	-0.37192	3.30056
				H	-1.79278	-0.36975	4.74444
				H	-3.47779	-2.18140	4.54130
				H	4.53946	1.64865	-1.31773
				H	6.01376	3.06246	0.07252
				H	5.79448	3.03397	2.54155
				H	4.10414	1.58079	3.62485
				H	2.61700	0.16242	2.24421
				H	2.49510	-1.29891	-3.32476
				H	3.54453	-3.35177	-4.22460
				H	4.91474	-4.79317	-2.74463
				H	5.30059	-4.14867	-0.38469
				H	4.29358	-2.07023	0.51572
				H	0.62068	-2.97575	-1.60053
				H	0.85759	-5.17213	-2.70408
				H	1.54525	-7.16167	-1.38942
84							
<b>16H<sub>2</sub></b>							
P	2.41100	-0.16101	-0.68555				
C	0.86372	-0.76057	0.01278				
C	-0.26562	-0.07471	-0.31540				
B	-0.32606	1.35495	-1.14305				
C	-1.59111	-0.68832	-0.01239				
C	-2.10521	-1.68740	-0.83146				
C	-3.37863	-2.21178	-0.64594				
C	-4.17812	-1.72178	0.37477				
C	-3.70806	-0.69495	1.18408				
C	-2.44257	-0.17669	0.96469				
F	-2.03677	0.83210	1.73368				
F	-4.46536	-0.23030	2.17402				
F	-5.38585	-2.23536	0.58441				
F	-3.83087	-3.17651	-1.44342				
F	-1.39329	-2.14962	-1.86298				
C	3.49598	0.80747	0.38160				
C	3.32783	-1.56431	-1.34764				
P	1.18835	-2.10910	1.24863				
C	-0.33793	-2.18349	2.26170				
C	1.19748	-3.70111	0.33913				
C	-0.51732	-1.17813	3.21774				
C	-1.64813	-1.17188	4.02856				
C	-2.59362	-2.18748	3.91248				
C	4.45559	1.61754	-0.23391				
C	5.28643	2.41342	0.54791				
C	5.15877	2.39778	1.93502				
C	4.21019	1.58048	2.54585				
C	3.37194	0.78331	1.77331				
C	3.12104	-1.91621	-2.68511				



H	2.00946	-6.93358	1.03993	C	-0.70625	2.14523	2.30833
H	1.81946	-4.72775	2.13368	F	-2.28664	4.74661	4.22327
H	-3.14540	-3.99637	2.88234	F	0.00304	3.29371	4.24267
H	-1.15782	-3.98984	1.41278	F	0.43312	1.44281	2.36317
				F	-3.75455	2.48529	0.41677
				F	-4.15794	4.33504	2.30862
				F	-1.24473	-0.14266	-2.53412
				F	-3.08042	-1.68525	-3.70151
				F	-5.29940	-2.43293	-2.33428
				F	-5.70852	-1.56037	0.19712
				F	-3.88623	0.00159	1.38761
				C	3.34042	-1.21480	1.75455
				C	4.28028	-1.56179	2.72083
				C	5.30224	-2.45889	2.41892
				C	5.38055	-3.02139	1.14720
				C	4.42716	-2.69877	0.18688
				C	4.73482	1.11041	-2.72171
				C	4.21407	0.19297	-1.81187
				H	-1.27852	-1.34670	1.48811
				H	1.14127	-0.25210	-3.21513
				H	2.06117	1.40683	-4.79889
				H	4.36318	2.28223	-4.48733
				H	-2.69938	-3.50519	1.13409
				H	-4.08479	-4.92751	-0.33275
				H	-3.42112	-5.29949	-2.69315
				H	-1.35708	-4.25775	-3.58598
				H	0.04651	-2.83053	-2.13243
				H	0.04096	-1.63928	3.53921
				H	1.44348	-2.81724	5.20187
				H	2.83518	-4.74495	4.50420
				H	2.78127	-5.54646	2.16220
				H	1.33929	-4.41367	0.49458
				H	2.55695	-0.50146	1.99121
				H	4.21809	-1.12146	3.71086
				H	6.03769	-2.71777	3.17344
				H	6.17525	-3.71929	0.90583
				H	4.47495	-3.16110	-0.79642
				H	5.74257	1.48776	-2.58519
				H	4.81073	-0.12719	-0.96366
				83			
				<b>[16H]<sup>-</sup></b>			
				P	1.49362	1.84924	-1.22861
				C	1.21905	0.29732	-0.20320
				C	-0.04613	-0.20840	-0.22062
				B	-1.30016	0.50978	-1.01223
				C	-0.40966	-1.48392	0.47149
				C	0.25795	-2.68711	0.24460
				C	-0.09058	-3.88250	0.85667
				C	-1.18851	-3.92883	1.69769
				C	-1.93142	-2.77587	1.89368
83							
<b>[16H]<sup>+</sup></b>							
P	-0.31620	-2.01119	0.71193				
C	0.70125	-0.72544	-0.06567				
C	0.13899	0.51099	-0.17785				
B	-1.37958	0.84154	0.18466				
C	0.85972	1.70002	-0.68021				
C	2.17875	2.02113	-0.36202				
C	2.82004	3.11948	-0.91470				
C	2.12617	3.96260	-1.77405				
C	0.78547	3.71782	-2.05564				
C	0.17761	2.61123	-1.49104				
F	-1.12494	2.40395	-1.73853				
F	0.10761	4.53636	-2.84657				
F	2.73465	5.00316	-2.31266				
F	4.09068	3.36202	-0.62880				
F	2.86652	1.26176	0.48468				
C	-1.23811	-3.07839	-0.41073				
C	0.61055	-2.95696	1.91719				
P	2.17971	-1.52448	-0.84902				
C	2.91274	-0.29076	-1.97733				
C	3.40678	-1.78464	0.48054				
C	2.14880	0.13255	-3.07271				
C	2.66381	1.06846	-3.96230				
C	3.95872	1.55835	-3.78758				
C	-2.39807	-3.67252	0.10240				
C	-3.17914	-4.47540	-0.72243				
C	-2.80424	-4.68178	-2.04928				
C	-1.64363	-4.09720	-2.55277				
C	-0.85387	-3.29035	-1.73895				
C	0.63001	-2.50275	3.24048				
C	1.42600	-3.15722	4.17235				
C	2.20442	-4.24374	3.77762				
C	2.17578	-4.69778	2.45985				
C	1.36831	-4.06394	1.52321				
C	-2.51024	0.04346	-0.53697				
C	-1.64700	1.88296	1.30433				
C	-3.68630	-0.34706	0.11522				
C	-4.63676	-1.16329	-0.47444				
C	-4.42987	-1.61130	-1.77604				
C	-3.29018	-1.23222	-2.47250				
C	-2.35199	-0.42881	-1.84299				
C	-2.81731	2.65171	1.34497				
C	-3.04455	3.61913	2.31093				
C	-2.08215	3.83605	3.29269				
C	-0.90589	3.09258	3.29855				

C	-1.55389	-1.59379	1.27245	C	2.61121	-3.78386	2.79706
F	-2.35648	-0.54921	1.47951	C	2.91895	-2.78563	1.87361
F	-3.01188	-2.80903	2.67841	H	-0.86926	0.95304	-2.05292
F	-1.52447	-5.06481	2.31053	H	0.86429	-0.34005	3.02857
F	0.63748	-4.98167	0.64843	H	0.29700	-2.12209	4.64249
F	1.31916	-2.73256	-0.56233	H	1.41132	-4.33991	4.49622
C	1.05522	3.22225	-0.06718	H	0.18541	4.32366	-1.69345
C	3.34053	2.06040	-1.29505	H	-0.46407	6.26584	-0.29734
P	2.69027	-0.12914	0.82869	H	0.00503	6.25067	2.14076
C	2.29082	-1.53871	1.94253	H	1.12001	4.28671	3.16707
C	3.86342	-0.88844	-0.37505	H	1.77233	2.35621	1.77193
C	1.36470	-1.30514	2.96975	H	3.35292	1.13032	-3.23243
C	1.04137	-2.30912	3.87419	H	5.80205	1.27213	-3.52360
C	1.66668	-3.55411	3.79195	H	7.20052	2.33579	-1.76429
C	0.41573	4.33106	-0.63112	H	6.11979	3.25028	0.27533
C	0.04802	5.42140	0.15455	H	3.68408	3.07028	0.57766
C	0.31125	5.41327	1.52111	H	2.44646	-1.37060	-1.92073
C	0.93792	4.30987	2.09706	H	4.14531	-2.29562	-3.45948
C	1.30363	3.22132	1.31095	H	6.54118	-2.32192	-2.80581
C	3.96271	1.58969	-2.45836	H	7.22523	-1.40092	-0.60304
C	5.34119	1.67388	-2.62628	H	5.52128	-0.46165	0.92729
C	6.12375	2.26668	-1.63930	H	3.09429	-4.75311	2.71894
C	5.51751	2.77615	-0.49424	H	3.62816	-2.98848	1.07729
C	4.13909	2.67386	-0.32358				
C	-1.92963	1.78134	-0.19780	82			
C	-2.41189	-0.61356	-1.44732	<b>16PB</b>			
C	-2.77461	2.65248	-0.88148	P	0.88206	1.52835	0.01410
C	-3.30148	3.81388	-0.33718	C	-0.71385	0.88524	-0.54674
C	-2.99088	4.14659	0.97314	C	-0.49947	-0.39607	-0.11818
C	-2.17312	3.30552	1.70621	B	1.05884	-0.48487	0.34084
C	-1.66045	2.15603	1.11383	C	-1.46313	-1.50264	-0.04426
C	-3.77169	-0.62230	-1.15647	C	-2.80739	-1.31360	0.28969
C	-4.64440	-1.61549	-1.59421	C	-3.72501	-2.35137	0.29712
C	-4.16268	-2.66734	-2.35494	C	-3.29300	-3.64439	0.03385
C	-2.81062	-2.71346	-2.66368	C	-1.94711	-3.88689	-0.20747
C	-1.98131	-1.69747	-2.21152	C	-1.04963	-2.82921	-0.20791
F	-4.98743	-3.63002	-2.78221	F	0.23925	-3.12139	-0.37879
F	-2.33027	-3.73003	-3.39044	F	-1.52445	-5.13161	-0.40998
F	-0.67785	-1.81187	-2.52557	F	-4.15866	-4.64965	0.03950
F	-4.32981	0.33796	-0.40462	F	-5.00373	-2.12131	0.57941
F	-5.94563	-1.56796	-1.28361	F	-3.24673	-0.10605	0.63770
F	-0.84434	1.42828	1.90066	C	1.91072	2.25106	-1.29326
F	-1.86264	3.62312	2.96990	C	0.79408	2.77457	1.32501
F	-3.46525	5.27332	1.51800	P	-1.90105	1.75984	-1.62541
F	-4.10087	4.61665	-1.05328	C	-3.04855	0.42291	-2.15431
F	-3.13228	2.36953	-2.14395	C	-2.87941	2.78751	-0.45927
C	3.49071	-1.39397	-1.62541	C	-2.50572	-0.62035	-2.91447
C	4.45028	-1.90810	-2.49192	C	-3.30367	-1.68316	-3.32507
C	5.79455	-1.92202	-2.12591	C	-4.66055	-1.69995	-3.00695
C	6.17774	-1.41043	-0.88962	C	3.04135	2.99682	-0.94358
C	5.21765	-0.88949	-0.02533	C	3.96116	3.35959	-1.92203

C	3.75460	2.98442	-3.24778	H	-3.47416	3.45172	2.82135
C	2.62300	2.25198	-3.60020	H	-4.88704	5.22220	1.80690
C	1.70303	1.87959	-2.62533	H	-5.00676	5.44126	-0.66346
C	1.47361	2.53521	2.52273	H	-3.69402	3.92056	-2.10371
C	1.45172	3.49207	3.53377	H	-6.26900	-0.65714	-2.02823
C	0.74989	4.68035	3.35007	H	-4.84359	1.20656	-1.25597
C	0.08006	4.92472	2.15204				
C	0.10759	3.97841	1.13411	82			
C	2.11398	-0.85518	-0.82172	<b>16</b>			
C	1.30725	-1.03331	1.82886	P	0.88246	1.52794	0.01549
C	3.43707	-0.44609	-0.66052	C	-0.71369	0.88600	-0.54596
C	4.39252	-0.50445	-1.65935	C	-0.49979	-0.39573	-0.11843
C	4.03147	-1.01238	-2.90257	B	1.05853	-0.48558	0.34029
C	2.72641	-1.42276	-3.11892	C	-1.46392	-1.50197	-0.04533
C	1.79560	-1.32498	-2.08873	C	-2.80798	-1.31259	0.28922
C	2.29373	-1.94924	2.19026	C	-3.72607	-2.34996	0.29610
C	2.44378	-2.43139	3.48632	C	-3.29470	-3.64297	0.03172
C	1.57637	-2.00690	4.48153	C	-1.94899	-3.88588	-0.21018
C	0.57000	-1.10254	4.17017	C	-1.05104	-2.82858	-0.21011
C	0.45322	-0.65083	2.86415	F	0.23766	-3.12119	-0.38164
F	1.70798	-2.45898	5.72410	F	-1.52694	-5.13062	-0.41378
F	-0.26970	-0.68704	5.11711	F	-4.16081	-4.64785	0.03678
F	-0.53749	0.22599	2.62182	F	-5.00461	-2.11950	0.57886
F	3.15622	-2.42324	1.28750	F	-3.24669	-0.10509	0.63824
F	3.40669	-3.30330	3.77714	C	1.91180	2.25130	-1.29096
F	0.53022	-1.64674	-2.41251	C	0.79531	2.77278	1.32775
F	2.36224	-1.87547	-4.31886	P	-1.90057	1.76174	-1.62410
F	4.92806	-1.08127	-3.88214	C	-3.04885	0.42569	-2.15353
F	5.63364	-0.06868	-1.45388	C	-2.87838	2.78929	-0.45739
F	3.79415	0.11959	0.50470	C	-2.50665	-0.61721	-2.91465
C	-2.82203	2.66805	0.93329	C	-3.30516	-1.67942	-3.32574
C	-3.53599	3.54820	1.74211	C	-4.66194	-1.69590	-3.00718
C	-4.32736	4.54222	1.17260	C	3.04365	2.99464	-0.94002
C	-4.39577	4.66552	-0.21334	C	3.96445	3.35692	-1.91772
C	-3.66278	3.80352	-1.02298	C	3.75763	2.98374	-3.24400
C	-5.21372	-0.64773	-2.28122	C	2.62476	2.25388	-3.59770
C	-4.41303	0.40933	-1.85454	C	1.70383	1.88188	-2.62356
H	-1.44555	-0.62167	-3.15505	C	1.47546	2.53199	2.52483
H	-2.86462	-2.49721	-3.89306	C	1.45473	3.48794	3.53675
H	-5.28454	-2.52890	-3.32526	C	0.75343	4.67676	3.35456
H	3.20824	3.27817	0.09249	C	0.08292	4.92255	2.15719
H	4.84266	3.92929	-1.64801	C	0.10929	3.97716	1.13839
H	4.47752	3.26217	-4.00777	C	2.11322	-0.85512	-0.82293
H	2.46022	1.96084	-4.63274	C	1.30716	-1.03555	1.82769
H	0.82841	1.29390	-2.89550	C	3.43641	-0.44632	-0.66170
H	2.02149	1.60612	2.65650	C	4.39151	-0.50356	-1.66092
H	1.97862	3.30702	4.46371	C	4.03000	-1.01011	-2.90458
H	0.72726	5.42202	4.14201	C	2.72486	-1.42027	-3.12092
H	-0.46602	5.85123	2.00967	C	1.79438	-1.32348	-2.09034
H	-0.41123	4.17120	0.19879	C	2.29345	-1.95209	2.18805
H	-2.21660	1.88903	1.38583	C	2.44351	-2.43559	3.48361

C	1.57632	-2.01190	4.47935	C	-1.81230	0.51162	1.98932
C	0.57015	-1.10696	4.16903	F	-1.18132	-0.04469	3.02302
C	0.45336	-0.65387	2.86349	F	-3.51052	1.24926	3.45674
F	1.70794	-2.46532	5.72143	F	-4.87941	2.31737	1.36674
F	-0.26931	-0.69221	5.11651	F	-3.88964	2.11899	-1.15372
F	-0.53713	0.22349	2.62216	F	-1.52824	0.87877	-1.58293
F	3.15572	-2.42540	1.28473	C	1.06816	1.97969	-0.33079
F	3.40624	-3.30804	3.77343	C	0.93873	2.35538	-1.65964
F	0.52885	-1.64476	-2.41403	P	-1.30659	-2.88074	0.76389
F	2.36029	-1.87165	-4.32124	C	-2.74553	-2.15761	-0.13579
F	4.92622	-1.07785	-3.88456	C	-3.88289	-1.83684	0.61104
F	5.63263	-0.06777	-1.45550	C	-4.98348	-1.23998	-0.00153
F	3.79388	0.11815	0.50400	C	-4.95390	-0.96217	-1.36534
C	-2.82117	2.66905	0.93510	C	0.70055	3.67017	-2.03515
C	-3.53492	3.54898	1.74435	C	0.57754	4.64569	-1.05269
C	-4.32594	4.54354	1.17531	C	0.68570	4.30276	0.28942
C	-4.39417	4.66765	-0.21058	C	0.92512	2.97721	0.62238
C	-3.66138	3.80587	-1.02062	F	1.00496	2.64552	1.91954
C	-5.21447	-0.64400	-2.28050	F	0.55678	5.23531	1.22898
C	-4.41322	0.41245	-1.85331	F	0.34978	5.90750	-1.39781
H	-1.44657	-0.61875	-3.15559	F	0.58252	4.00398	-3.31693
H	-2.86662	-2.49322	-3.89448	F	1.02366	1.42939	-2.61782
H	-5.28637	-2.52438	-3.32587	C	2.71382	-0.08555	0.32638
H	3.21069	3.27442	0.09645	C	3.08523	-0.85418	1.43444
H	4.84692	3.92464	-1.64273	C	4.38582	-1.29472	1.63822
H	4.48133	3.26104	-4.00340	C	5.36665	-0.97391	0.70867
H	2.46177	1.96434	-4.63065	C	5.04461	-0.20994	-0.40613
H	0.82823	1.29811	-2.89472	C	3.73886	0.22761	-0.57013
H	2.02295	1.60249	2.65737	F	3.47654	0.95852	-1.65396
H	1.98215	3.30178	4.46618	F	5.98403	0.09403	-1.29534
H	0.73174	5.41775	4.14715	C	-3.82871	-1.29415	-2.11886
H	-0.46275	5.84948	2.01601	C	-2.73217	-1.89463	-1.50921
H	-0.41002	4.17108	0.20358	C	-0.77290	-4.24131	-0.35281
H	-2.21599	1.88959	1.38722	C	-1.19826	-5.53444	-0.03054
H	-3.47321	3.45189	2.82353	C	-0.85797	-6.61508	-0.83893
H	-4.88551	5.22330	1.80993	C	-0.07508	-6.41718	-1.97271
H	-5.00488	5.44383	-0.66030	C	0.36321	-5.13605	-2.29847
H	-3.69246	3.92350	-2.10129	C	0.01429	-4.05401	-1.49593
H	-6.26967	-0.65319	-2.02717	F	6.60988	-1.39498	0.88541
H	-4.84325	1.20943	-1.25404	F	4.70055	-2.01304	2.71079
				F	2.19248	-1.16931	2.37278
				H	1.00640	-2.16362	0.33721
				H	-3.89966	-2.04344	1.67810
				H	-5.85743	-0.98344	0.58915
				H	-5.80409	-0.48470	-1.84139
				H	-3.80207	-1.07642	-3.18151
				H	-1.85687	-2.14355	-2.10192
				H	-1.79557	-5.69418	0.86297
				H	-1.19679	-7.61229	-0.57784
				H	0.19694	-7.25991	-2.59983
				H	0.97550	-4.97752	-3.18036
60							
<b>16B</b>							
C	0.03230	-1.68752	0.46084				
C	-0.00369	-0.33479	0.47523				
B	1.26289	0.48489	0.14895				
C	-1.28297	0.39232	0.70926				
C	-1.99284	0.97803	-0.33448				
C	-3.20192	1.62260	-0.12953				
C	-3.71178	1.71836	1.15979				
C	-3.01590	1.16509	2.22475				

H	0.35968	-3.05843	-1.76346	F	4.69461	-1.57555	0.84530
				F	2.68343	0.18124	0.86564
61				H	-1.45429	-0.01169	-2.56785
[16BH] <sup>-</sup>				H	0.59267	1.13373	-2.56842
C	-1.37739	-0.46270	-1.57765	H	-2.63963	-3.51215	0.94446
C	-0.29235	-0.15402	-0.85557	H	-2.90351	-3.33527	3.40425
B	0.88871	0.82854	-1.43445	H	-3.44261	-1.14212	4.43614
C	-0.05702	-0.82464	0.45543	H	-3.71581	0.86274	2.99945
C	-0.27395	-0.19603	1.67792	H	-3.42382	0.68809	0.55513
C	-0.03632	-0.82659	2.88909	H	-5.36635	-2.39497	-2.12139
C	0.48148	-2.11358	2.90233	H	-7.34545	-1.16994	-2.96571
C	0.74260	-2.75877	1.70397	H	-7.24972	1.29519	-3.24922
C	0.47173	-2.11185	0.50491	H	-5.17082	2.52074	-2.66837
F	0.72024	-2.77799	-0.62717	H	-3.20535	1.30126	-1.80545
F	1.23946	-3.99910	1.71242				
F	0.70871	-2.73334	4.06344	60			
F	-0.32170	-0.21574	4.04195	16P			
F	-0.78253	1.03878	1.71760	P	-1.91919	0.93100	-1.70505
C	1.01680	2.22517	-0.58147	C	-0.31463	0.27014	-1.00991
C	-0.12579	2.94617	-0.23549	C	0.70211	1.13300	-1.20650
P	-2.73939	-1.63432	-1.23621	C	2.13827	0.95865	-0.91558
C	-3.03531	-1.43098	0.58170	C	2.89793	-0.08197	-1.44056
C	-2.89179	-2.55675	1.39786	C	4.23394	-0.25338	-1.10918
C	-3.03979	-2.45702	2.78003	C	4.85510	0.66477	-0.27322
C	-3.34384	-1.22773	3.35841	C	4.13661	1.74143	0.23108
C	-0.10979	4.16493	0.42913	C	2.79783	1.87590	-0.10158
C	1.10525	4.73992	0.76654	F	2.10784	2.89135	0.42940
C	2.27444	4.08134	0.42573	F	4.72939	2.61763	1.03894
C	2.20760	2.86117	-0.23929	F	6.13204	0.50491	0.05600
F	3.39634	2.32535	-0.56196	F	4.91950	-1.28953	-1.58289
F	3.45683	4.63390	0.72693	F	2.32917	-0.97867	-2.24738
F	1.14715	5.91697	1.40168	C	-3.17757	-0.37183	-1.36849
F	-1.25046	4.79656	0.73689	C	-2.39613	2.27820	-0.53526
F	-1.34872	2.47945	-0.54667	P	-0.24533	-1.50373	-0.49086
C	2.23532	-0.10316	-1.44595	C	1.33099	-1.70489	0.45273
C	2.97477	-0.41142	-0.30729	C	2.17075	-2.74931	0.05747
C	4.02215	-1.32191	-0.28418	C	3.38943	-2.96541	0.70021
C	4.37121	-1.97982	-1.45431	C	3.77782	-2.13466	1.74541
C	3.66587	-1.71326	-2.61626	C	-3.17589	-1.46797	-2.23949
C	2.62070	-0.79557	-2.58931	C	-4.08270	-2.51093	-2.07055
F	1.97717	-0.61325	-3.75152	C	-5.02693	-2.45215	-1.04996
F	3.99700	-2.34596	-3.74980	C	-5.05538	-1.35109	-0.19654
C	-3.50058	-0.10225	2.55127	C	-4.13431	-0.32062	-0.34907
C	-3.34787	-0.20275	1.17215	C	-3.66553	2.84110	-0.73530
C	-4.15343	-0.63507	-1.89341	C	-4.10296	3.91133	0.03601
C	-5.32890	-1.31402	-2.23203	C	-3.26925	4.45821	1.00927
C	-6.44063	-0.62630	-2.71018	C	-1.99791	3.92725	1.19695
C	-6.38689	0.75585	-2.86989	C	-1.56169	2.84794	0.43009
C	-5.21984	1.44296	-2.54558	C	2.94009	-1.09653	2.15755
C	-4.11038	0.75510	-2.05987	C	1.72159	-0.88988	1.52142
F	5.37843	-2.86045	-1.46031	C	-1.43985	-1.52074	0.91170

C	-1.66870	-0.43322	1.76097
C	-2.58869	-0.52959	2.79992
C	-3.28342	-1.71963	3.00863
C	-3.05741	-2.80921	2.17263
C	-2.14520	-2.70749	1.12517
H	0.46479	2.11344	-1.62598
H	1.87773	-3.38056	-0.77640
H	4.03732	-3.77242	0.37422
H	4.73134	-2.29067	2.24005
H	-2.45272	-1.50911	-3.05035
H	-4.05875	-3.36042	-2.74556
H	-5.74167	-3.25905	-0.92216
H	-5.78365	-1.30299	0.60699
H	-4.14546	0.51352	0.34467
H	-4.32214	2.42794	-1.49764
H	-5.09321	4.32362	-0.12952
H	-3.60547	5.29833	1.60805
H	-1.33399	4.35379	1.94228
H	-0.55752	2.46501	0.58352
H	3.24057	-0.44733	2.97430
H	1.07840	-0.07411	1.84152
H	-1.15007	0.50542	1.59148
H	-2.76721	0.32794	3.44148
H	-4.00221	-1.79473	3.81858
H	-3.60367	-3.73496	2.32421
H	-1.99591	-3.54746	0.45194

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**[16PH]<sup>+</sup>**

P	-1.87397	0.84617	-1.31305
C	-0.24633	0.18534	-0.85167
C	0.75056	1.03970	-1.17466
C	2.19385	0.83498	-1.00770
C	2.85743	-0.32305	-1.40345
C	4.20462	-0.51422	-1.13951
C	4.92598	0.49300	-0.50762
C	4.29995	1.68059	-0.13879
C	2.94961	1.83790	-0.40115
F	2.33404	2.95421	-0.00178
F	4.98876	2.63431	0.47087
F	6.20880	0.31805	-0.24666
F	4.80122	-1.64632	-1.48139
F	2.18256	-1.29189	-2.02150
C	-3.17975	-0.38005	-1.39822
C	-2.35007	2.28961	-0.34547
P	-0.19033	-1.57309	-0.25235
C	1.34302	-1.63322	0.75813
C	2.17419	-2.73717	0.54678
C	3.37871	-2.85571	1.23855
C	3.76088	-1.86668	2.13886
C	-3.08032	-1.35869	-2.39498

C	-4.04165	-2.35983	-2.46335
C	-5.09596	-2.37444	-1.55147
C	-5.19218	-1.39515	-0.56498
C	-4.23194	-0.39373	-0.47846
C	-3.61486	2.84602	-0.58027
C	-3.99570	3.99339	0.10512
C	-3.12028	4.58618	1.01358
C	-1.85859	4.03980	1.23426
C	-1.46463	2.89211	0.55353
C	2.93337	-0.76386	2.35967
C	1.72726	-0.65150	1.67820
C	-1.51590	-1.50776	1.02439
C	-1.75202	-0.41806	1.87122
C	-2.79585	-0.45118	2.79176
C	-3.60356	-1.58330	2.88705
C	-3.36538	-2.67906	2.06075
C	-2.33231	-2.63825	1.12781
H	-1.71241	1.29231	-2.63397
H	0.49801	2.02771	-1.56726
H	1.88995	-3.49403	-0.17854
H	4.01979	-3.71279	1.06324
H	4.70291	-1.95074	2.67066
H	-2.25757	-1.34889	-3.10555
H	-3.97085	-3.12280	-3.23034
H	-5.84708	-3.15492	-1.61116
H	-6.00875	-1.41621	0.14831
H	-4.28542	0.34714	0.31307
H	-4.30028	2.38657	-1.28740
H	-4.97422	4.42530	-0.07259
H	-3.42105	5.48208	1.54601
H	-1.17500	4.50948	1.93265
H	-0.47168	2.48336	0.71499
H	3.23086	0.00641	3.06394
H	1.09828	0.21951	1.84445
H	-1.12196	0.46490	1.81616
H	-2.97156	0.40147	3.43997
H	-4.41186	-1.61334	3.61028
H	-3.98981	-3.56330	2.13600
H	-2.16694	-3.48304	0.46453

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**16PHBH**

C	-4.369750	0.422509	-1.069631
C	-3.123164	0.012833	-0.799932
B	-1.945570	1.002362	-0.257448
C	-2.729628	-1.420134	-0.801594
C	-3.101001	-2.290709	0.217969
C	-2.729545	-3.628098	0.221332
C	-1.941724	-4.118062	-0.807672
C	-1.503892	-3.265768	-1.809803
C	-1.885212	-1.933269	-1.782923

F	-1.439271	-1.138074	-2.765331	H	-5.319001	0.129298	1.281322
F	-0.715349	-3.732131	-2.783799	P	1.910775	0.781158	-0.210646
F	-1.584161	-5.406444	-0.816319	C	3.627649	0.170547	-0.245773
F	-3.125977	-4.447511	1.194416	C	4.522013	0.980674	0.355212
F	-3.868568	-1.856024	1.222040	C	5.985432	0.848496	0.367958
C	-2.009733	0.825308	1.366383	C	6.742278	0.613700	-0.776442
C	-3.026531	1.375784	2.143282	C	8.113836	0.419943	-0.715294
P	-5.937976	-0.368323	-1.592139	C	8.762420	0.508123	0.510293
C	-5.719318	-2.189066	-1.383821	C	8.040100	0.786652	1.665463
C	-5.116122	-2.884166	-2.440981	C	6.668590	0.961035	1.578242
C	-4.931580	-4.261113	-2.375843	F	5.975558	1.191030	2.695162
C	-5.371433	-4.971085	-1.259099	F	8.662956	0.867322	2.835762
C	-3.153420	1.162825	3.508850	F	10.071756	0.318569	0.579818
C	-2.237462	0.345650	4.161740	F	8.805182	0.149210	-1.815455
C	-1.231082	-0.259282	3.426869	F	6.143251	0.538137	-1.964138
C	-1.160734	-0.028061	2.058798	C	1.620458	1.904816	-1.577355
F	-0.177685	-0.701252	1.414779	C	1.579401	1.554494	1.381292
F	-0.339973	-1.056445	4.030980	P	3.843416	-1.337297	-1.304521
F	-2.335034	0.138188	5.475086	C	5.456730	-2.038054	-0.760572
F	-4.154090	1.714550	4.200503	C	6.384277	-2.347001	-1.758435
F	-3.961494	2.142940	1.566268	C	7.639646	-2.851915	-1.422222
C	-2.071980	2.511983	-0.870291	C	7.973475	-3.044651	-0.085658
C	-2.056982	2.626976	-2.262003	C	2.127438	3.208999	-1.539070
C	-2.036747	3.833022	-2.945718	C	1.901929	4.057760	-2.614702
C	-2.058763	5.022667	-2.232688	C	1.187996	3.601224	-3.723364
C	-2.094008	4.971105	-0.849383	C	0.696773	2.300034	-3.761730
C	-2.100213	3.734751	-0.208680	C	0.903430	1.443183	-2.684330
F	-2.065289	3.795535	1.137803	C	0.653883	2.597822	1.448059
F	-2.098433	6.102912	-0.140913	C	0.284821	3.111101	2.691057
C	-5.994042	-4.294192	-0.214573	C	0.815658	2.567686	3.854008
C	-6.168965	-2.912394	-0.275167	C	1.737000	1.520817	3.788016
C	-6.951459	0.069894	-0.115093	C	2.126851	1.016914	2.556504
C	-8.331295	0.231415	-0.273144	C	7.046458	-2.750749	0.916139
C	-9.132441	0.576230	0.812849	C	5.790167	-2.260203	0.579503
C	-8.558277	0.781486	2.064933	C	2.665972	-2.474477	-0.456764
C	-7.183597	0.627611	2.232945	C	2.301185	-2.385952	0.891523
C	-6.387465	0.264693	1.151074	C	1.390841	-3.280434	1.445050
F	-2.021986	6.193583	-2.868650	C	0.869481	-4.307082	0.662942
F	-1.940117	3.859164	-4.279640	C	1.243938	-4.422225	-0.673924
F	-1.991802	1.523205	-3.021696	C	2.116087	-3.496349	-1.238573
H	-4.539872	1.501237	-1.009102	H	1.077138	-0.316857	-0.430074
H	-0.869055	0.573487	-0.643603	H	4.153250	1.824749	0.939080
H	-4.783108	-2.335584	-3.319526	H	6.131306	-2.168328	-2.799402
H	-4.449240	-4.781542	-3.198028	H	8.356705	-3.081251	-2.203259
H	-5.229248	-6.045942	-1.205458	H	8.953995	-3.426602	0.179881
H	-6.338020	-4.840717	0.657918	H	2.672317	3.564050	-0.667957
H	-6.644137	-2.393722	0.551310	H	2.271817	5.076744	-2.585155
H	-8.776430	0.094327	-1.255199	H	0.989445	4.273311	-4.551825
H	-10.202763	0.697767	0.678349	H	0.101777	1.964902	-4.603330
H	-9.180736	1.066185	2.907566	H	0.457904	0.452006	-2.686150
H	-6.723367	0.798247	3.201443	H	0.208280	2.993991	0.541052

H	-0.440477	3.913643	2.734265	C	3.06685	-3.22409	-0.04163
H	0.509256	2.955538	4.819990	C	2.84854	-2.73697	-1.32091
H	2.149102	1.095701	4.696367	C	1.74716	-1.92272	-1.55885
H	2.862919	0.221591	2.512728	F	4.15203	-3.94996	0.22497
H	7.303949	-2.908578	1.958684	F	3.73114	-2.99915	-2.28812
H	5.070533	-2.032701	1.362235	F	1.65127	-1.41573	-2.79933
H	2.708969	-1.596688	1.516719	F	0.33136	-1.72356	1.72702
H	1.073567	-3.153247	2.474796	F	2.41946	-3.30478	2.21890
H	0.147450	-5.001772	1.080866	F	-2.50729	0.90519	-2.13000
H	0.812364	-5.202275	-1.290728	F	-5.02546	0.05064	-2.45513
H	2.360896	-3.561627	-2.295269	F	-5.77351	-2.39213	-1.50908
				F	-3.95283	-3.95985	-0.23152
				F	-1.44925	-3.12458	0.10844
				H	1.96905	0.65659	-1.54603
				H	-0.08344	0.10074	-1.91249
				H	0.56729	3.56207	1.18494
				H	0.03343	2.40360	2.41471
				H	1.75897	2.66312	2.12682
				H	0.98486	3.54211	-1.41645
				H	1.79452	5.81287	-1.98925
				H	4.14938	6.44299	-1.53267
				H	5.70115	4.80513	-0.51167
				H	4.90906	2.52541	0.04810
				H	4.70317	0.01423	-1.27643
				H	6.37815	-1.42694	-0.16582
				H	6.11045	-2.02791	2.22341
				H	4.16182	-1.19651	3.50868
				H	2.45879	0.22159	2.39846
65				64			
<b>17H<sub>2</sub></b>				<b>[17H]<sup>+</sup></b>			
P	2.24929	1.24592	-0.30748	P	-1.77332	1.44197	0.55836
C	0.73868	1.47113	0.61876	C	-0.39282	1.64428	-0.58601
C	-0.34180	0.73729	0.26196	C	0.54844	0.67653	-0.64511
B	-0.35204	-0.46333	-0.87077	B	0.41796	-0.74670	0.05754
C	-1.65112	1.18186	0.81772	C	1.80827	0.86397	-1.39871
C	-2.49175	0.34711	1.55381	C	2.33183	-0.21084	-2.12025
C	-3.76972	0.73529	1.93186	C	3.52969	-0.13699	-2.80947
C	-4.24673	1.98602	1.56186	C	4.26710	1.04268	-2.74914
C	-3.43837	2.84067	0.82579	C	3.80550	2.11673	-1.99644
C	-2.16198	2.43130	0.46794	C	2.59729	2.01291	-1.31963
F	-1.42249	3.28277	-0.25299	F	2.22509	3.03243	-0.54785
F	-3.88721	4.04149	0.46999	F	4.52927	3.22165	-1.90563
F	-5.46623	2.36743	1.92118	F	5.41577	1.13338	-3.39150
F	-4.53797	-0.08135	2.64593	F	3.98155	-1.17151	-3.49962
F	-2.07883	-0.86181	1.92248	F	1.65581	-1.36695	-2.12263
C	2.90680	2.89142	-0.66790	C	-2.00500	2.99242	1.43149
C	3.50364	0.24621	0.51070	C	-3.27965	0.84966	-0.21759
C	0.78052	2.58987	1.64023	C	-0.40420	2.95746	-1.33115
C	2.02260	3.81692	-1.23718	C	-0.87507	3.58376	2.01452
C	2.47523	5.09271	-1.54858	C	-1.01975	4.77843	2.70662
C	3.79981	5.44497	-1.28984				
C	4.67348	4.52576	-0.71721				
C	4.23045	3.24308	-0.40278				
C	4.59969	-0.22569	-0.22051				
C	5.54064	-1.03803	0.40275				
C	5.38559	-1.37701	1.74636				
C	4.29412	-0.90697	2.47241				
C	3.34525	-0.09649	1.85582				
C	-1.84032	-1.08862	-1.04484				
C	0.83486	-1.54704	-0.57507				
C	-2.28046	-2.31534	-0.56276				
C	-3.58643	-2.77112	-0.71246				
C	-4.51795	-1.97422	-1.36024				
C	-4.13277	-0.73118	-1.84454				
C	-2.81702	-0.32318	-1.67839				
C	1.09825	-2.07134	0.68753				
C	2.17874	-2.89541	0.97105				



C	-2.27711	5.37596	2.81078	C	-1.53578	-1.30748	-0.63945
C	-3.39371	4.78588	2.22552	C	-2.32801	-0.56334	-1.51408
C	-3.26473	3.58628	1.53019	C	-3.57721	-0.99342	-1.94198
C	-4.24428	0.22409	0.58122	C	-4.07889	-2.20568	-1.49212
C	-5.39323	-0.28873	-0.01368	C	-3.32176	-2.97535	-0.62264
C	-5.57405	-0.17430	-1.39136	C	-2.07605	-2.52112	-0.21082
C	-4.61288	0.45384	-2.18250	F	-1.39658	-3.30095	0.63428
C	-3.45660	0.96300	-1.60149	F	-3.79692	-4.14623	-0.18852
C	1.50666	-1.17336	1.07289	F	-5.27456	-2.63354	-1.90273
C	-0.86168	-1.58719	-0.24637	F	-4.29695	-0.25315	-2.78880
C	1.76568	-2.51878	1.37061	F	-1.90338	0.61332	-1.97215
C	2.76687	-2.91383	2.24341	C	3.18238	-2.77354	0.74301
C	3.54540	-1.94251	2.86617	C	3.40383	-0.21305	-0.50645
C	3.32212	-0.59247	2.61022	C	0.91572	-2.72991	-1.19554
C	2.32215	-0.23550	1.72207	C	2.52787	-3.78626	1.45995
C	-1.48646	-1.54728	-1.49670	C	3.08674	-5.05268	1.58119
C	-2.69138	-2.18463	-1.75439	C	4.32564	-5.32839	1.00332
C	-3.33187	-2.86310	-0.72628	C	4.98933	-4.32952	0.29888
C	-2.74964	-2.93174	0.53709	C	4.42098	-3.06303	0.16488
C	-1.53161	-2.30867	0.75042	C	4.54613	0.43522	-0.02319
F	-4.51270	-3.41433	-0.93682	C	5.33329	1.21946	-0.86376
F	-3.38041	-3.55544	1.52180	C	4.97857	1.37572	-2.20056
F	-1.03679	-2.34031	1.98913	C	3.84053	0.73997	-2.69225
F	-0.94918	-0.84771	-2.49670	C	3.05953	-0.04909	-1.85323
F	-3.26174	-2.09740	-2.94907	C	-1.90571	1.07280	0.99277
F	2.13379	1.07543	1.51946	C	0.76668	1.62497	0.66306
F	4.05821	0.32890	3.21446	C	-2.37092	2.22307	0.36563
F	4.49628	-2.30103	3.70378	C	-3.70258	2.62836	0.38936
F	2.99009	-4.19494	2.48791	C	-4.64097	1.85774	1.05574
F	1.05516	-3.47827	0.78668	C	-4.23379	0.68991	1.68457
H	-1.41587	0.47711	1.51187	C	-2.89347	0.33104	1.63985
H	0.00461	3.77171	-0.72826	C	1.09944	2.06885	-0.61294
H	0.18858	2.87087	-2.24423	C	2.13402	2.95521	-0.88490
H	-1.42391	3.24194	-1.61016	C	2.91002	3.42999	0.15893
H	0.10491	3.11900	1.91915	C	2.61915	3.02783	1.45314
H	-0.15415	5.24597	3.16237	C	1.56111	2.15384	1.67925
H	-2.38366	6.31062	3.35088	F	3.93606	4.25478	-0.07913
H	-4.36615	5.25828	2.30722	F	3.36481	3.48472	2.46982
H	-4.13192	3.12291	1.06931	F	1.35435	1.81488	2.95858
H	-4.09896	0.12462	1.65449	F	0.43014	1.61199	-1.68015
H	-6.13908	-0.78724	0.59567	F	2.40680	3.33145	-2.14118
H	-6.46569	-0.58537	-1.85236	F	-2.57437	-0.83028	2.23590
H	-4.75183	0.52534	-3.25523	F	-5.13476	-0.06883	2.32154
H	-2.68621	1.40543	-2.22589	F	-5.92496	2.23114	1.08827
				F	-4.08984	3.75021	-0.23015
				F	-1.54190	3.01168	-0.33335
64				H	-0.15917	0.06357	2.08744
[17H] <sup>-</sup>				H	0.77977	-3.67414	-0.65723
P	2.35949	-1.11538	0.71921	H	1.89099	-2.78766	-1.69017
C	0.85113	-1.54101	-0.25802	H	0.14095	-2.66588	-1.96513
C	-0.26137	-0.80598	-0.04131	H	1.55929	-3.57531	1.91054
B	-0.37339	0.49115	0.97692				

H	2.55749	-5.82548	2.13090	C	-2.24394	-0.61613	1.45145
H	4.76790	-6.31513	1.10229	F	-4.33264	-3.53471	1.80241
H	5.95289	-4.53601	-0.15847	F	-4.38298	-0.88416	2.42793
H	4.94327	-2.29614	-0.39993	F	-2.32257	0.70018	1.71589
H	4.80170	0.34725	1.03065	F	-0.18116	-3.00278	-0.27911
H	6.20474	1.73137	-0.46685	F	-2.20534	-4.56517	0.45615
H	5.57322	2.00869	-2.85193	F	1.71551	2.11653	-0.54955
H	3.54296	0.88268	-3.72646	F	3.02378	3.77337	1.08336
H	2.14364	-0.49428	-2.23027	F	2.75336	3.53538	3.78352
				F	1.15070	1.59530	4.81187
				F	-0.15334	-0.07127	3.21305
63				H	0.70053	0.40376	-4.18242
<b>17PB</b>				H	0.70429	-1.33120	-3.85660
P	-1.12652	0.84091	-1.28372	H	-0.83460	-0.47636	-4.07961
C	0.08592	-0.12955	-2.18746	H	-1.28226	3.06471	0.50442
C	0.80170	-0.50916	-1.09470	H	-1.25629	5.52521	0.15769
B	-0.05381	-0.02628	0.21029	H	-1.02108	6.44913	-2.12957
C	2.10569	-1.18850	-1.04757	H	-0.82974	4.92682	-4.07462
C	2.49870	-1.87346	0.11050	H	-0.87804	2.47349	-3.73922
C	3.73530	-2.48870	0.23094	H	-3.75590	2.14261	-1.00259
C	4.65258	-2.39337	-0.80718	H	-6.05225	1.21876	-1.07014
C	4.32112	-1.68324	-1.95219	H	-6.41807	-1.16238	-1.65076
C	3.07461	-1.08165	-2.05068	H	-4.48565	-2.62172	-2.18981
F	2.84176	-0.35832	-3.14657	H	-2.18487	-1.70803	-2.11365
F	5.20699	-1.55924	-2.93650				
F	5.84253	-2.96852	-0.70059				
F	4.05612	-3.14729	1.33966	63			
F	1.68054	-1.95352	1.15852	<b>17</b>			
C	-1.08330	2.62107	-1.59590	P	-1.73156	1.19497	0.91428
C	-2.82745	0.27861	-1.56525	C	-0.46894	1.66235	-0.36702
C	0.17264	-0.39843	-3.65767	C	0.49689	0.73928	-0.55926
C	-1.19099	3.47937	-0.49678	B	0.40349	-0.69541	0.10419
C	-1.17405	4.85735	-0.69315	C	1.72212	0.98090	-1.35794
C	-1.04176	5.37472	-1.97919	C	2.24882	-0.04693	-2.14351
C	-0.93333	4.51958	-3.07446	C	3.41578	0.08447	-2.87757
C	-0.95725	3.14191	-2.88649	C	4.12673	1.27644	-2.80598
C	-3.91727	1.10206	-1.26989	C	3.66834	2.30342	-1.99291
C	-5.20695	0.58091	-1.30553	C	2.49606	2.13958	-1.26453
C	-5.41162	-0.75743	-1.63329	F	2.14917	3.12439	-0.43885
C	-4.32718	-1.57875	-1.93583	F	4.37082	3.42735	-1.88888
C	-3.03559	-1.06431	-1.90097	F	5.24921	1.42419	-3.49768
C	0.69424	0.95131	1.24242	F	3.86588	-0.91650	-3.62706
C	-1.12250	-1.09288	0.77555	F	1.61922	-1.22947	-2.16948
C	0.60223	0.86445	2.63078	C	-2.14064	2.86305	1.57025
C	1.27844	1.72123	3.49241	C	-3.21260	0.75357	-0.08485
C	2.10059	2.70949	2.97205	C	-0.53603	3.02014	-1.01156
C	2.23492	2.83011	1.59601	C	-1.16698	3.48000	2.36671
C	1.54482	1.95267	0.77209	C	-1.39082	4.74369	2.90098
C	-1.15764	-2.44274	0.45263	C	-2.59955	5.39637	2.66363
C	-2.21847	-3.27623	0.79663	C	-3.57593	4.78352	1.88473
C	-3.30671	-2.75347	1.47647	C	-3.34798	3.52353	1.33405
C	-3.32726	-1.40171	1.80272	C	-4.24105	0.07823	0.58329

C	-5.35651	-0.38455	-0.11115	F	2.67240	-1.97015	-2.17658
C	-5.45071	-0.18666	-1.48637	F	5.13066	-1.81125	-1.09940
C	-4.43259	0.48362	-2.16142	F	5.43684	-1.14319	1.51400
C	-3.32005	0.95029	-1.46683	F	3.25425	-0.63397	3.05429
C	1.55094	-1.15135	1.06650	F	0.77832	-0.80790	1.97741
C	-0.81615	-1.61599	-0.24603	C	-0.03033	1.15481	-0.28720
C	1.88245	-2.49575	1.26400	C	-0.50860	2.12766	0.59261
C	2.91671	-2.90249	2.09294	C	0.53517	-3.79948	-1.72758
C	3.66048	-1.94348	2.76958	C	0.06230	3.38583	0.70668
C	3.36975	-0.59539	2.60713	C	1.14723	3.71259	-0.09808
C	2.33597	-0.22332	1.76008	C	1.64819	2.78367	-1.00065
C	-1.45537	-1.55316	-1.48510	C	1.05822	1.53001	-1.07761
C	-2.62987	-2.24058	-1.76205	F	1.55965	0.68336	-1.98165
C	-3.22403	-2.99548	-0.76369	F	2.67536	3.10400	-1.78112
C	-2.62119	-3.09221	0.48662	F	1.69991	4.91307	-0.00771
C	-1.43458	-2.41848	0.71825	F	-0.41439	4.27772	1.56873
F	-4.37095	-3.61867	-0.99450	F	-1.55000	1.86046	1.38302
F	-3.19926	-3.81309	1.44410	C	-2.20998	-0.46891	-0.20652
F	-0.91248	-2.50892	1.94278	C	-3.12410	0.46997	-0.69281
F	-0.96597	-0.79487	-2.46836	C	-4.49580	0.33296	-0.55257
F	-3.20604	-2.14504	-2.95732	C	-4.99855	-0.77305	0.12265
F	2.10448	1.08712	1.64651	C	-4.12990	-1.72252	0.64281
F	4.08217	0.31941	3.25772	C	-2.76130	-1.56130	0.46991
F	4.64911	-2.31535	3.56829	F	-1.97936	-2.49059	1.01923
F	3.20617	-4.19078	2.24368	F	-4.61275	-2.77130	1.30169
F	1.21392	-3.45558	0.62689	F	-6.30646	-0.91881	0.27216
H	-0.15607	3.79428	-0.33925	F	-5.32913	1.24130	-1.04919
H	0.04385	3.05243	-1.93816	F	-2.68781	1.55130	-1.34247
H	-1.57567	3.28071	-1.23147	H	-1.22981	-2.49494	-1.71116
H	-0.22536	2.96806	2.55713	H	-0.12265	-4.66497	-1.61203
H	-0.62612	5.21634	3.50891	H	0.84619	-3.76298	-2.77698
H	-2.77882	6.37920	3.08725	H	1.42671	-3.94800	-1.11590
H	-4.51822	5.28873	1.69761				
H	-4.11003	3.05571	0.71766	42			
H	-4.15690	-0.10340	1.65246	[17BH] <sup>-</sup>			
H	-6.14078	-0.91583	0.41857	C	-0.01723	-2.53220	-2.00249
H	-6.30906	-0.56327	-2.03289	C	0.19781	-1.47458	-1.20850
H	-4.49376	0.62421	-3.23560	B	-0.73060	-0.13228	-1.31308
H	-2.51290	1.42775	-2.01354	C	1.31689	-1.49627	-0.23348
				C	1.15480	-1.05482	1.08373
41				C	2.20926	-0.95804	1.98036
17B				C	3.49347	-1.28659	1.57042
C	-0.20006	-2.55309	-1.35809	C	3.70315	-1.70335	0.26591
C	0.25883	-1.50392	-0.64685	C	2.62982	-1.78718	-0.61245
B	-0.66157	-0.28069	-0.37462	F	2.90885	-2.15885	-1.86492
C	1.64291	-1.45782	-0.11399	F	4.94007	-2.00746	-0.14169
C	1.84292	-1.08627	1.21473	F	4.51622	-1.20479	2.42590
C	3.10428	-0.98001	1.77957	F	2.00118	-0.55037	3.23539
C	4.22017	-1.23778	0.99235	F	-0.04967	-0.69070	1.52790
C	4.06095	-1.58736	-0.34226	C	-2.19307	-0.29637	-0.58989
C	2.78412	-1.67970	-0.88084	C	-3.15991	0.68206	-0.81568

C	0.66149	-3.87186	-1.97938	C	-3.87801	1.61304	-0.92190
C	-4.46006	0.62314	-0.33950	C	-4.36903	2.90016	-0.73476
C	-4.85201	-0.47235	0.41729	C	-3.50377	3.93553	-0.38647
C	-3.93077	-1.46988	0.68133	C	-2.14712	3.67291	-0.22861
C	-2.63247	-1.36502	0.18427	C	-1.65316	2.38266	-0.41235
F	-1.82068	-2.38346	0.51173	H	0.69878	-0.51604	-2.00313
F	-4.29748	-2.52953	1.41663	H	-0.99917	-1.06340	1.72065
F	-6.10306	-0.55840	0.88812	H	0.65111	-0.41581	1.75530
F	-5.34066	1.60135	-0.59423	H	-0.74317	0.67954	1.65992
F	-2.83460	1.77682	-1.52194	H	-2.67587	-3.09259	-1.35776
C	0.11290	1.17774	-0.79362	H	-4.05058	-4.63656	0.00317
C	-0.22729	2.06410	0.22284	H	-5.17822	-3.81207	2.05408
C	0.56594	3.14416	0.60203	H	-4.91274	-1.44342	2.74110
C	1.77264	3.36839	-0.03852	H	-3.52800	0.09434	1.39107
C	2.16930	2.50456	-1.04880	H	-4.56155	0.81137	-1.19104
C	1.34175	1.44590	-1.39633	H	-5.42893	3.09560	-0.86355
F	1.79755	0.63566	-2.36663	H	-3.88609	4.94066	-0.24131
F	3.33899	2.70422	-1.67048	H	-1.46550	4.47321	0.04185
F	2.54810	4.40069	0.31429	H	-0.59055	2.19417	-0.28402
F	0.17883	3.96631	1.58601				
F	-1.36207	1.91850	0.92454	42			
H	-0.81703	-2.42794	-2.73697	[17PH] <sup>+</sup>			
H	-0.96352	0.04889	-2.49332	P	-2.06979	0.13277	-1.05035
H	-0.08361	-4.67449	-2.00840	C	-0.32552	-0.29635	-1.11722
H	1.31666	-4.00435	-2.84827	C	0.51751	0.41231	-0.34639
H	1.26811	-4.00976	-1.08058	C	1.93840	0.10234	-0.15256
				C	2.40020	-1.18872	0.11051
41				C	3.74192	-1.45067	0.34576
17P				C	4.65453	-0.40083	0.33403
P	-1.90200	-0.36240	-1.13998	C	4.22279	0.90168	0.09776
C	-0.32309	-0.35279	-0.17559	C	2.87615	1.13718	-0.12750
C	0.78873	-0.37794	-0.92765	F	2.46549	2.38454	-0.34173
C	2.16994	-0.23032	-0.42785	F	5.09274	1.89823	0.09295
C	2.55730	0.79442	0.43517	F	5.93274	-0.63938	0.55403
C	3.87047	0.94445	0.86108	F	4.15023	-2.68422	0.59922
C	4.84329	0.06575	0.40424	F	1.53616	-2.20412	0.18735
C	4.49715	-0.95352	-0.47425	C	-2.98186	-1.22697	-0.32347
C	3.17760	-1.08226	-0.88097	C	-2.38490	1.67962	-0.20509
F	2.87158	-2.06313	-1.72984	C	0.01429	-1.45338	-2.01987
F	5.42814	-1.79402	-0.91501	C	-4.35122	-1.35580	-0.58624
F	6.10200	0.20111	0.80303	C	-5.06466	-2.38141	0.02114
F	4.20370	1.93316	1.68571	C	-4.41553	-3.26668	0.88179
F	1.66288	1.68897	0.86416	C	-3.05320	-3.13424	1.14117
C	-2.99402	-1.39776	-0.07115	C	-2.32572	-2.11239	0.53941
C	-2.51486	1.33550	-0.75344	C	-2.00932	2.88049	-0.82323
C	-0.34331	-0.28361	1.32410	C	-2.22327	4.08086	-0.15887
C	-3.15751	-2.73381	-0.45181	C	-2.80698	4.08070	1.10874
C	-3.93392	-3.60258	0.31153	C	-3.17901	2.88535	1.71870
C	-4.56671	-3.13967	1.46087	C	-2.97099	1.67490	1.06457
C	-4.41873	-1.80831	1.84610	H	-2.51500	0.27356	-2.37359
C	-3.63696	-0.94315	1.08720	H	0.15507	1.29070	0.18503

H	-0.53387	-1.37908	-2.96416	F	3.236477	0.666085	4.599019
H	1.08159	-1.45160	-2.24863	F	3.529097	-0.843416	2.442453
H	-0.23670	-2.41333	-1.56050	H	2.825395	-3.830620	0.884606
H	-4.85609	-0.66563	-1.25698	H	5.253433	-4.026912	0.778422
H	-6.12429	-2.49324	-0.17916	H	4.735429	-4.388864	-0.866700
H	-4.97655	-4.06793	1.35068	H	5.394290	-2.792732	-0.481643
H	-2.55482	-3.82869	1.80812	H	0.899889	-0.751862	-0.365321
H	-1.26051	-2.01082	0.73267	P	-0.155436	1.871240	-0.327075
H	-1.55422	2.87995	-1.81047	C	-1.897297	2.039534	-0.749637
H	-1.93992	5.01561	-0.62937	C	-2.618218	0.908838	-0.667104
H	-2.97478	5.02149	1.62195	C	-4.063758	0.806326	-0.908987
H	-3.63495	2.89368	2.70230	C	-4.563981	-0.297231	-1.604456
H	-3.26600	0.74020	1.53216	C	-6.354328	1.555534	-0.591550

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**17PHBH**

C	3.382480	-3.142048	0.252667	F	-3.716147	-1.199265	-2.084162
C	2.779769	-1.983496	-0.055338	C	0.863868	2.208326	-1.765231
B	1.294155	-1.557723	0.463536	C	0.220358	2.900653	1.097144
C	3.476882	-1.016049	-0.949433	C	-2.359223	3.395878	-1.205542
C	3.554101	0.347359	-0.658917	C	0.984734	1.152220	-2.682216
C	4.174896	1.278399	-1.474979	C	1.713009	1.347222	-3.849046
C	4.721185	0.874237	-2.682146	C	2.324766	2.577687	-4.092154
C	4.635210	-0.462684	-3.040195	C	2.200201	3.622272	-3.179867
C	4.021897	-1.375340	-2.187102	C	1.461086	3.445315	-2.013155
F	3.953860	-2.636858	-2.615162	C	-0.820774	3.205401	1.982003
F	5.121197	-0.862625	-4.215551	C	-0.531983	3.840609	3.184697
F	5.271625	1.764715	-3.507009	C	0.783967	4.169548	3.499949
F	4.210794	2.567071	-1.113281	C	1.816572	3.874479	2.611493
F	2.979137	0.838344	0.450837	C	1.544480	3.237602	1.405465
C	0.199326	-2.765779	0.424830	H	0.084654	0.503831	-0.065648
C	-0.841667	-2.782522	-0.496352	H	-2.125134	-0.029021	-0.422161
C	4.765624	-3.602853	-0.104370	H	-1.609499	3.842520	-1.866863
C	-1.824052	-3.763058	-0.538423	H	-2.510268	4.074070	-0.360711
C	-1.786353	-4.797360	0.385544	H	-3.298233	3.319751	-1.756846
C	-0.778897	-4.819795	1.339563	H	0.527330	0.187002	-2.473233
C	0.173645	-3.808108	1.344100	H	1.821487	0.533807	-4.558571
F	1.102983	-3.865334	2.313919	H	2.913986	2.717156	-4.992330
F	-0.745160	-5.799724	2.243486	H	2.686879	4.572406	-3.370106
F	-2.714531	-5.753063	0.362752	H	1.369726	4.253496	-1.292783
F	-2.802859	-3.717918	-1.445996	H	-1.842366	2.910199	1.755643
F	-0.979800	-1.783044	-1.402068	H	-1.332447	4.054310	3.883969
C	1.211560	-0.787603	1.916118	H	1.008160	4.644530	4.449001
C	2.285108	-0.456174	2.742556	H	2.841126	4.124791	2.863871
C	2.162941	0.341153	3.875843	H	2.352235	2.984677	0.726797
C	0.917545	0.823131	4.253693	C	-5.922258	-0.471398	-1.821612
C	-0.189136	0.490035	3.491793	F	-6.372230	-1.514149	-2.506320
C	-0.010473	-0.293337	2.359791	C	-6.818348	0.462275	-1.312344
F	-1.127563	-0.492724	1.613064	F	-8.118379	0.307255	-1.511909
F	-1.397848	0.963894	3.816251				
F	0.791194	1.618739	5.317384				

88			H	2.647294	0.327861	1.919428	
<b>18H<sub>2</sub></b>			H	1.380969	0.944795	-0.983183	
P	-5.084281	0.003658	0.030839	H	0.794502	1.924901	1.810956
F	4.363391	-1.528954	2.170402	H	-0.233179	3.252167	-1.489115
F	6.630446	-2.541286	1.200239	H	0.545856	4.814051	-1.355311
F	7.292048	-2.180951	-1.418652	H	1.801486	2.401798	-2.475795
F	5.617789	-0.780486	-3.049519	H	2.584217	3.952597	-2.183831
F	3.347832	0.231168	-2.111846	H	3.718845	2.328884	-0.607985
F	0.359408	-0.285269	2.890148	H	2.751293	5.746631	1.068167
F	-1.791254	-1.855387	2.807055	H	2.477491	5.494211	-0.656796
F	-2.210598	-3.513451	0.685146	H	4.004042	4.995419	0.078072
F	-0.535695	-3.414605	-1.449413	H	3.983179	3.505497	2.014397
F	1.609518	-1.811223	-1.416114	H	2.746572	2.285896	2.270470
B	2.393169	0.066693	0.765989	H	2.448550	3.976855	2.743316
C	3.743162	-0.567264	0.094448	H	0.114372	4.323037	2.318267
C	4.631154	-1.303033	0.875747	H	-1.092124	4.377701	1.022420
C	5.817550	-1.846895	0.396883	H	0.234795	5.545483	1.039436
C	6.158004	-1.667785	-0.935094	H	-0.502354	0.861949	-1.524719
C	5.304232	-0.952326	-1.760417	H	-2.768896	0.000666	-1.792603
C	4.127408	-0.431823	-1.235851	H	-3.674876	1.161479	2.273451
C	1.159402	-1.031365	0.777847	H	-1.369824	1.986736	2.520839
C	0.235334	-1.084558	1.817432	H	-7.710957	1.343995	0.071982
C	-0.902710	-1.882283	1.798943	H	-7.926096	-0.010148	-1.057973
C	-1.137098	-2.703076	0.708646	H	-7.996615	1.652007	-1.642758
C	-0.269950	-2.666094	-0.371705	H	-6.112533	-0.498819	-2.822131
C	0.846229	-1.838848	-0.313429	H	-4.647592	0.507508	-2.902224
C	1.779117	1.356388	-0.048267	H	-6.210272	1.177370	-3.369077
C	0.621705	2.044875	0.734267	H	-6.051514	3.099000	-1.765701
C	0.823970	3.559920	0.414178	H	-4.415644	2.545027	-1.353918
C	0.667049	3.752401	-1.115862	H	-5.605289	2.837971	-0.073603
C	1.980233	3.168381	-1.717342	H	-4.350711	-3.488722	-1.103151
C	2.660262	2.570048	-0.471925	H	-3.242218	-2.137764	-0.927632
C	2.374248	3.662367	0.590150	H	-4.558793	-2.060851	-2.126852
C	2.921971	5.052836	0.237391	H	-4.749360	-3.411282	1.339586
C	2.903308	3.325257	1.986921	H	-5.554158	-2.027909	2.102557
C	-0.025837	4.501822	1.246026	H	-3.831582	-1.945259	1.655119
C	-0.770514	1.522447	0.511121	H	-6.991179	-2.021792	-1.348254
C	-1.198663	0.948270	-0.697898	H	-7.383727	-1.832488	0.379540
C	-2.484411	0.454508	-0.847363	H	-6.730039	-3.357100	-0.225145
C	-3.394694	0.533063	0.218847				
C	-2.988085	1.102864	1.433190				
C	-1.693315	1.579108	1.567982	87			
C	-5.986038	1.017440	-1.241065	<b>[18H]<sup>+</sup></b>			
C	-7.492290	0.983764	-0.937886	P	-5.177013	-0.093148	-0.152943
C	-5.713929	0.506222	-2.661114	F	3.934019	-2.036186	1.249855
C	-5.472504	2.459338	-1.092451	F	6.342362	-2.834707	0.365454
C	-5.230266	-1.840445	-0.049722	F	7.379118	-1.755239	-1.894800
C	-4.283836	-2.397104	-1.122829	F	5.999356	0.124797	-3.277351
C	-4.812430	-2.319703	1.352062	F	3.594152	0.935333	-2.407554
C	-6.674901	-2.269284	-0.331426	F	1.961840	-0.917262	2.786928
H	-5.708749	0.359684	1.237615	F	-0.062180	-2.475823	3.666009
				F	-1.901870	-3.432909	1.901943

F	-1.675236	-2.864207	-0.742196	H	2.848696	1.303916	2.095534
F	0.345802	-1.291378	-1.612844	H	2.743060	2.680010	3.192487
B	2.281447	-0.048264	-0.026629	H	0.373993	3.214665	3.213761
C	3.685058	-0.495858	-0.523991	H	-0.963598	3.757851	2.187165
C	4.418799	-1.485069	0.136466	H	0.401827	4.834116	2.495006
C	5.664459	-1.909668	-0.299664	H	-0.782891	1.601616	-1.606570
C	6.199012	-1.354769	-1.457819	H	-3.064086	0.841564	-1.999336
C	5.493665	-0.383893	-2.161676	H	-3.554718	0.145701	2.237070
C	4.260269	0.030296	-1.683709	H	-1.243086	0.890473	2.604466
C	1.254627	-1.116009	0.552883	H	-7.817955	0.975545	0.579272
C	1.109278	-1.432143	1.895108	H	-8.096166	0.061323	-0.919793
C	0.062507	-2.213118	2.371259	H	-8.296085	1.812148	-0.898999
C	-0.875539	-2.703433	1.470700	H	-6.469839	0.342163	-2.904178
C	-0.760385	-2.408236	0.119713	H	-5.066532	1.427352	-2.767634
C	0.294330	-1.619901	-0.312559	H	-6.697703	2.089690	-2.823011
C	1.666241	1.376492	-0.229752	H	-6.431747	3.357475	-0.663826
C	0.578791	1.735766	0.835500	H	-4.741663	2.823763	-0.628539
C	0.835342	3.249419	1.091505	H	-5.790064	2.565322	0.779646
C	0.532751	4.021117	-0.214249	H	-4.421733	-2.884489	-2.529557
C	1.723455	3.672134	-1.153635	H	-3.315811	-1.657376	-1.917135
C	2.526269	2.666303	-0.309377	H	-4.717124	-1.188763	-2.918557
C	2.401664	3.252463	1.116420	H	-4.530014	-3.717020	-0.185476
C	2.996500	4.657523	1.268822	H	-5.302881	-2.770067	1.095094
C	3.056240	2.374340	2.188487	H	-3.652910	-2.381734	0.549958
C	0.123926	3.791120	2.316108	H	-7.104760	-1.655008	-2.004255
C	-0.837408	1.314368	0.535128	H	-7.328362	-2.117893	-0.298121
C	-1.383438	1.292447	-0.757071	H	-6.669390	-3.273732	-1.456689
C	-2.683230	0.860413	-0.982416				
C	-3.481197	0.442788	0.092324				
C	-2.954907	0.465626	1.389279				
C	-1.649249	0.891616	1.596379				
C	-6.230198	1.235651	-0.913397				
C	-7.692966	0.987545	-0.507497				
C	-6.096376	1.259025	-2.441320				
C	-5.756647	2.570539	-0.314790				
C	-5.231144	-1.801349	-0.868880				
C	-4.365000	-1.865508	-2.134807				
C	-4.642433	-2.709036	0.224889				
C	-6.675795	-2.217481	-1.171176				
H	-5.684278	-0.227277	1.149449				
H	1.194897	1.220608	-1.218408				
H	0.824459	1.235188	1.779405				
H	-0.440224	3.739392	-0.628373				
H	0.477866	5.094914	-0.015575				
H	1.406997	3.236589	-2.106336				
H	2.316519	4.558501	-1.390010				
H	3.550477	2.506404	-0.651356				
H	2.915504	4.990498	2.308276				
H	2.513968	5.409384	0.642682				
H	4.060528	4.643243	1.012826				
H	4.142903	2.491608	2.138824				
				87			
				[18H]			
				P	-5.287102	0.136538	0.182115
				F	4.400219	-1.549078	2.069733
				F	6.634998	-2.543303	1.016277
				F	7.219995	-2.139764	-1.615337
				F	5.497749	-0.713538	-3.172675
				F	3.257906	0.281691	-2.153980
				F	0.465103	-0.350354	2.977971
				F	-1.637055	-1.984741	2.987768
				F	-2.138059	-3.607875	0.854846
				F	-0.568799	-3.443318	-1.358922
				F	1.533413	-1.787047	-1.408768
				B	2.376073	0.072899	0.758945
				C	3.710237	-0.550802	0.029915
				C	4.622809	-1.299760	0.769948
				C	5.794829	-1.835390	0.247900
				C	6.096621	-1.634932	-1.089630
				C	5.218520	-0.906466	-1.876007
				C	4.056434	-0.394940	-1.309292
				C	1.162946	-1.038771	0.811976
				C	0.293146	-1.127145	1.894371
				C	-0.820418	-1.958493	1.924880

C	-1.093257	-2.768462	0.834544	H	-6.001255	-0.768519	-2.842060
C	-0.280383	-2.694206	-0.285849	H	-4.538025	0.222844	-2.954167
C	0.814917	-1.839038	-0.272181	H	-6.070231	0.833780	-3.580007
C	1.729950	1.367508	-0.017024	H	-6.018372	2.914471	-2.226505
C	0.580565	2.038873	0.795841	H	-4.409248	2.433942	-1.646182
C	0.795160	3.559857	0.521496	H	-5.675021	2.857731	-0.486598
C	0.605218	3.805184	-0.996750	H	-4.126831	-3.374657	-0.981574
C	1.895436	3.222024	-1.645944	H	-3.126550	-1.940506	-0.773086
C	2.604189	2.588535	-0.433275	H	-4.365548	-1.975828	-2.039808
C	2.348219	3.654638	0.663208	H	-4.669406	-3.321908	1.399674
C	2.900282	5.049227	0.332204	H	-5.526631	-1.946433	2.134813
C	2.906043	3.283611	2.039599	H	-3.807602	-1.815384	1.717459
C	-0.031950	4.480133	1.399268	H	-6.854448	-2.086744	-1.363631
C	-0.827146	1.536605	0.566171	H	-7.313713	-1.916842	0.343163
C	-1.289119	1.038285	-0.659687	H	-6.534326	-3.402848	-0.229677
C	-2.597976	0.595689	-0.814519				
C	-3.516434	0.640774	0.244344				
C	-3.052625	1.129196	1.472064	86			
C	-1.737035	1.554622	1.629592	18			
C	-5.961676	0.904429	-1.427623	P	-5.328741	-0.034197	0.104092
C	-7.493137	0.917063	-1.278866	F	3.924716	-1.912346	1.272766
C	-5.613670	0.251013	-2.768536	F	6.335429	-2.681647	0.364058
C	-5.480765	2.363159	-1.444648	F	7.282766	-1.684136	-1.973568
C	-5.161595	-1.748469	-0.008466	F	5.810535	0.088069	-3.404798
C	-4.136470	-2.278289	-1.014995	F	3.404504	0.871637	-2.507107
C	-4.768238	-2.230421	1.398216	F	1.861261	-0.876972	2.768962
C	-6.550049	-2.311108	-0.336663	F	-0.065653	-2.551593	3.645120
H	2.690791	0.320175	1.901877	F	-1.802903	-3.670028	1.878647
H	1.311785	0.968372	-0.948281	F	-1.588269	-3.115656	-0.778312
H	0.763919	1.883005	1.866607	F	0.311870	-1.393352	-1.641925
H	-0.309200	3.327063	-1.359646	B	2.169655	-0.037536	-0.050899
H	0.495783	4.876350	-1.200726	C	3.579678	-0.475946	-0.570089
H	1.685920	2.472386	-2.413655	C	4.360685	-1.404407	0.118741
H	2.495764	4.009406	-2.114743	C	5.608681	-1.811895	-0.329302
H	3.659971	2.350870	-0.603216	C	6.096778	-1.299582	-1.525486
H	2.737559	5.729180	1.176708	C	5.344273	-0.386248	-2.254233
H	2.449837	5.507713	-0.550374	C	4.109215	0.012821	-1.764712
H	3.981749	4.991234	0.163450	C	1.171294	-1.125872	0.530340
H	3.992632	3.428233	2.040533	C	1.036155	-1.439130	1.873436
H	2.719896	2.247343	2.314358	C	0.042015	-2.284294	2.346787
H	2.490687	3.940292	2.814584	C	-0.850169	-2.852034	1.445112
H	0.137122	4.271135	2.462072	C	-0.744233	-2.564108	0.090582
H	-1.101785	4.349684	1.202295	C	0.251679	-1.698307	-0.336632
H	0.218522	5.531183	1.213145	C	1.576479	1.393046	-0.216608
H	-0.609304	0.974769	-1.503998	C	0.546949	1.760043	0.904062
H	-2.898972	0.199437	-1.779053	C	0.881664	3.250802	1.193239
H	-3.736617	1.170058	2.316159	C	0.530532	4.082831	-0.060984
H	-1.396076	1.899783	2.602646	C	1.637286	3.709501	-1.089251
H	-7.793592	1.437250	-0.364837	C	2.463651	2.658557	-0.324354
H	-7.911251	-0.093015	-1.244396	C	2.445746	3.207339	1.122302
H	-7.942440	1.435953	-2.135491	C	3.100088	4.585585	1.274019
				C	3.134858	2.279679	2.128791



C	0.259317	3.768396	2.475260	H	-7.114002	-2.258787	-0.333254
C	-0.892430	1.390721	0.632653	H	-6.274957	-3.332352	-1.465817
C	-1.492703	1.487389	-0.628691				
C	-2.810169	1.090572	-0.831021	60			
C	-3.591258	0.587439	0.218274	<b>18B</b>			
C	-2.991970	0.503839	1.480822	C	0.251012	3.670298	-1.088840
C	-1.668259	0.885569	1.679985	C	-1.192078	3.889574	-0.548549
C	-6.228590	1.167753	-1.063811	C	0.828025	2.654404	-0.086014
C	-7.728859	0.946047	-0.798136	C	0.073760	1.321954	-0.333294
C	-5.990502	1.067939	-2.573951	C	-1.312214	1.549938	0.356223
C	-5.873509	2.584928	-0.588465	C	-1.246356	3.049914	0.749314
C	-5.044138	-1.699673	-0.765549	C	0.232118	3.139674	1.257153
C	-4.101297	-1.696136	-1.972098	C	0.650781	4.561154	1.650352
C	-4.435845	-2.591423	0.329210	C	0.591586	2.229309	2.436735
C	-6.403742	-2.285326	-1.166604	B	0.691906	-0.083677	-0.064385
H	1.043741	1.253532	-1.176745	C	-2.337698	3.469997	1.714300
H	0.810484	1.219049	1.820775	C	2.219459	-0.409396	-0.156711
H	-0.479446	3.859072	-0.413116	C	-0.373890	-1.245166	0.110641
H	0.546052	5.150987	0.175117	C	2.814232	-1.389733	0.639204
H	1.234746	3.301151	-2.021439	C	4.164238	-1.699806	0.562186
H	2.244137	4.578512	-1.356846	C	4.959202	-1.032675	-0.361980
H	3.460527	2.483209	-0.736826	C	4.404908	-0.064762	-1.190954
H	3.063322	4.907229	2.319990	C	3.055272	0.232589	-1.071909
H	2.626862	5.363261	0.672848	C	-1.026741	-1.703784	-1.025393
H	4.154909	4.534841	0.984103	C	-2.138515	-2.530338	-0.971105
H	4.219565	2.330092	1.988056	C	-2.613602	-2.931006	0.271124
H	2.849575	1.226620	2.053034	C	-1.983228	-2.499182	1.431275
H	2.924249	2.594651	3.156592	C	-0.880405	-1.661965	1.330373
H	0.553385	3.157863	3.336387	F	6.248518	-1.322574	-0.455865
H	-0.833526	3.745621	2.409504	F	4.700582	-2.624300	1.351668
H	0.562244	4.802497	2.668837	F	2.083898	-2.051662	1.537055
H	-0.923411	1.860915	-1.476237	F	5.166397	0.556686	-2.085579
H	-3.225027	1.160051	-1.830973	F	2.556309	1.145857	-1.910084
H	-3.573442	0.123916	2.317036	F	-0.336417	-1.194358	2.463995
H	-1.223294	0.788731	2.668461	F	-2.455178	-2.867702	2.619803
H	-7.965183	1.078965	0.261171	F	-3.685315	-3.711724	0.351021
H	-8.055568	-0.054795	-1.093866	F	-2.755394	-2.925566	-2.080031
H	-8.313755	1.672242	-1.375538	F	-0.604618	-1.283120	-2.228329
H	-6.308207	0.102753	-2.976469	C	-2.525747	1.050272	-0.397169
H	-4.946605	1.227101	-2.853407	C	-3.561232	0.449683	0.328883
H	-6.582982	1.841789	-3.078541	C	-4.660401	-0.117661	-0.309125
H	-6.543030	3.306869	-1.071015	C	-4.745148	-0.096752	-1.698694
H	-4.844294	2.854542	-0.838094	C	-3.734133	0.513655	-2.436081
H	-5.995501	2.685127	0.495436	C	-2.638893	1.082930	-1.791920
H	-4.004369	-2.720066	-2.354597	H	0.823697	4.601537	-1.088839
H	-3.098915	-1.358304	-1.699113	H	0.271209	3.280887	-2.111260
H	-4.469048	-1.070772	-2.788526	H	-1.967137	3.573029	-1.251604
H	-4.209571	-3.582984	-0.079370	H	-1.383682	4.944492	-0.330659
H	-5.123456	-2.710663	1.171856	H	1.917961	2.573376	-0.101351
H	-3.500664	-2.171422	0.711540	H	-0.073962	1.210918	-1.425769
H	-6.847072	-1.754697	-2.014254	H	-1.326703	0.999810	1.305039

H	1.740681	4.623017	1.738197
H	0.228331	4.820616	2.626638
H	0.329268	5.323842	0.939346
H	0.496253	1.159190	2.232189
H	1.630746	2.408462	2.731204
H	-0.036099	2.450268	3.307010
H	-2.221028	4.518562	2.006862
H	-3.324172	3.357983	1.252262
H	-2.324702	2.857307	2.622829
H	-3.485809	0.405209	1.413534
H	-5.439433	-0.593542	0.278476
H	-5.588548	-0.556357	-2.203129
H	-3.789351	0.535604	-3.519692
H	-1.851963	1.531611	-2.392377

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**[18BH]<sup>-</sup>**

C	-0.27109	3.60928	-1.13948
C	-1.82279	3.48626	-1.08773
C	0.15390	2.92347	0.17505
C	-0.14260	1.40839	-0.00993
C	-1.68560	1.34236	0.22731
C	-2.10685	2.84085	0.28983
C	-0.94267	3.42265	1.15481
C	-0.99702	4.95045	1.30472
C	-0.84677	2.85886	2.57627
B	0.72019	0.30448	0.84859
C	-3.52084	3.06337	0.79285
C	2.26900	0.09826	0.32976
C	-0.09611	-1.11193	0.67607
C	3.05804	-0.85922	0.96744
C	4.38183	-1.12442	0.64445
C	4.98623	-0.40777	-0.37788
C	4.25106	0.55605	-1.04621
C	2.92501	0.78333	-0.68684
C	-0.20555	-1.74777	-0.55627
C	-1.05947	-2.81331	-0.80760
C	-1.84442	-3.30473	0.22428
C	-1.76526	-2.71639	1.47636
C	-0.90518	-1.64112	1.67396
F	6.26288	-0.64165	-0.70948
F	5.08368	-2.05895	1.30118
F	2.54056	-1.58927	1.96859
F	4.82500	1.25732	-2.03437
F	2.30509	1.74494	-1.39920
F	-0.93871	-1.08280	2.89763
F	-2.54047	-3.17485	2.47087
F	-2.69054	-4.31955	0.00651
F	-1.15258	-3.35669	-2.02797
F	0.48940	-1.28448	-1.61258
C	-2.47637	0.46322	-0.72028

C	-3.54129	-0.29367	-0.21609
C	-4.26068	-1.17291	-1.02119
C	-3.92997	-1.31549	-2.36532
C	-2.88373	-0.56095	-2.89061
C	-2.16958	0.31641	-2.08032
H	0.04326	4.65778	-1.18687
H	0.16733	3.10083	-2.00241
H	-2.23464	2.88045	-1.89947
H	-2.30965	4.46594	-1.15558
H	1.18091	3.14445	0.48419
H	0.04403	1.17352	-1.06279
H	-1.88315	0.92421	1.22368
H	-0.04656	5.31735	1.70911
H	-1.78405	5.23440	2.01326
H	-1.18718	5.48247	0.37080
H	-0.74621	1.77671	2.61997
H	0.03372	3.27967	3.07549
H	-1.72691	3.15704	3.16034
H	0.79869	0.56871	2.02858
H	-3.74753	4.13260	0.88050
H	-4.25004	2.61954	0.10565
H	-3.66751	2.60036	1.77563
H	-3.78187	-0.21369	0.84211
H	-5.06223	-1.76592	-0.58996
H	-4.47004	-2.01759	-2.99304
H	-2.60514	-0.67185	-3.93442
H	-1.33247	0.86330	-2.50279

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**18P**

C	-4.242114	1.929716	-0.596301
C	-3.685802	0.753617	-1.448332
C	-4.557813	1.254536	0.749124
C	-3.211270	0.905898	1.410418
C	-2.704279	-0.330359	0.590510
C	-3.792705	-0.476579	-0.509741
C	-5.087557	-0.128848	0.308927
C	-5.393734	-1.069226	1.480279
C	-6.357912	-0.063839	-0.547021
C	-3.848413	-1.828679	-1.204976
C	-1.236597	-0.236819	0.208905
C	-0.712082	-0.535624	-1.048998
C	0.659335	-0.458746	-1.295062
C	1.568705	-0.102134	-0.296235
C	1.041417	0.186966	0.972019
C	-0.323829	0.125598	1.211702
P	3.347254	-0.058431	-0.793913
C	4.058940	-1.525048	0.180976
C	4.015830	1.577423	-0.087094
C	3.640338	-1.663789	1.647478
C	3.552290	-2.762950	-0.578127

C	5.588726	-1.486047	0.076756	C	-3.80690	-0.43129	-0.56529
C	4.315894	1.673222	1.411644	C	-5.11749	-0.15994	0.25894
C	2.991671	2.659069	-0.463131	C	-5.44728	-1.21009	1.32616
C	5.313106	1.868243	-0.862577	C	-6.36933	-0.00746	-0.61266
H	-3.515726	2.738586	-0.479711	C	-3.85151	-1.71082	-1.38794
H	-5.140140	2.362667	-1.045341	C	-1.27472	-0.27896	0.24149
H	-4.274133	0.596073	-2.357546	C	-0.72723	-0.46290	-1.03244
H	-2.658225	0.937997	-1.764909	C	0.64488	-0.38232	-1.24881
H	-5.232197	1.828755	1.391897	C	1.51245	-0.12717	-0.18314
H	-3.324700	0.664467	2.471290	C	0.98367	0.05373	1.10455
H	-2.510551	1.743484	1.342531	C	-0.38533	-0.01940	1.29969
H	-2.774967	-1.221950	1.227317	P	3.27337	-0.02844	-0.49713
H	-5.587057	-2.085664	1.121121	C	4.14009	-1.54148	0.13363
H	-4.599729	-1.122778	2.226603	C	3.97798	1.64210	-0.08799
H	-6.299826	-0.729794	1.993082	C	3.82683	-1.75936	1.62050
H	-6.702167	-1.072606	-0.797667	C	3.57304	-2.71073	-0.69030
H	-7.160850	0.422824	0.016974	C	5.65218	-1.42411	-0.09574
H	-6.230354	0.483495	-1.482260	C	4.32826	1.75884	1.40067
H	-3.941361	-2.637867	-0.472677	C	2.90120	2.67327	-0.46510
H	-4.713748	-1.876846	-1.874587	C	5.22767	1.87200	-0.95431
H	-2.961087	-2.038712	-1.805266	H	-3.52767	2.76873	-0.21687
H	-1.367495	-0.817568	-1.863987	H	-5.13732	2.45098	-0.84985
H	1.032743	-0.678205	-2.291964	H	-4.24820	0.81629	-2.30724
H	1.702569	0.458924	1.788262	H	-2.64605	1.10178	-1.66016
H	-0.696955	0.356428	2.206663	H	-5.28125	1.68445	1.52260
H	2.560549	-1.805802	1.739507	H	-3.40286	0.41685	2.52586
H	4.128105	-2.547937	2.077484	H	-2.56520	1.60218	1.52571
H	3.928511	-0.801850	2.253238	H	-2.82891	-1.34292	1.11944
H	3.933318	-3.671083	-0.095583	H	-5.63733	-2.18500	0.86572
H	2.458375	-2.811945	-0.572661	H	-4.67141	-1.34155	2.08280
H	3.890017	-2.758802	-1.618601	H	-6.36202	-0.91867	1.85130
H	6.003412	-2.435459	0.436432	H	-6.71321	-0.98537	-0.96369
H	6.022172	-0.687586	0.685853	H	-7.18044	0.42664	-0.01959
H	5.917195	-1.346356	-0.958722	H	-6.22416	0.62651	-1.48861
H	5.094696	0.971750	1.722099	H	-3.93757	-2.58934	-0.74015
H	4.679013	2.683878	1.638381	H	-4.71897	-1.69807	-2.05498
H	3.431590	1.501866	2.029757	H	-2.97034	-1.85821	-2.01704
H	3.428111	3.648916	-0.283752	H	-1.37172	-0.66296	-1.87809
H	2.076332	2.575673	0.128186	H	1.03123	-0.52111	-2.25497
H	2.716604	2.598800	-1.521765	H	1.63214	0.24774	1.95425
H	5.702170	2.850998	-0.569548	H	-0.78341	0.12272	2.29999
H	6.091287	1.128096	-0.657188	H	3.38012	-0.11195	-1.89464
H	5.132807	1.878008	-1.941094	H	2.76062	-1.93256	1.78574
65				H	4.36342	-2.65363	1.95136
<b>[18PH]<sup>+</sup></b>				H	4.15587	-0.92732	2.24859
C	-4.25027	1.97510	-0.42562	H	4.01995	-3.63821	-0.32023
C	-3.67838	0.88479	-1.37637	H	2.48773	-2.79703	-0.58598
C	-4.59608	1.17395	0.84042	H	3.82253	-2.62131	-1.75191
C	-3.26563	0.76129	1.49738	H	6.11027	-2.38545	0.15542
C	-2.74810	-0.39422	0.57192	H	6.10967	-0.66576	0.54441
				H	5.89794	-1.20564	-1.13976

H	5.13432	1.08014	1.69090	H	6.566228	-0.424522	-0.747430
H	4.67305	2.77973	1.59059	H	5.718513	-1.007298	0.678583
H	3.46411	1.58258	2.04723	H	5.615972	-3.194638	-0.332782
H	3.32803	3.67211	-0.33485	H	6.436564	-2.558481	-1.742443
H	2.01550	2.59154	0.16865	H	4.393165	0.791527	-0.840472
H	2.58903	2.57872	-1.51033	H	3.549314	-1.143790	0.917454
H	5.59491	2.88317	-0.75517	H	2.171654	-2.360696	-1.442933
H	6.03747	1.17764	-0.72474	H	5.392300	0.603897	-3.424604
H	4.99966	1.80916	-2.02239	H	5.290279	-0.961309	-4.234663

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**18PHBH**

C	5.676612	-0.968207	-0.414368	H	2.924099	-1.014074	-4.052515
C	5.598950	-2.380360	-1.060020	H	1.680690	0.677075	-0.921343
C	4.369309	-0.298678	-0.895087	H	4.978529	-3.356632	-3.633771
C	3.201068	-0.958456	-0.106274	H	4.211484	-4.424579	-2.448005
C	3.083696	-2.346922	-0.834413	H	3.212548	-3.362686	-3.448082
C	4.273221	-2.349290	-1.847926	H	1.510351	-4.477935	-1.238918
C	4.235140	-0.867772	-2.334448	H	1.263641	-6.528976	0.117635
C	5.399639	-0.479362	-3.256684	H	2.607083	-6.817363	2.189782
C	2.957598	-0.486847	-3.091506	H	4.187210	-5.029872	2.878112
B	1.795587	-0.077829	0.032020	H	4.403967	-2.978728	1.541509
C	4.162792	-3.430971	-2.906033	C	-5.394593	-2.547288	-0.793037
C	1.858772	0.905066	1.380401	C	-4.790169	-1.827451	0.442911
C	0.507985	-1.090744	0.030209	C	-6.491996	-1.567713	-1.228236
C	1.158959	0.769060	2.582354	C	-5.783943	-0.293876	-1.746939
C	1.362791	1.564831	3.709099	C	-5.366393	0.455712	-0.435206
C	2.283779	2.599660	3.666380	C	-5.698432	-0.584775	0.660971
C	2.956365	2.835060	2.476719	C	-7.079175	-1.111239	0.128873
C	2.721529	2.004956	1.388690	C	-8.184954	-0.058048	-0.013649
C	0.383999	-2.134769	0.946192	C	-7.654868	-2.246729	0.982759
C	-0.633420	-3.078544	0.917457	C	-5.723989	-0.042492	2.080878
C	-1.599437	-3.000242	-0.078376	C	-3.996817	1.099360	-0.516578
C	-1.519794	-1.987651	-1.019275	C	-2.928942	0.851557	0.350113
C	-0.471823	-1.077256	-0.952797	C	-1.710523	1.507195	0.196448
F	2.482669	3.380391	4.726480	C	-1.537608	2.449067	-0.820388
F	0.660983	1.352813	4.822438	C	-2.605229	2.731879	-1.681361
F	0.161675	-0.121003	2.712333	C	-3.805337	2.056453	-1.528413
F	3.779286	3.882913	2.365764	P	0.064563	3.255506	-0.923560
F	3.339984	2.391648	0.249017	C	0.046621	4.746458	0.183344
F	-0.480112	-0.126428	-1.911636	C	0.725191	3.489809	-2.645633
F	-2.468887	-1.867464	-1.959758	C	-1.025618	5.752392	-0.252241
F	-2.612633	-3.870302	-0.111034	C	-0.306912	4.212245	1.582874
F	-0.692652	-4.058548	1.818165	C	1.439693	5.389833	0.212673
F	1.284053	-2.254748	1.928305	C	0.303338	2.275158	-3.486304
C	2.989874	-3.583827	0.032906	C	2.261674	3.491272	-2.539195
C	2.110546	-4.606803	-0.339985	C	0.231298	4.789407	-3.290711
C	1.967226	-5.761234	0.424804	H	-4.650032	-2.713058	-1.572794
C	2.717854	-5.923072	1.584902	H	-5.812971	-3.521152	-0.526132
C	3.603382	-4.919547	1.969318	H	-4.778212	-2.467407	1.330229
C	3.732854	-3.764250	1.205476	H	-3.756698	-1.541393	0.250745







H	2.107618	1.038063	-1.310847	F	0.973306	-1.711114	-0.967742
H	1.187511	2.375265	1.231508	F	4.410942	-0.339858	-2.484539
H	1.288190	3.234193	-2.415985	F	6.723738	-1.637788	-2.883709
H	2.139183	4.750647	-2.215304	F	7.957099	-2.884558	-0.815201
H	4.237887	3.611977	-2.210512	F	6.859953	-2.835850	1.665473
H	3.368730	2.142732	-2.664391	F	4.542133	-1.546132	2.082117
H	4.523084	2.010667	-0.259551	B	3.038535	-0.128474	0.056996
H	3.724526	5.712299	0.758883	C	1.918234	-0.780195	0.976423
H	3.825849	5.339764	-0.962506	C	1.750154	-0.505504	2.323922
H	5.044380	4.706126	0.152786	C	0.627544	-0.911097	3.036332
H	4.251240	3.607250	2.173160	C	-0.373960	-1.614838	2.378152
H	2.968124	2.409773	2.126372	C	-0.240754	-1.906865	1.025308
H	2.578650	4.129736	2.384783	C	0.896819	-1.487703	0.354790
H	0.635731	4.878587	1.193813	C	4.397601	-0.865957	-0.176407
H	-0.110646	4.912522	-0.413367	C	4.999931	-0.918681	-1.434668
H	1.341967	5.869424	-0.098433	C	6.188055	-1.595267	-1.668410
H	-4.061617	-1.800119	0.554514	C	6.817552	-2.240988	-0.610964
H	-6.149346	-2.060132	-1.597621	C	6.252823	-2.216941	0.658724
H	-6.450125	0.033529	0.650726	C	5.053480	-1.546872	0.850681
H	-4.012161	1.197565	2.007566	C	2.580950	1.141615	-0.721541
H	-2.167992	-1.913253	-0.826169	C	1.536968	2.012834	0.055676
H	-2.736304	-4.264950	-1.930957	C	1.925097	3.460781	-0.329597
H	-3.117811	-4.052269	-0.222532	C	1.687880	3.643762	-1.845768
H	-7.184710	-3.571950	0.081388	C	2.833056	2.829256	-2.514032
H	-6.758723	-2.041430	0.861684	C	3.550486	2.204612	-1.301748
H	-5.734951	-3.461255	1.092801	C	3.485083	3.342921	-0.254464
H	-5.225889	2.928213	2.897936	C	4.206486	4.626239	-0.681845
H	-6.313134	1.775400	3.658034	C	4.060818	2.943059	1.108735
H	-7.839107	1.815751	1.801790	C	1.260761	4.508944	0.541983
H	-7.280872	3.493521	1.753825	C	0.098857	1.572446	-0.061957
H	-4.772734	-0.224548	3.883257	C	-0.504582	1.030141	-1.194682
H	-4.630885	-1.202061	2.421196	C	-1.751922	0.418756	-1.152028
H	-6.228445	-0.670228	2.977951	C	-2.506111	0.306285	0.013835
H	-5.053109	-3.847764	-2.578111	C	-1.919061	0.901663	1.134550
H	-5.288844	-4.744013	-1.083046	C	-0.678515	1.519999	1.094045
H	-2.819832	-0.646509	-2.844702	C	-4.243907	-2.111475	-0.788808
H	-2.296663	-2.263615	-3.315475	C	-5.675516	-2.693782	-0.634447
H	-4.026889	-1.858616	-3.271675	C	-5.451730	0.557034	0.112888
H	-7.043053	2.029240	-0.477330	C	-5.438613	1.630549	1.238076
H	-4.857797	3.018567	-1.062227	F	0.125633	1.044581	-2.380994
H	-5.796842	4.195950	-0.136278	F	-2.214596	-0.045620	-2.318255
H	-4.480692	3.303070	0.640071	F	-2.524553	0.849003	2.326225
H	2.558783	0.400192	1.827229	F	-0.182040	1.991534	2.247660
				C	-3.959518	-2.257455	-2.300060
				C	-4.441269	-3.702285	-2.535726
				C	-6.058691	-3.127523	0.777567
				C	-6.419965	2.725718	0.736231
				C	-6.900442	2.265887	-0.654033
				C	-5.803467	1.075959	2.611033
				C	-5.697840	-3.864991	-1.650794
				C	-4.714077	-1.291506	-3.208446
100							
<b>19</b>							
P	-4.054343	-0.654237	0.370745				
F	2.666503	0.235486	2.961159				
F	0.494235	-0.614087	4.323543				
F	-1.470127	-1.980825	3.027089				
F	-1.222736	-2.535157	0.378111				



C	-5.776515	1.351014	-1.169787	C	-1.173609	-1.434669	-0.421439
C	-4.612914	2.177972	-1.715975	C	-1.201796	-2.878604	-0.994990
H	2.084214	0.635220	-1.569785	C	0.290969	-3.014751	-1.448821
H	1.745915	1.933157	1.126213	C	0.725789	-2.014590	-2.525675
H	0.695512	3.292607	-2.137874	C	0.646211	-4.408875	-1.979354
H	1.736508	4.703643	-2.112884	B	0.998155	-0.019821	0.058038
H	3.505273	3.477362	-3.082393	C	-2.276797	-3.074013	-2.046998
H	2.458677	2.064774	-3.199349	C	0.179239	1.265638	-0.370324
H	4.556829	1.834845	-1.513372	C	2.531542	0.174922	0.366956
H	4.149984	5.373112	0.116793	C	0.389106	1.862363	-1.606676
H	3.796055	5.077958	-1.586161	C	-0.408096	2.893305	-2.086529
H	5.266551	4.419354	-0.862462	C	-1.450469	3.362445	-1.297498
H	5.154191	2.939545	1.054835	C	-1.675444	2.809142	-0.042173
H	3.755495	1.953631	1.461584	C	-0.853772	1.784168	0.401584
H	3.774759	3.664760	1.881514	C	3.578819	-0.500701	-0.249520
H	1.457195	4.330180	1.604115	C	4.910312	-0.263052	0.064613
H	0.174424	4.495455	0.400447	C	5.221991	0.676279	1.038976
H	1.616278	5.512224	0.286576	C	4.206304	1.373094	1.682382
H	-3.572116	-2.830326	-0.296461	C	2.890076	1.119196	1.327725
H	-6.389937	-1.929848	-0.968824	F	-2.227121	4.342407	-1.738710
H	-6.327225	-0.081964	0.313930	F	-0.188881	3.425440	-3.284454
H	-4.431108	2.059943	1.302752	F	1.369641	1.404875	-2.398215
H	-2.888793	-2.172748	-2.493853	F	-2.679191	3.250660	0.710462
H	-4.639527	-3.898383	-3.593558	F	-1.080423	1.282119	1.621571
H	-3.664875	-4.404453	-2.216077	F	1.929880	1.796158	1.968389
H	-7.030776	-3.629835	0.769845	F	4.503308	2.266913	2.619471
H	-6.119045	-2.285408	1.473490	F	6.488257	0.906855	1.356816
H	-5.317307	-3.830490	1.173016	F	5.883423	-0.920593	-0.557761
H	-5.914904	3.693927	0.673523	F	3.330576	-1.399932	-1.207834
H	-7.256945	2.850207	1.429916	C	-2.375102	-0.962152	0.360686
H	-7.824824	1.685808	-0.557697	C	-3.266582	-0.079263	-0.252898
H	-7.106785	3.099379	-1.332219	C	-4.317674	0.516157	0.430487
H	-5.791508	1.868821	3.364554	C	-4.552200	0.223396	1.762701
H	-5.104006	0.296877	2.924961	C	-3.689405	-0.659195	2.388795
H	-6.812650	0.647480	2.590901	C	-2.624153	-1.231458	1.705617
H	-6.618220	-3.844583	-2.241259	F	-3.078031	0.275483	-1.532857
H	-5.683406	-4.823538	-1.122209	F	-5.094785	1.382344	-0.219789
H	-4.462170	-0.253131	-2.994428	F	-3.858281	-0.964829	3.676302
H	-4.459538	-1.489673	-4.254010	F	-1.801573	-2.022985	2.412431
H	-5.798668	-1.412370	-3.109134	H	0.082073	-3.498050	1.879780
H	-6.147100	0.685541	-1.955431	H	0.659112	-4.747494	0.781807
H	-3.828219	1.551383	-2.141717	H	-1.473274	-4.887764	-0.212065
H	-4.967766	2.847500	-2.505395	H	-2.083511	-3.648194	0.862625
H	-4.158982	2.796360	-0.933598	H	1.937450	-2.750458	0.057136
60				H	0.070722	-1.282699	1.397873
19B				H	-1.143855	-0.774738	-1.291992
C	0.132533	-3.790608	0.829029	H	0.063398	-2.079729	-3.395725
C	-1.272140	-3.883252	0.171984	H	0.734081	-0.967774	-2.205034
C	0.849299	-2.726805	-0.027919	H	1.738524	-2.243383	-2.864766
C	0.212447	-1.349222	0.303043	H	1.732929	-4.503001	-2.072935
				H	0.294285	-5.224122	-1.346186

H 0.218253 -4.553501 -2.976817  
H -2.200970 -2.329171 -2.845772  
H -2.210345 -4.071022 -2.493951  
H -3.272257 -2.977161 -1.599871  
H -5.372961 0.679759 2.300703

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[19BH]<sup>-</sup>

C -0.356348 3.682764 0.993606  
C 1.196316 3.718484 0.878897  
C -0.767476 2.945843 -0.299320  
C -0.339180 1.463404 -0.110622  
C 1.196936 1.549844 -0.399600  
C 1.487384 3.072732 -0.494978  
C 0.243695 3.528012 -1.325561  
C 0.157588 2.939397 -2.737975  
C 0.148181 5.051691 -1.494575  
B -1.107330 0.278121 -0.951798  
C 2.858522 3.395730 -1.059054  
C -0.140880 -1.047651 -0.820630  
C -2.604095 -0.092267 -0.377771  
C 0.674265 -1.490493 -1.855442  
C 1.644808 -2.477538 -1.705123  
C 1.829498 -3.064110 -0.463311  
C 1.040208 -2.658972 0.604069  
C 0.081105 -1.676734 0.401153  
C -3.300947 0.539686 0.646202  
C -4.580774 0.172761 1.054558  
C -5.222707 -0.882751 0.430246  
C -4.574112 -1.550396 -0.598213  
C -3.299760 -1.145734 -0.970980  
F 2.788052 -3.979737 -0.280259  
F 2.416147 -2.850458 -2.733235  
F 0.601149 -0.925747 -3.072153  
F 1.253869 -3.181907 1.819778  
F -0.592044 -1.271957 1.494961  
F -2.734925 -1.834026 -1.976456  
F -5.186384 -2.571844 -1.213251  
F -6.453485 -1.250949 0.808875  
F -5.198970 0.827946 2.047033  
F -2.772296 1.582622 1.315074  
C 2.094732 0.738029 0.509895  
C 3.131650 -0.002558 -0.064809  
C 3.905634 -0.902712 0.653875  
C 3.704725 -1.088261 2.009512  
C 2.703338 -0.344768 2.609812  
C 1.924632 0.549763 1.885583  
F 3.377074 0.098404 -1.380113  
F 4.839105 -1.610602 0.006914  
F 2.472321 -0.475805 3.921772  
F 0.990893 1.216865 2.578262

H -0.696052 3.138483 1.877295  
H -0.773833 4.694032 1.048198  
H 1.582890 4.743842 0.901262  
H 1.693050 3.180997 1.689669  
H -1.820247 3.072274 -0.571541  
H -0.475456 1.219798 0.944060  
H 1.394026 1.138765 -1.394290  
H 0.974265 3.330065 -3.358232  
H 0.180207 1.852511 -2.774364  
H -0.784305 3.250331 -3.204059  
H -0.837591 5.316916 -1.893264  
H 0.292676 5.612714 -0.569928  
H 0.896003 5.401651 -2.215827  
H -1.254493 0.534558 -2.126377  
H 3.013108 2.907129 -2.026870  
H 2.988021 4.476357 -1.189643  
H 3.647758 3.045744 -0.382995  
H 4.290450 -1.801163 2.574408

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19P

C 4.992505 2.172024 -0.343821  
C 4.203354 1.638332 0.883641  
C 5.470613 0.877832 -1.016182  
C 4.227615 0.171137 -1.589646  
C 3.543290 -0.462324 -0.325863  
C 4.402050 0.097491 0.836826  
C 5.834579 -0.007979 0.196386  
C 6.284943 -1.420161 -0.196556  
C 6.936596 0.573992 1.089215  
C 4.261427 -0.632611 2.162650  
C 2.029665 -0.312682 -0.341094  
C 1.177720 0.201127 0.635313  
C -0.203990 0.246319 0.465566  
C -0.852554 -0.219895 -0.671335  
C -0.003399 -0.764349 -1.636681  
C 1.371804 -0.811728 -1.469079  
P -2.677218 -0.287018 -1.005684  
C -3.363953 1.442385 -0.740333  
C -3.240221 -1.481927 0.323899  
C -4.902599 1.359186 -0.471145  
C -2.812870 2.559020 0.174349  
C -2.603316 -2.868836 0.058798  
C -3.036124 -1.311456 1.839023  
F 1.633122 0.685624 1.800815  
F -0.496049 -1.279600 -2.766234  
F 2.095519 -1.379630 -2.444015  
F -0.899675 0.789799 1.474610  
C -5.214967 2.593246 0.411122  
C -4.010245 3.518158 0.238480  
C -3.121820 -3.710378 1.238659

C	-3.362345	-2.716647	2.397121	C	5.031108	-2.205687	0.061998
C	-5.701720	1.346481	-1.773445	C	4.268521	-1.503222	-1.095206
C	-1.554334	3.235978	-0.356493	C	5.492374	-1.019850	0.918834
C	-2.889742	-3.496719	-1.299474	C	4.237397	-0.396816	1.559705
C	-3.859990	-0.220244	2.504064	C	3.589162	0.414315	0.378150
H	4.367165	2.768974	-1.013370	C	4.468867	0.016194	-0.833915
H	5.835610	2.799443	-0.042432	C	5.885261	0.026743	-0.147860
H	4.585920	2.042688	1.825524	C	6.325483	1.368991	0.449404
H	3.151259	1.915380	0.836528	C	7.007264	-0.428219	-1.088326
H	6.271939	1.017825	-1.748086	C	4.364961	0.926899	-2.046992
H	4.482061	-0.599231	-2.319551	C	2.076274	0.280873	0.343644
H	3.563275	0.881032	-2.092091	C	1.248247	-0.089382	-0.721165
H	3.704078	-1.546910	-0.357264	C	-0.133775	-0.147319	-0.588164
H	6.315795	-2.077985	0.678444	C	-0.782222	0.172195	0.597735
H	5.657377	-1.893982	-0.953234	C	0.025935	0.571548	1.662404
H	7.300676	-1.375454	-0.602805	C	1.401959	0.628887	1.523908
H	7.189867	-0.130531	1.888071	P	-2.573886	0.156705	0.739986
H	7.844727	0.739365	0.499716	C	-3.323062	-1.510409	0.659229
H	6.666571	1.521246	1.558809	C	-3.296987	1.529137	-0.226294
H	3.260107	-0.538913	2.582244	C	-4.887259	-1.426997	0.607593
H	4.478220	-1.699547	2.041387	C	-2.860914	-2.517298	-0.423882
H	4.967461	-0.227061	2.894806	C	-2.564976	2.861457	0.073074
H	-3.256687	1.844140	-1.760675	C	-3.308632	1.453961	-1.766557
H	-4.321437	-1.589588	0.131980	F	1.716932	-0.410873	-1.924560
H	-5.145908	0.450885	0.089499	F	-0.522334	0.915514	2.829452
H	-2.619451	2.179236	1.179938	F	2.099756	1.048115	2.575948
H	-1.515376	-2.750482	0.174069	F	-0.860442	-0.543987	-1.640493
H	-1.973711	-1.110758	2.013680	C	-5.288793	-2.558660	-0.371387
H	-5.299690	2.293218	1.461242	C	-4.065514	-3.469920	-0.461371
H	-6.162223	3.063184	0.129304	C	-3.237686	3.799484	-0.944599
H	-3.912352	4.261749	1.035159	C	-3.603936	2.923172	-2.162657
H	-4.082450	4.062171	-0.713444	C	-5.495118	-1.593158	1.999538
H	-2.422963	-4.510508	1.497688	C	-1.555818	-3.235576	-0.098168
H	-4.061682	-4.191750	0.944319	C	-2.634906	3.361935	1.510465
H	-4.409707	-2.747517	2.717750	C	-4.298831	0.467108	-2.368302
H	-2.755886	-2.939321	3.279334	H	4.394257	-2.892336	0.626389
H	-6.771255	1.223686	-1.579408	H	5.881459	-2.783813	-0.306670
H	-5.376530	0.532402	-2.429086	H	4.667685	-1.774577	-2.076263
H	-5.562458	2.289574	-2.314084	H	3.215842	-1.786242	-1.107330
H	-0.712392	2.546942	-0.450465	H	6.273494	-1.261250	1.644767
H	-1.246972	4.051230	0.305103	H	4.476337	0.263151	2.394845
H	-1.746484	3.663150	-1.347516	H	3.561704	-1.169351	1.941020
H	-2.528213	-4.529548	-1.321857	H	3.748876	1.483593	0.567129
H	-2.409902	-2.950028	-2.114355	H	6.379860	2.142859	-0.323020
H	-3.968720	-3.513996	-1.491038	H	5.684187	1.736881	1.252898
H	-3.599938	0.770630	2.127807	H	7.330603	1.262962	0.868473
H	-3.699406	-0.220781	3.586583	H	7.284233	0.382583	-1.769098
H	-4.930118	-0.383377	2.326659	H	7.898374	-0.682538	-0.505790
				H	6.748644	-1.296145	-1.696813
				H	3.378702	0.904157	-2.511211
				H	4.584007	1.964162	-1.772375

H	5.090639	0.622340	-2.807209	C	-2.145438	-3.375242	-0.964174
H	-2.769813	0.551257	2.067525	C	-2.003133	-2.013553	-1.186827
H	-3.030275	-1.932337	1.633125	C	-0.847371	-1.385271	-0.748085
H	-4.330592	1.608951	0.145997	F	4.270929	1.814595	-3.650034
H	-5.214605	-0.465989	0.195154	F	3.491267	3.109807	-1.360893
H	-2.772339	-2.016225	-1.393633	F	2.243898	1.807740	0.564075
H	-1.513891	2.729311	-0.219437	F	3.636700	-0.810101	-3.978304
H	-2.296817	1.197908	-2.098585	F	2.267269	-2.121283	-2.092213
H	-5.519620	-2.142284	-1.356397	F	-0.770553	-0.057155	-1.041132
H	-6.182809	-3.081457	-0.022749	F	-2.973829	-1.322645	-1.808425
H	-4.059519	-4.101160	-1.352886	F	-3.229340	-4.027560	-1.390785
H	-4.017889	-4.133269	0.411852	F	-1.266575	-5.354250	-0.058041
H	-2.582283	4.635369	-1.197612	F	0.878472	-4.104939	0.815536
H	-4.139350	4.224163	-0.490370	C	4.956765	-1.273314	0.141245
H	-4.664171	3.030076	-2.410409	C	5.571317	-0.097500	-0.298321
H	-3.039744	3.194221	-3.057166	C	6.307521	-0.022845	-1.471958
H	-6.582749	-1.502542	1.958506	C	6.504867	-1.143837	-2.258505
H	-5.124367	-0.838937	2.702290	C	5.936291	-2.330456	-1.827620
H	-5.254112	-2.580338	2.407211	C	5.186149	-2.397067	-0.658425
H	-0.696626	-2.564266	-0.041737	F	5.401681	1.043941	0.390558
H	-1.339604	-3.981901	-0.866240	F	6.793404	1.164144	-1.849311
H	-1.639500	-3.758269	0.860466	F	6.100975	-3.446614	-2.541398
H	-2.255441	4.385161	1.565308	F	4.678936	-3.596974	-0.345205
H	-2.034323	2.762404	2.201359	H	3.290378	-4.457384	1.748481
H	-3.670258	3.374715	1.868267	H	3.277121	-4.444595	3.511067
H	-4.053588	-0.569783	-2.123980	H	5.431990	-3.478283	3.527086
H	-4.301841	0.553963	-3.457600	H	5.458993	-3.435282	1.775616
H	-5.315989	0.673017	-2.015925	H	1.475186	-2.810137	2.877340

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**19PHBH**

C	3.443144	-3.824321	2.624947	H	3.258491	0.441755	4.241193
C	4.856659	-3.171787	2.647273	H	2.380256	0.227914	2.711989
C	2.510075	-2.594974	2.593652	H	1.660891	-0.317178	4.219422
C	2.664635	-1.969779	1.176626	H	2.438329	-2.300266	5.431943
C	4.018331	-1.198046	1.326659	H	3.968432	-3.085415	5.037838
C	4.570776	-1.654158	2.704698	H	3.954714	-1.409639	5.589448
C	3.251944	-1.616621	3.543764	H	0.946460	-0.300501	1.324706
C	2.606958	-0.232836	3.671505	H	5.484617	0.249570	3.207781
C	3.421771	-2.143894	4.974943	H	6.035890	-1.113046	4.207432
B	1.443786	-1.085613	0.529944	H	6.606766	-0.942849	2.542809
C	5.736119	-0.816476	3.196517	H	7.070935	-1.094912	-3.179446
C	2.114807	-0.219052	-0.696355	C	-6.015310	-2.827856	-1.646338
C	0.184491	-1.990346	-0.039436	C	-5.570651	-2.738689	-0.162141
C	2.515263	1.102172	-0.571762	C	-7.165577	-1.814163	-1.704041
C	3.214119	1.812260	-1.540542	C	-6.548015	-0.413297	-1.532274
C	3.585223	1.169270	-2.708582	C	-6.242283	-0.330907	0.008417
C	3.241447	-0.167699	-2.879515	C	-6.582639	-1.761794	0.496689
C	2.518115	-0.820190	-1.889394	C	-7.877455	-2.038888	-0.351069
C	-0.016804	-3.354713	0.158340	C	-9.047634	-1.077460	-0.111239
C	-1.143084	-4.046512	-0.283413	C	-8.422903	-3.458482	-0.159919
				C	-6.780926	-1.909431	1.996751

C	-4.882019	0.289917	0.277838	H	-1.438433	6.371750	3.271935
C	-3.818214	-0.206138	1.032504	H	-0.793658	5.058785	4.261587
C	-2.605379	0.468740	1.123987	H	-2.186075	3.929856	-3.560800
C	-2.381197	1.684824	0.490414	H	-0.487277	4.337295	-3.766716
C	-3.460417	2.228967	-0.192317	H	-1.164438	6.172879	-2.391775
C	-4.661770	1.552297	-0.289715	H	-2.326180	5.199019	-1.501381
P	-0.717123	2.383197	0.557691	H	2.710085	3.911978	3.294709
C	-0.531442	3.333041	2.103575	H	1.918268	2.358598	3.005703
C	-0.162996	3.272935	-0.958502	H	1.278000	3.462935	4.237879
C	0.847223	4.070902	2.198128	H	-3.389892	3.031100	2.580608
C	-1.654026	4.360401	2.415164	H	-3.547558	4.566405	3.438864
C	-0.804190	2.781138	-2.298183	H	-2.507608	3.293877	4.093265
C	-0.256947	4.828961	-0.932493	H	-0.296958	1.683342	-4.089250
F	-3.881342	-1.356785	1.704032	H	0.493007	1.054985	-2.634764
F	-3.340753	3.424440	-0.779128	H	1.060843	2.566279	-3.377251
F	-5.647886	2.147552	-0.966785	H	1.891642	5.125207	-0.629653
F	-1.630021	-0.084561	1.842472	H	1.046758	6.515569	-1.338947
C	0.475178	5.524485	2.569629	H	1.399562	5.083315	-2.319602
C	-0.899357	5.421734	3.230866				
C	-1.246974	4.075393	-3.021413				
C	-1.340067	5.180817	-1.965502				
C	1.740762	3.409619	3.245897				
C	-2.844726	3.773727	3.168348				
C	0.173474	1.966837	-3.143493				
C	1.099581	5.423521	-1.322427				
H	-5.201966	-2.568431	-2.327392				
H	-6.352589	-3.833717	-1.909029				
H	-5.589503	-3.711805	0.336640				
H	-4.546446	-2.379274	-0.088251				
H	-7.806223	-1.901358	-2.586694				
H	-7.225580	0.386944	-1.835260				
H	-5.634087	-0.310932	-2.125702				
H	-6.956693	0.362518	0.469526				
H	-9.384032	-1.122082	0.929962				
H	-8.826319	-0.035439	-0.350216				
H	-9.894743	-1.376848	-0.736745				
H	-8.966524	-3.532773	0.787492				
H	-9.129875	-3.696199	-0.961746				
H	-7.648970	-4.227464	-0.158401				
H	-5.870244	-1.706560	2.560559				
H	-7.558549	-1.225565	2.354472				
H	-7.095004	-2.930241	2.236537				
H	0.076657	1.235677	0.705548				
H	-0.563049	2.544541	2.870655				
H	0.899316	2.999444	-0.948473				
H	1.378891	4.044032	1.240985				
H	-2.014674	4.818568	1.483259				
H	-1.677783	2.154857	-2.092175				
H	-0.527480	5.208235	0.055422				
H	0.417758	6.152680	1.674133				
H	1.228506	5.968807	3.225617				
				85			
				<b>20H<sub>2</sub></b>			
				P	2.806334	0.295049	0.072537
				C	2.598917	2.029550	0.457358
				C	3.646767	2.955480	0.545401
				C	3.358042	4.318162	0.647358
				C	2.043463	4.793948	0.632221
				C	0.987171	3.889038	0.538284
				C	1.303675	2.523221	0.476764
				O	0.221513	1.737911	0.421687
				C	-0.880892	2.591136	0.404757
				C	-0.464592	3.926898	0.470694
				C	-1.439485	4.929158	0.454035
				C	-2.762286	4.520984	0.368350
				C	-3.113499	3.160175	0.318248
				C	-2.181997	2.115810	0.346064
				B	-2.540413	0.541944	0.502811
				C	-1.626598	-0.517946	-0.359015
				C	-0.786208	-0.269266	-1.439535
				F	-0.627426	0.968363	-1.933778
				C	-0.032478	-1.259706	-2.065133
				F	0.865522	-0.938979	-3.019756
				C	-0.163899	-2.581685	-1.675421
				F	0.568668	-3.540565	-2.254792
				C	-1.017288	-2.886053	-0.627942
				C	-1.701175	-1.861223	0.009196
				F	-2.464952	-2.229398	1.049474
				F	-1.098558	-4.148119	-0.186140
				C	-4.095713	0.243991	0.123003
				C	-4.554617	0.435481	-1.176631
				F	-3.705624	0.890877	-2.112984



C	0.519887	-1.671827	2.813289	O	-0.222441	1.709895	-0.145042
C	1.221473	-0.629161	2.208769	C	0.867927	2.552831	-0.234549
C	1.047194	0.749800	2.800232	C	0.452620	3.890302	-0.287785
C	4.645382	0.078568	-0.076226	C	1.421676	4.895309	-0.365660
C	5.238680	0.134874	-1.356821	C	2.749671	4.497267	-0.390948
C	4.453739	0.422712	-2.614745	C	3.106537	3.137329	-0.368040
C	6.611213	-0.073040	-1.446952	C	2.180222	2.090848	-0.305804
C	7.400280	-0.318181	-0.320884	B	2.550319	0.525520	-0.522229
C	8.884622	-0.517243	-0.458672	C	1.710779	-0.563491	0.367923
C	6.786285	-0.336027	0.930821	C	1.018727	-0.329344	1.552009
C	5.415267	-0.138538	1.083231	F	1.002307	0.889112	2.108846
C	4.817577	-0.166801	2.469029	C	0.303892	-1.314733	2.227766
H	4.533304	2.628788	0.706434	F	-0.408581	-1.026640	3.326404
H	3.994290	5.032612	0.821213	C	0.323408	-2.617114	1.757611
H	1.689369	5.846675	0.427421	F	-0.368180	-3.579097	2.385332
H	-1.198454	5.954983	-0.199472	C	1.036923	-2.910761	0.608205
H	-3.547485	5.315711	-0.693301	C	1.687703	-1.887694	-0.064199
H	-4.199097	2.961580	-0.857276	F	2.326775	-2.241736	-1.194324
H	2.342406	0.011551	-1.219259	F	1.042076	-4.166698	0.134291
H	3.029483	-3.760985	-0.640862	C	4.141593	0.253662	-0.252384
H	2.921344	-2.172575	-1.375164	C	4.680400	0.375769	1.025566
H	4.186453	-2.505481	-0.182307	F	3.889118	0.739322	2.045925
H	1.603223	-4.313246	1.006346	C	6.015851	0.141274	1.325911
H	-0.167732	-4.012946	4.112731	F	6.484310	0.274388	2.573789
H	-1.270957	-3.930058	2.734826	C	6.878612	-0.239273	0.307678
H	0.086707	-5.060700	2.703133	F	8.170884	-0.470398	0.569825
H	-0.127467	-1.437012	3.654643	C	6.391226	-0.375256	-0.982158
H	0.752991	0.656242	3.846701	C	5.044859	-0.127841	-1.237115
H	0.256305	1.303131	2.285655	F	4.655186	-0.275414	-2.510336
H	1.955821	1.352353	2.766299	F	7.224558	-0.739852	-1.966452
H	5.133237	0.549316	-3.458024	C	-2.108277	-0.966565	-0.784203
H	3.867168	1.343530	-2.526625	C	-2.193118	-2.297144	-0.295743
H	3.765105	-0.390423	-2.871005	C	-2.916992	-2.648672	0.984789
H	7.082308	-0.037032	-2.425696	C	-1.559125	-3.332246	-0.978165
H	9.304289	-1.006456	0.421776	C	-0.779445	-3.097989	-2.106957
H	9.387223	0.447657	-0.578523	C	0.030127	-4.193717	-2.746657
H	9.119770	-1.121433	-1.337614	C	-0.716477	-1.795869	-2.584375
H	7.391288	-0.506023	1.817369	C	-1.375562	-0.727732	-1.967334
H	5.602288	-0.051605	3.217986	C	-1.234946	0.601825	-2.672356
H	4.098416	0.645299	2.622815	C	-4.692980	0.054653	0.202573
H	4.298330	-1.110078	2.664957	C	-5.437856	-0.029045	1.399488
				C	-4.788379	0.104655	2.757732
				C	-6.818809	-0.224584	1.342688
				C	-7.494168	-0.335498	0.130933
				C	-8.979152	-0.589676	0.089534
				C	-6.754872	-0.217376	-1.042429
				C	-5.372513	-0.018427	-1.031631
				C	-4.667332	0.153101	-2.351589
				H	-4.672743	2.619467	-0.149721
				H	-4.172416	5.020235	-0.355564
				H	-1.832349	5.846792	-0.407712

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[20H]<sup>-</sup>

P	-2.854879	0.249379	0.399964
C	-2.619477	1.989306	-0.114034
C	-3.637090	2.945809	-0.188141
C	-3.348885	4.315122	-0.298795
C	-2.040587	4.784070	-0.330403
C	-0.999578	3.853960	-0.265060
C	-1.323005	2.495496	-0.163728

H	1.141963	5.943750	-0.405734	C	-1.029137	-2.808091	-0.413855
H	3.532891	5.248336	-0.444080	C	-1.818515	-1.705415	-0.135360
H	4.162954	2.883953	-0.423403	F	-2.707644	-1.833046	0.855593
H	2.307152	0.275146	-1.685448	F	-1.166808	-3.943002	0.268900
H	-2.832067	-3.719226	1.180536	C	-4.196926	0.325308	-0.257962
H	-2.477070	-2.119175	1.838158	C	-4.886857	-0.571712	-1.072691
H	-3.980271	-2.389512	0.946360	F	-4.283033	-1.100715	-2.140924
H	-1.618098	-4.339664	-0.572165	C	-6.205383	-0.936527	-0.843845
H	-0.043870	-4.160583	-3.837589	F	-6.833580	-1.779660	-1.657844
H	1.082520	-4.071189	-2.474892	C	-6.871096	-0.410682	0.256223
H	-0.294647	-5.179172	-2.404034	F	-8.129978	-0.753029	0.495348
H	-0.119126	-1.584558	-3.469612	C	-6.217839	0.473052	1.105005
H	-1.354916	0.450313	-3.749459	C	-4.902645	0.826875	0.835014
H	-0.235514	1.013631	-2.500990	F	-4.309542	1.657490	1.696107
H	-1.964838	1.341361	-2.354323	F	-6.852321	0.964963	2.165499
H	-5.542767	0.038635	3.545575	C	2.064624	-0.942458	0.914806
H	-4.269028	1.061931	2.857854	C	2.281949	-2.301601	0.570368
H	-4.039622	-0.674584	2.924640	C	3.171745	-2.715584	-0.579624
H	-7.379997	-0.288022	2.272819	C	1.652885	-3.313813	1.295181
H	-9.432502	-0.144692	-0.800080	C	0.785929	-3.035274	2.346482
H	-9.190532	-1.664149	0.064037	C	0.044129	-4.125822	3.072412
H	-9.476428	-0.177331	0.971262	C	0.605527	-1.700461	2.692661
H	-7.267781	-0.272715	-2.000775	C	1.233219	-0.648181	2.019416
H	-5.392951	0.209072	-3.166528	C	0.970047	0.733722	2.573841
H	-4.078206	1.074468	-2.354120	C	4.621996	0.090434	-0.134961
H	-3.979456	-0.672094	-2.553701	C	5.361703	0.086387	-1.338524
				C	4.702042	0.270396	-2.685950
				C	6.745601	-0.075163	-1.292019
				C	7.426716	-0.232836	-0.086895
				C	8.917516	-0.447545	-0.063728
				C	6.687791	-0.197482	1.091979
				C	5.300354	-0.034695	1.094549
				C	4.595232	0.021241	2.426200
				H	4.533048	2.578425	0.553174
				H	4.026232	4.974060	0.779065
				H	1.718736	5.836743	0.488137
				H	-1.206666	5.963673	-0.017032
				H	-3.576191	5.342322	-0.427906
				H	-4.232613	2.994321	-0.678384
				H	3.106928	-3.793298	-0.735436
				H	2.873435	-2.225152	-1.514054
				H	4.218503	-2.456586	-0.396086
				H	1.823171	-4.347682	1.003599
				H	0.191843	-4.054141	4.153721
				H	-1.029347	-4.048613	2.875933
				H	0.373984	-5.113893	2.744681
				H	-0.044205	-1.458939	3.531904
				H	0.705734	0.653784	3.630544
				H	0.131748	1.217275	2.063445
				H	1.830970	1.396398	2.493804
				H	5.451366	0.249948	-3.480013

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P	2.788859	0.228687	-0.323533
C	2.512509	1.976285	0.158150
C	3.507716	2.917225	0.436858
C	3.217204	4.285935	0.558260
C	1.927785	4.776010	0.397342
C	0.909610	3.861252	0.113699
C	1.237463	2.509389	0.005386
O	0.135329	1.740550	-0.250790
C	-0.928884	2.586853	-0.313679
C	-0.525368	3.917502	-0.113411
C	-1.486874	4.924407	-0.158052
C	-2.815658	4.570787	-0.383701
C	-3.183583	3.233443	-0.529565
C	-2.253670	2.176015	-0.496401
B	-2.687793	0.692216	-0.541840
C	-1.707887	-0.497885	-0.830534
C	-0.731026	-0.453954	-1.827775
F	-0.577891	0.643355	-2.567507
C	0.082785	-1.536944	-2.127878
F	1.009349	-1.457794	-3.081546
C	-0.077982	-2.720208	-1.420295
F	0.682427	-3.771953	-1.697468



H	4.173180	1.226796	-2.742854
H	3.961118	-0.508913	-2.886625
H	7.306981	-0.075408	-2.223674
H	9.350224	-0.122741	0.885287
H	9.408911	0.099866	-0.871773
H	9.157560	-1.508212	-0.191392
H	7.204570	-0.292014	2.044645
H	5.316592	0.193940	3.227848
H	3.860267	0.830128	2.449355
H	4.060070	-0.908444	2.640440

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**20B**

C	2.262128	3.170687	3.783784
C	1.003710	2.604032	3.958229
C	0.150259	3.021111	4.989637
C	0.532501	4.018393	5.878145
C	1.791823	4.599119	5.721623
C	2.621226	4.162451	4.681874
O	3.812889	4.839813	4.671274
C	3.772137	5.717813	5.716306
C	2.552595	5.630952	6.403539
C	2.329266	6.463467	7.498764
C	3.324373	7.364653	7.865047
C	4.518316	7.437556	7.145911
C	4.801104	6.606337	6.046150
B	6.163440	6.680580	5.311739
C	6.789500	5.432979	4.592831
C	6.615795	4.130670	5.069688
F	5.917687	3.903716	6.181476
C	7.169030	3.021013	4.448005
F	6.985296	1.799946	4.942367
C	7.927421	3.193882	3.297598
F	8.457665	2.142943	2.688540
C	8.132484	4.469208	2.787636
C	7.575760	5.556027	3.444321
F	7.807195	6.758898	2.911972
F	8.859259	4.634844	1.686216
C	6.962897	8.037790	5.319050
C	8.351949	8.076502	5.462643
F	9.040595	6.942223	5.612333
C	9.078250	9.256732	5.476234
F	10.398227	9.246498	5.634466
C	8.409330	10.464412	5.317445
F	9.087779	11.602822	5.320401
C	7.031304	10.476840	5.152388
C	6.334568	9.275353	5.159308
F	5.016864	9.347737	4.968163
F	6.394393	11.632141	4.985486
H	2.933932	2.860370	2.992414
H	0.676930	1.822480	3.280672

H	-0.823637	2.555324	5.093420
H	-0.131445	4.337603	6.674953
H	1.397178	6.410227	8.052616
H	3.170726	8.020852	8.714409
H	5.273055	8.153178	7.459917

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**[20BH]**

C	2.158913	3.044816	3.895667
C	1.042862	2.309282	4.283573
C	0.333721	2.623805	5.450778
C	0.725503	3.684453	6.260991
C	1.841758	4.435848	5.891995
C	2.534390	4.098814	4.716297
O	3.588090	4.924009	4.498467
C	3.607668	5.825106	5.546661
C	2.555603	5.575306	6.436076
C	2.411952	6.386700	7.566246
C	3.337853	7.402198	7.741728
C	4.381193	7.604616	6.820201
C	4.569794	6.827175	5.674381
B	5.700868	7.086065	4.541503
C	6.534661	5.746398	4.089409
C	6.645082	4.555167	4.798982
F	6.033975	4.397074	5.981143
C	7.375112	3.458975	4.349669
F	7.437989	2.330769	5.070418
C	8.057250	3.537102	3.146340
F	8.769939	2.493889	2.701026
C	7.996856	4.710351	2.410071
C	7.251734	5.777270	2.895833
F	7.253252	6.889399	2.143400
F	8.661832	4.799037	1.248976
C	6.806556	8.187227	5.038131
C	7.656927	7.921284	6.108154
F	7.550302	6.756179	6.765816
C	8.631973	8.801861	6.558324
F	9.421803	8.497377	7.596857
C	8.787839	10.020749	5.913801
F	9.720852	10.887708	6.326753
C	7.968003	10.332882	4.841382
C	7.001240	9.420335	4.427229
F	6.247670	9.801488	3.387693
F	8.116748	11.510880	4.219603
H	2.721518	2.815838	2.997979
H	0.717434	1.475183	3.669608
H	-0.532159	2.029144	5.724720
H	0.174348	3.924490	7.165473
H	1.607010	6.221980	8.276424
H	3.263066	8.053540	8.608070
H	5.078667	8.417482	7.009349

H 5.148381 7.507865 3.550490

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**20P**

P 0.519144 -0.147898 0.798518  
C -0.683598 -1.002326 -0.298820  
C -0.366122 -1.961397 -1.265878  
C -1.354963 -2.664207 -1.969535  
C -2.705389 -2.445003 -1.732059  
C -3.058396 -1.510508 -0.756652  
C -2.046944 -0.834011 -0.065036  
O -2.562731 0.049467 0.845660  
C -3.924871 -0.056316 0.753040  
C -4.304287 -0.997399 -0.213813  
C -5.661689 -1.230176 -0.441056  
C -6.589889 -0.514636 0.305022  
C -6.179700 0.420526 1.266141  
C -4.832669 0.668008 1.509337  
C 0.799453 1.594988 0.229340  
C 1.801852 2.264338 0.970805  
C 2.571721 1.602066 2.090691  
C 2.119844 3.590140 0.670357  
C 1.464121 4.295891 -0.330193  
C 1.834104 5.717673 -0.663144  
C 0.453475 3.637001 -1.024829  
C 0.102706 2.310192 -0.771641  
C -1.021034 1.741305 -1.605683  
C 2.089935 -1.014618 0.328356  
C 2.550663 -1.981945 1.250554  
C 1.766051 -2.343841 2.490479  
C 3.757264 -2.638506 1.016939  
C 4.533282 -2.370377 -0.108837  
C 5.852109 -3.066835 -0.320916  
C 4.054563 -1.438066 -1.022761  
C 2.848090 -0.757393 -0.832789  
C 2.417081 0.206963 -1.911192  
H 0.678864 -2.168600 -1.475188  
H -1.051960 -3.392119 -2.714670  
H -3.465583 -2.988038 -2.284138  
H -5.983385 -1.953379 -1.183550  
H -7.649646 -0.680335 0.144052  
H -6.928316 0.963691 1.833172  
H -4.497344 1.386042 2.248177  
H 3.121349 2.352473 2.662574  
H 1.902913 1.072315 2.777148  
H 3.292424 0.870054 1.712193  
H 2.900192 4.082413 1.246653  
H 0.944206 6.323102 -0.854396  
H 2.394856 6.181537 0.151511  
H 2.457633 5.759108 -1.562309  
H -0.086793 4.174691 -1.801211

H -1.307139 2.460861 -2.375493  
H -1.905528 1.541365 -0.994875  
H -0.749554 0.807556 -2.103215  
H 2.273026 -3.139700 3.040238  
H 0.758952 -2.690748 2.240896  
H 1.647569 -1.483694 3.155677  
H 4.099148 -3.382384 1.733377  
H 6.164996 -3.013851 -1.366084  
H 5.793908 -4.119535 -0.032359  
H 6.637418 -2.603883 0.285538  
H 4.631082 -1.234709 -1.922763  
H 2.937863 -0.022035 -2.843940  
H 1.342025 0.148003 -2.097202  
H 2.640938 1.243350 -1.640241

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**[20PH]<sup>+</sup>**

P 0.663227 -0.122034 0.439999  
C -0.534599 -1.183760 -0.360049  
C -0.168753 -2.199471 -1.251724  
C -1.144560 -3.005261 -1.843247  
C -2.498330 -2.828298 -1.560948  
C -2.880524 -1.829252 -0.665825  
C -1.887681 -1.032129 -0.083230  
O -2.398872 -0.089118 0.748136  
C -3.771475 -0.270135 0.725192  
C -4.131093 -1.322983 -0.124294  
C -5.481146 -1.648171 -0.271861  
C -6.415350 -0.905313 0.437316  
C -6.020984 0.143813 1.280835  
C -4.681894 0.484876 1.443067  
C 0.572484 1.643622 0.083476  
C 1.286274 2.465143 0.990313  
C 2.010809 1.924093 2.201636  
C 1.310086 3.837243 0.762983  
C 0.648234 4.417094 -0.318645  
C 0.669945 5.906242 -0.525801  
C -0.053849 3.582606 -1.185747  
C -0.116351 2.200034 -1.015565  
C -0.941561 1.418972 -2.010842  
C 2.306613 -0.839892 0.257765  
C 2.737662 -1.764086 1.237781  
C 1.872760 -2.193985 2.399006  
C 4.015736 -2.298613 1.117415  
C 4.864758 -1.958357 0.062266  
C 6.232492 -2.574345 -0.044606  
C 4.400162 -1.064698 -0.900576  
C 3.130515 -0.493074 -0.831899  
C 2.702943 0.455085 -1.925321  
H 0.359931 -0.209857 1.800946  
H 0.881335 -2.359700 -1.478443

H	-0.838631	-3.783921	-2.532165	F	1.472044	4.404608	4.061228
H	-3.242679	-3.461519	-2.032175	C	0.601562	2.508409	2.960041
H	-5.791525	-2.459163	-0.921892	C	0.539175	1.732524	1.807359
H	-7.469541	-1.138549	0.340111	F	-0.296953	0.670266	1.877107
H	-6.776937	0.703167	1.820870	F	-0.104184	2.179357	4.048951
H	-4.362475	1.291627	2.091472	C	2.427619	0.350391	-1.213832
H	2.553006	2.727508	2.700743	C	3.743606	0.545892	-0.796840
H	1.310092	1.506306	2.934079	F	4.051144	1.461429	0.132208
H	2.738773	1.147602	1.945826	C	4.817829	-0.205958	-1.260704
H	1.862412	4.471483	1.451067	F	6.050688	0.003552	-0.791824
H	1.618286	6.337330	-0.198743	C	4.599688	-1.224395	-2.174301
H	-0.127005	6.379679	0.056389	F	5.610893	-1.997973	-2.578138
H	0.513163	6.163779	-1.574785	C	3.310653	-1.463933	-2.622595
H	-0.574741	4.022054	-2.032094	C	2.270973	-0.682418	-2.136690
H	-1.140918	2.040047	-2.884983	F	1.040376	-1.008774	-2.580259
H	-1.907486	1.141444	-1.576928	F	3.074739	-2.481524	-3.460105
H	-0.462250	0.501831	-2.357488	H	-3.412700	3.385952	1.277695
H	2.345251	-3.020137	2.930957	H	-5.394227	4.745180	0.586212
H	0.885273	-2.537388	2.073366	H	-5.600586	5.579205	-1.725497
H	1.730557	-1.382246	3.121845	H	-3.842553	5.096863	-3.410098
H	4.358729	-3.007658	1.866301	H	-1.427684	4.131994	-4.741248
H	6.866110	-2.020140	-0.738720	H	0.741837	3.002016	-5.197868
H	6.157709	-3.604852	-0.405537	H	1.893427	1.724852	-3.454381
H	6.726217	-2.603115	0.929410	H	0.263437	0.281164	-0.508730
H	5.043405	-0.804059	-1.736625	P	-1.638815	-1.723814	0.254276
H	3.373930	0.363075	-2.780381	C	-0.238973	-2.733319	-0.232122
H	1.690253	0.240650	-2.281468	C	-0.329452	-3.712527	-1.227210
H	2.722381	1.496187	-1.589270	C	0.806849	-4.404647	-1.652698

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**20PHBH**

C	-3.530857	3.738424	0.259345	O	1.288212	-1.550961	1.245013
C	-4.622687	4.505132	-0.138041	C	2.651751	-1.583513	1.436117
C	-4.737792	4.981760	-1.450571	C	3.253299	-2.577127	0.654156
C	-3.756818	4.712521	-2.398522	C	4.639367	-2.739636	0.704882
C	-2.653794	3.944948	-2.022405	C	5.368991	-1.889274	1.524689
C	-2.572058	3.466294	-0.705749	C	4.736334	-0.890330	2.280715
O	-1.441510	2.727678	-0.506321	C	3.356669	-0.718350	2.255720
C	-0.748521	2.739641	-1.709889	C	-2.125243	-1.769370	1.996193
C	-1.448964	3.468785	-2.677832	C	-2.976023	-0.705266	2.381181
C	-0.914656	3.572516	-3.965349	C	-3.393331	0.394824	1.434577
C	0.293568	2.937188	-4.211221	C	-3.421284	-0.655781	3.698071
C	0.950622	2.206661	-3.206831	C	-3.042603	-1.609743	4.640464
C	0.455656	2.065544	-1.907318	C	-3.515959	-1.509092	6.065375
B	1.085955	1.149473	-0.726589	C	-2.192788	-2.634549	4.235833
C	1.240852	2.017229	0.644232	C	-1.710313	-2.738906	2.930357
C	1.994605	3.186922	0.693502	C	-0.742380	-3.861896	2.643493
F	2.668738	3.582671	-0.392095	C	-3.007933	-2.063387	-0.879238
C	2.096705	3.991214	1.820304	C	-3.179122	-1.201197	-1.985923
F	2.848592	5.094057	1.816645	C	-2.281013	-0.019272	-2.246584
C	1.394136	3.645048	2.967155	C	-4.231801	-1.463507	-2.860995

C	-5.099845	-2.538162	-2.677457	C	1.068282	4.132685	0.290171
C	-6.243568	-2.769678	-3.628085	C	-0.237586	4.870758	0.005353
C	-4.891252	-3.382497	-1.588169	C	-0.248825	6.287062	0.577825
C	-3.858157	-3.169352	-0.678368	C	-0.419418	4.938624	-1.528796
C	-3.683094	-4.139944	0.462642	B	1.975995	0.304755	0.358371
H	-1.216579	-0.406939	0.033539	C	1.350568	-0.358608	-1.009635
H	-1.291040	-3.915629	-1.689025	C	1.067599	-1.724612	-0.999621
H	0.709934	-5.144536	-2.438733	F	1.259687	-2.434425	0.131575
H	2.938519	-4.668200	-1.463228	C	0.549757	-2.424853	-2.079295
H	5.135761	-3.483448	0.089406	F	0.272839	-3.732053	-1.992173
H	6.448973	-1.976448	1.560486	C	0.242528	-1.737411	-3.243505
H	5.339051	-0.223072	2.886940	F	-0.300663	-2.379199	-4.281961
H	2.854742	0.068739	2.806559	C	0.467802	-0.372793	-3.298984
H	-4.101216	1.061755	1.928627	C	1.032960	0.279294	-2.206003
H	-2.526540	0.993670	1.128875	F	1.228774	1.597179	-2.369992
H	-3.882749	0.014940	0.531501	F	0.111089	0.310600	-4.390922
H	-4.076252	0.158427	3.997131	C	3.339492	-0.498774	0.735117
H	-3.410790	-2.461827	6.588048	C	3.474587	-1.275091	1.879121
H	-2.928808	-0.761547	6.607936	F	2.462960	-1.384701	2.758533
H	-4.563347	-1.201316	6.111900	C	4.629254	-1.985675	2.186151
H	-1.882090	-3.380842	4.962473	F	4.708880	-2.719967	3.299877
H	-0.809211	-4.612917	3.432449	C	5.711004	-1.933661	1.319329
H	0.283863	-3.481667	2.631779	F	6.827803	-2.607376	1.597818
H	-0.915332	-4.360667	1.689457	C	5.622626	-1.176281	0.159426
H	-2.552881	0.472955	-3.181887	C	4.446436	-0.486722	-0.106111
H	-1.222432	-0.294892	-2.313546	F	4.401814	0.230029	-1.240692
H	-2.370683	0.727778	-1.449465	F	6.659955	-1.125152	-0.679868
H	-4.370833	-0.806049	-3.715116	C	-2.319620	-0.769527	-1.026216
H	-6.590065	-3.804369	-3.589315	C	-2.608510	-0.029281	-2.193390
H	-5.954109	-2.538452	-4.655711	C	-2.463293	1.468392	-2.307553
H	-7.089152	-2.123742	-3.371060	C	-2.984147	-0.730166	-3.338351
H	-5.547930	-4.236403	-1.442760	C	-3.064768	-2.120535	-3.373324
H	-4.321553	-5.012420	0.315040	C	-3.430574	-2.838007	-4.642820
H	-2.650330	-4.497258	0.528576	C	-2.709386	-2.826192	-2.227674
H	-3.939441	-3.687267	1.424752	C	-2.319945	-2.183453	-1.053403
				C	-1.873997	-3.055627	0.099095
				C	-2.891887	-0.841971	1.883107
				C	-2.207541	-1.220154	3.059103
				C	-2.925934	-1.889851	4.045894
				C	-4.282606	-2.183695	3.905877
				C	-5.027122	-2.890575	5.006899
				C	-4.930238	-1.786271	2.739145
				C	-4.261490	-1.118739	1.712023
				C	-5.042753	-0.773105	0.463373
				C	-0.738276	-0.947414	3.278920
				H	-0.580855	-0.172594	0.852769
				H	-4.220691	1.591333	1.702734
				H	-4.469868	4.034798	1.992350
				H	-2.678466	5.566831	1.278540
				H	4.278997	2.007805	0.781689
				H	4.372639	4.457513	0.986110
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<b>21H<sub>2</sub></b>							
P	-1.952511	-0.008302	0.582784				
C	-2.270380	1.754883	0.785720				
C	-3.439276	2.263705	1.364496				
C	-3.570813	3.633476	1.538738				
C	-2.547686	4.498824	1.138637				
C	-1.371470	4.022019	0.569946				
C	-1.248799	2.636183	0.423455				
O	-0.133812	2.090018	-0.100548				
C	1.077706	2.746409	0.179507				
C	2.179428	1.913358	0.346246				
C	3.372345	2.586364	0.629894				
C	3.428630	3.973782	0.755504				
C	2.283975	4.747454	0.593506				

H	2.341228	5.825250	0.701541	C	1.133323	-0.449078	-1.696170
H	0.560189	6.876464	0.140998	C	0.851953	-1.819891	-1.584986
H	-0.128119	6.282069	1.664983	F	1.383986	-2.547445	-0.597451
H	-1.182486	6.798310	0.326608	C	-0.006423	-2.495368	-2.436248
H	0.379567	5.545661	-1.964117	F	-0.259561	-3.789424	-2.261633
H	-0.358788	3.940481	-1.972151	C	-0.657690	-1.794313	-3.442443
H	-1.386161	5.385509	-1.783622	F	-1.492681	-2.421610	-4.254496
H	1.165688	0.069305	1.244669	C	-0.449885	-0.429000	-3.573837
H	-2.650935	1.773581	-3.337970	C	0.439918	0.211628	-2.722329
H	-3.155804	2.014793	-1.661206	F	0.616131	1.512703	-2.947340
H	-1.442701	1.772805	-2.053543	F	-1.117034	0.256394	-4.495026
H	-3.196423	-0.165671	-4.242437	C	3.280476	-0.583345	-0.025592
H	-2.532510	-2.977904	-5.251679	C	3.598812	-0.305535	1.304745
H	-3.854267	-3.822805	-4.435379	F	2.920014	0.634971	1.974593
H	-4.150491	-2.264002	-5.230368	C	4.565407	-1.009078	2.009264
H	-2.694973	-3.912786	-2.252461	F	4.816222	-0.730386	3.283061
H	-1.501913	-4.000984	-0.297823	C	5.270204	-2.018438	1.364557
H	-2.691527	-3.266703	0.795223	F	6.200982	-2.693410	2.016093
H	-1.049395	-2.613619	0.665894	C	4.987437	-2.329572	0.037891
H	-2.408331	-2.191653	4.952968	C	3.997265	-1.620752	-0.623504
H	-5.987424	-3.273322	4.656168	F	3.736966	-1.956081	-1.888917
H	-4.443922	-3.727319	5.399192	F	5.657836	-3.297453	-0.571711
H	-5.220571	-2.206945	5.839465	C	-2.430535	-0.765074	-0.531455
H	-5.988346	-2.004558	2.617292	C	-3.075167	-0.085192	-1.588007
H	-6.105020	-0.692622	0.703308	C	-3.042241	1.410998	-1.787816
H	-4.924726	-1.549825	-0.299790	C	-3.734611	-0.850153	-2.550350
H	-4.731446	0.169911	0.006057	C	-3.772212	-2.242547	-2.505526
H	-0.449641	-1.240161	4.289304	C	-4.490993	-3.041065	-3.556162
H	-0.094713	-1.500582	2.584882	C	-3.072320	-2.886698	-1.485267
H	-0.489650	0.112438	3.159422	C	-2.387633	-2.180818	-0.499919
				C	-1.606752	-2.982446	0.517797
				C	-2.201773	-0.663881	2.444417
				C	-1.214364	-0.905294	3.426618
				C	-1.612708	-1.500255	4.618364
				C	-2.942983	-1.849325	4.864578
				C	-3.327638	-2.505258	6.162404
				C	-3.894123	-1.571969	3.885366
				C	-3.554970	-0.982083	2.667123
				C	-4.653602	-0.735878	1.657533
				C	0.241857	-0.547970	3.234399
				H	-0.297456	-0.144296	0.793352
				H	-3.491147	1.791347	2.460755
				H	-3.587384	4.255009	2.691014
				H	-1.998304	5.683736	1.471630
				H	4.457321	1.800299	-0.700401
				H	4.693176	4.251638	-0.513601
				H	2.698046	5.679656	-0.311132
				H	0.893881	6.820692	-0.476264
				H	0.594894	6.276781	1.188381
				H	-0.740089	6.825895	0.149333
				H	0.133123	5.468541	-2.438660

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[21H]<sup>+</sup>

P	-1.676427	0.067108	0.886467
C	-1.860607	1.848334	1.043947
C	-2.813378	2.421530	1.894009
C	-2.855469	3.801623	2.032809
C	-1.949431	4.608158	1.341149
C	-0.985565	4.062755	0.495793
C	-0.960523	2.674276	0.370433
O	-0.042444	2.057862	-0.428529
C	1.208550	2.665166	-0.499959
C	2.305698	1.811652	-0.631233
C	3.570566	2.421835	-0.617737
C	3.707385	3.800602	-0.512656
C	2.577524	4.605582	-0.399587
C	1.297026	4.049306	-0.393313
C	-0.000461	4.852584	-0.357516
C	0.202324	6.273126	0.167581
C	-0.558866	4.914406	-1.798540
B	2.201630	0.264451	-0.791367

H	-0.677578	3.911438	-2.218967	F	0.105903	-3.205196	-3.519462
H	-1.529477	5.418958	-1.808069	C	0.795637	-1.037543	-2.872051
H	-3.556495	1.665218	-2.715289	C	1.274109	-0.185005	-1.881467
H	-3.525606	1.960052	-0.975467	F	1.517045	1.075967	-2.283285
H	-2.010404	1.768107	-1.874180	F	0.557428	-0.583886	-4.110920
H	-4.224467	-0.335859	-3.372298	C	3.549421	-0.354282	1.028795
H	-3.795394	-3.720813	-4.055274	C	3.850162	-0.959267	2.243314
H	-5.281685	-3.647816	-3.106267	F	2.953204	-0.993751	3.237156
H	-4.941085	-2.394747	-4.310853	C	5.077315	-1.558664	2.513942
H	-3.031812	-3.972964	-1.470376	F	5.320484	-2.128497	3.702574
H	-1.313578	-3.934767	0.072940	C	6.063997	-1.567180	1.541079
H	-2.198308	-3.187862	1.415269	F	7.250587	-2.137020	1.786337
H	-0.683611	-2.487263	0.834526	C	5.812174	-0.977439	0.310684
H	-0.864840	-1.692066	5.383452	C	4.571788	-0.394837	0.084758
H	-4.411081	-2.576019	6.268774	F	4.380655	0.160208	-1.123039
H	-2.914254	-3.516782	6.216369	F	6.763523	-0.982384	-0.632941
H	-2.932615	-1.945071	7.013680	C	-2.223509	-0.967258	-0.847462
H	-4.935871	-1.818401	4.072734	C	-2.322324	-0.492447	-2.173303
H	-5.617027	-0.678758	2.167010	C	-2.121356	0.951457	-2.562276
H	-4.708146	-1.547131	0.923860	C	-2.576687	-1.397685	-3.204785
H	-4.521102	0.194718	1.096965	C	-2.713790	-2.765065	-2.983837
H	0.790090	-0.690836	4.166284	C	-2.946953	-3.715277	-4.128096
H	0.722064	-1.181608	2.477501	C	-2.529127	-3.228579	-1.686965
H	0.381453	0.495151	2.933028	C	-2.263143	-2.363687	-0.623140

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[21H]-

P	-1.977315	0.026567	0.702022	C	-1.986396	-2.987369	0.726474
C	-2.310349	1.816087	0.383402	C	-3.521640	-0.409255	1.648276
C	-3.515404	2.470286	0.657469	C	-3.344535	-0.552712	3.043538
C	-3.629056	3.850025	0.515865	C	-4.415795	-0.955334	3.839955
C	-2.541012	4.600762	0.079341	C	-5.671509	-1.222496	3.299585
C	-1.319806	3.990371	-0.199275	C	-6.804461	-1.695135	4.174298
C	-1.221366	2.609211	-0.005328	C	-5.842309	-1.048021	1.930820
O	-0.045175	1.967426	-0.236534	C	-4.797327	-0.643402	1.093510
C	1.132718	2.673106	-0.000278	C	-5.119518	-0.459457	-0.371977
C	2.231722	1.911369	0.404828	C	-2.015559	-0.275758	3.708251
C	3.392182	2.652582	0.651908	H	-4.368185	1.895837	1.003880
C	3.441975	4.039229	0.516364	H	-4.571397	4.339915	0.739838
C	2.320722	4.741025	0.091385	H	-2.648381	5.673456	-0.045414
C	1.138411	4.054118	-0.190411	H	4.284872	2.127529	0.982309
C	-0.106662	4.694481	-0.792805	H	4.362568	4.573877	0.733349
C	-0.155708	6.205798	-0.571538	H	2.369324	5.818621	-0.027707
C	-0.089161	4.409714	-2.312542	H	0.716116	6.684002	-1.024761
B	2.094210	0.315762	0.674912	H	-0.175909	6.454112	0.493942
C	1.487888	-0.577316	-0.564261	H	-1.039448	6.636956	-1.050808
C	1.187293	-1.915445	-0.312858	H	0.766874	4.913904	-2.772746
F	1.335512	-2.412069	0.929707	H	0.012334	3.337495	-2.501786
C	0.733881	-2.808108	-1.273444	H	-1.012442	4.768479	-2.781060
F	0.436895	-4.077240	-0.956443	H	1.350630	0.157462	1.618502
C	0.544294	-2.365002	-2.572629	H	-2.164696	1.050285	-3.649349
				H	-2.871876	1.617011	-2.125513
				H	-1.136487	1.299010	-2.235562
				H	-2.651253	-1.016473	-4.221229

H	-1.991665	-3.985576	-4.588387	C	2.977891	2.398032	1.724068
H	-3.428843	-4.635753	-3.788242	F	2.979837	2.076167	3.021254
H	-3.575113	-3.261855	-4.899828	C	3.366068	3.681771	1.373806
H	-2.557164	-4.298797	-1.492778	F	3.739392	4.562797	2.298430
H	-1.747074	-4.044886	0.597978	C	3.352651	4.050308	0.032787
H	-2.840523	-2.903936	1.406046	F	3.701809	5.281911	-0.318485
H	-1.126641	-2.511075	1.210548	C	2.975079	3.131554	-0.937073
H	-4.263332	-1.062971	4.912205	C	2.628895	1.843878	-0.550313
H	-7.771856	-1.529664	3.693437	F	2.279145	0.987188	-1.514312
H	-6.716872	-2.766710	4.383515	F	2.935862	3.490856	-2.218400
H	-6.806110	-1.174206	5.135819	C	-2.217914	1.195264	-2.001956
H	-6.823490	-1.223456	1.492909	C	-1.663058	2.394222	-2.503499
H	-6.192985	-0.290264	-0.494709	C	-0.218462	2.771868	-2.271270
H	-4.841861	-1.340482	-0.959661	C	-2.462109	3.266045	-3.241160
H	-4.585651	0.391313	-0.801610	C	-3.802080	2.990574	-3.504638
H	-2.094972	-0.418063	4.788777	C	-4.655139	3.966704	-4.271930
H	-1.226979	-0.929274	3.324103	C	-4.327119	1.793345	-3.029500
H	-1.679933	0.748675	3.521547	C	-3.565433	0.887507	-2.285693
				C	-4.247288	-0.386062	-1.841543
				C	-2.262567	-0.389146	0.398822
92				C	-2.599113	-1.713055	0.763075
<b>21</b>				C	-2.018018	-2.945461	0.113381
P	-1.099839	0.161706	-0.944580	C	-3.504432	-1.925920	1.805118
C	-0.721438	-1.222056	-2.109058	C	-4.098446	-0.882551	2.510149
C	-1.282428	-1.383208	-3.380109	C	-5.082894	-1.149253	3.617294
C	-0.780183	-2.335927	-4.262643	C	-3.725112	0.412906	2.172318
C	0.294112	-3.143971	-3.899545	C	-2.808966	0.678548	1.152046
C	0.885331	-3.013334	-2.643645	C	-2.432907	2.127618	0.934769
C	0.359555	-2.046168	-1.789367	H	-2.100866	-0.741823	-3.689836
O	0.914150	-1.875088	-0.541849	H	-1.226297	-2.443769	-5.245614
C	2.283471	-2.016187	-0.476120	H	0.673797	-3.876054	-4.604249
C	2.945307	-1.135477	0.374535	H	4.904905	-0.527019	1.027868
C	4.341593	-1.217260	0.405391	H	6.099364	-2.224614	-0.316125
C	5.017121	-2.165513	-0.357898	H	4.853070	-3.744566	-1.800353
C	4.310029	-3.026062	-1.195292	H	3.600076	-5.186316	-2.817411
C	2.918415	-2.964078	-1.272378	H	3.235023	-3.845500	-3.925791
C	2.026975	-3.876279	-2.109395	H	2.140416	-5.239245	-3.790076
C	2.798537	-4.569063	-3.231152	H	2.223349	-5.576112	-0.762509
C	1.426334	-4.946022	-1.169150	H	0.900791	-4.478478	-0.331649
B	2.141445	-0.022611	1.128895	H	0.719755	-5.576206	-1.717923
C	0.975697	-0.310502	2.128371	H	0.014134	3.715721	-2.769079
C	0.190616	0.705126	2.696054	H	-0.003454	2.886027	-1.202671
F	0.398705	1.989207	2.398058	H	0.467372	2.010586	-2.651681
C	-0.859947	0.461728	3.565689	H	-2.023966	4.185902	-3.622164
F	-1.582308	1.467332	4.053951	H	-5.519059	3.471149	-4.720629
C	-1.192157	-0.846388	3.884228	H	-5.030615	4.755658	-3.612008
F	-2.199617	-1.096949	4.707234	H	-4.083671	4.450194	-5.068201
C	-0.469040	-1.891750	3.328870	H	-5.364224	1.546606	-3.247537
C	0.594821	-1.614627	2.484125	H	-5.089935	-0.603593	-2.502467
F	1.249612	-2.677915	2.018138	H	-4.630770	-0.299360	-0.819739
F	-0.814549	-3.148416	3.595447	H	-3.569964	-1.242961	-1.858685
C	2.593408	1.447802	0.784354				

H -2.456850 -3.839890 0.560133  
H -0.935506 -2.993260 0.265079  
H -2.203766 -2.979358 -0.963242  
H -3.745332 -2.950807 2.078795  
H -6.103148 -1.218430 3.225696  
H -5.063853 -0.347976 4.359490  
H -4.856045 -2.089856 4.124616  
H -4.128900 1.249394 2.738428  
H -2.610402 2.692923 1.852421  
H -1.375712 2.240570 0.676079  
H -3.017466 2.582143 0.128695

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**21B**

C 3.135227 0.641358 2.217796  
C 4.258403 0.575616 3.033498  
C 5.314744 -0.265596 2.693791  
C 5.255858 -1.024388 1.527658  
C 4.149190 -0.960265 0.680639  
C 3.096846 -0.128679 1.062476  
O 1.957598 -0.037048 0.294593  
C 1.600378 -1.132519 -0.447329  
C 0.232581 -1.288497 -0.727687  
C -0.137987 -2.449110 -1.428141  
C 0.801949 -3.381504 -1.840794  
C 2.150777 -3.166859 -1.566050  
C 2.578329 -2.033777 -0.875973  
C 4.040859 -1.653425 -0.670777  
C 4.979149 -2.854612 -0.781934  
C 4.405847 -0.621783 -1.763894  
B -0.847108 -0.235584 -0.356510  
C -0.548502 1.308074 -0.325412  
C -1.232053 2.182472 0.523129  
F -2.173787 1.722667 1.351477  
C -0.972784 3.543972 0.580271  
F -1.640759 4.331257 1.419050  
C -0.005532 4.084061 -0.256090  
F 0.251154 5.383993 -0.222596  
C 0.691542 3.259274 -1.129298  
C 0.414830 1.900855 -1.147601  
F 1.111478 1.168263 -2.017598  
F 1.612660 3.778053 -1.936842  
C -2.315920 -0.734297 -0.074635  
C -2.576325 -1.904830 0.642925  
F -1.576931 -2.628258 1.147706  
C -3.863503 -2.359585 0.899518  
F -4.065375 -3.473755 1.597020  
C -4.947533 -1.636218 0.422545  
F -6.182081 -2.060147 0.652569  
C -4.737987 -0.464089 -0.294019  
C -3.440108 -0.033090 -0.517945

F -3.292750 1.101923 -1.205841  
F -5.777779 0.227564 -0.750730  
H 2.282374 1.266715 2.458664  
H 4.301646 1.171477 3.938918  
H 6.188533 -0.328594 3.333188  
H 6.090331 -1.668896 1.273389  
H -1.187167 -2.609919 -1.659702  
H 0.493338 -4.269448 -2.381176  
H 2.881085 -3.894817 -1.903152  
H 4.905423 -3.310042 -1.772438  
H 4.754062 -3.613277 -0.026774  
H 6.017932 -2.537807 -0.662042  
H 4.323129 -1.080634 -2.754122  
H 3.730815 0.237869 -1.727323  
H 5.431151 -0.267718 -1.619545

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**[21BH]<sup>-</sup>**

C 3.609187 0.991750 2.043153  
C 4.874022 1.092897 2.608795  
C 5.908895 0.278837 2.153790  
C 5.677303 -0.620633 1.115332  
C 4.422786 -0.725992 0.515394  
C 3.393724 0.082590 1.010584  
O 2.138857 0.015011 0.491900  
C 1.720741 -1.209544 -0.016909  
C 0.342794 -1.447161 0.022225  
C -0.048145 -2.698614 -0.462823  
C 0.864926 -3.636859 -0.943525  
C 2.219047 -3.330885 -0.993012  
C 2.668815 -2.088616 -0.540102  
C 4.099413 -1.583607 -0.699585  
C 5.106498 -2.717090 -0.889106  
C 4.129484 -0.668668 -1.946009  
B -0.673891 -0.358174 0.670082  
C -0.550401 1.163929 0.060798  
C -1.182116 2.200705 0.743839  
F -1.873217 1.938867 1.865634  
C -1.154451 3.529764 0.340653  
F -1.779102 4.483102 1.047223  
C -0.472910 3.870833 -0.817508  
F -0.431067 5.144786 -1.230031  
C 0.162126 2.876019 -1.542938  
C 0.102089 1.557545 -1.102803  
F 0.734440 0.664138 -1.880316  
F 0.817411 3.196393 -2.667778  
C -2.239050 -0.800622 0.465582  
C -3.108785 -1.085295 1.511540  
F -2.691031 -1.053597 2.783650  
C -4.446861 -1.420373 1.321639  
F -5.246597 -1.687987 2.363646



C	-4.961401	-1.479993	0.036556
F	-6.245102	-1.804245	-0.163588
C	-4.133333	-1.203772	-1.042023
C	-2.806379	-0.870134	-0.803989
F	-2.050093	-0.610664	-1.882602
F	-4.626359	-1.261718	-2.286738
H	2.769541	1.586734	2.385656
H	5.046916	1.798029	3.416021
H	6.895444	0.345695	2.601365
H	6.493231	-1.243759	0.762802
H	-1.104654	-2.955340	-0.449985
H	0.516869	-4.603486	-1.297088
H	2.922560	-4.053838	-1.393526
H	4.860814	-3.298358	-1.781338
H	5.119254	-3.389896	-0.026167
H	6.113450	-2.316471	-1.038212
H	3.890299	-1.254056	-2.839815
H	3.385015	0.126688	-1.854421
H	5.120919	-0.217822	-2.066153
H	-0.442694	-0.277088	1.856058

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**21P**

P	0.803204	-0.118648	0.654850
C	-0.355274	-0.918813	-0.532303
C	-0.002125	-1.965661	-1.388282
C	-0.975058	-2.657103	-2.104566
C	-2.316491	-2.310285	-1.983480
C	-2.712797	-1.268720	-1.143253
C	-1.716179	-0.608539	-0.425039
O	-2.039503	0.425426	0.423422
C	-3.272184	0.362967	1.033427
C	-3.381346	0.944496	2.290066
C	-4.604894	0.902464	2.947259
C	-5.692551	0.269570	2.350880
C	-5.560039	-0.303977	1.089130
C	-4.348599	-0.258400	0.397841
C	-4.144554	-0.752196	-1.030214
C	-5.171834	-1.814256	-1.424663
C	-4.288442	0.460655	-1.977191
C	1.284784	1.579856	0.087028
C	0.769666	2.314304	-1.004790
C	-0.293575	1.805003	-1.947981
C	1.258614	3.598457	-1.251400
C	2.234651	4.197393	-0.460617
C	2.720263	5.593850	-0.749226
C	2.716390	3.472892	0.622629
C	2.254909	2.189428	0.918658
C	2.844615	1.502770	2.129663
C	2.347091	-1.107992	0.367476
C	2.648444	-2.068081	1.360459

C	3.829307	-2.803618	1.275423
C	4.733373	-2.622970	0.231013
C	6.022755	-3.400441	0.181252
C	4.410225	-1.699083	-0.756946
C	3.235892	-0.941853	-0.715294
C	2.976818	0.001539	-1.864493
C	1.719139	-2.338160	2.521366
H	1.041182	-2.251069	-1.478822
H	-0.684844	-3.470195	-2.761538
H	-3.060062	-2.857029	-2.552936
H	-2.503052	1.405253	2.728403
H	-4.703868	1.352302	3.929506
H	-6.646640	0.224373	2.864907
H	-6.419050	-0.787256	0.636317
H	-6.184618	-1.409539	-1.359660
H	-5.103694	-2.696700	-0.782225
H	-5.026204	-2.122774	-2.462621
H	-5.298514	0.875999	-1.905603
H	-3.575380	1.246669	-1.713017
H	-4.099793	0.156016	-3.011390
H	-0.434129	2.516471	-2.764456
H	-0.045825	0.834882	-2.384617
H	-1.249784	1.694471	-1.430454
H	0.861569	4.147910	-2.102434
H	2.056475	6.338764	-0.297929
H	3.722317	5.756029	-0.345117
H	2.748379	5.788460	-1.824396
H	3.473011	3.916285	1.266460
H	3.389124	2.224790	2.741681
H	3.539734	0.705453	1.847436
H	2.065680	1.047244	2.749866
H	4.047540	-3.539929	2.045989
H	6.421619	-3.442227	-0.834853
H	6.782172	-2.933433	0.817016
H	5.881574	-4.423945	0.537800
H	5.087507	-1.564428	-1.597803
H	3.569313	-0.297943	-2.732241
H	3.240450	1.032679	-1.609917
H	1.923228	-0.000151	-2.153809
H	2.109976	-3.150516	3.137945
H	1.596834	-1.452390	3.151409
H	0.719791	-2.621203	2.177985

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**[21PH]<sup>+</sup>**

P	0.942093	-0.103822	0.306038
C	-0.258989	-1.066128	-0.614023
C	0.124886	-2.133452	-1.430199
C	-0.858013	-2.891605	-2.051374
C	-2.205323	-2.584456	-1.858863
C	-2.616407	-1.520011	-1.055435



F	-4.750036	5.464764	-1.107336	H	-2.318288	-4.660322	-0.766971
C	-2.822960	4.154660	-1.477075	H	-3.372546	-6.081129	-0.933750
C	-2.175458	2.931193	-1.342035	H	-0.840735	0.548570	-1.040935
F	-0.942840	2.853688	-1.886325	H	2.129174	-1.091077	0.277833
F	-2.208600	5.197496	-2.062511	H	3.803290	-0.272648	-3.147487
P	3.332395	-0.659360	-0.298645	H	3.311010	1.639992	-4.650776
C	2.947803	0.694246	-1.417059	H	2.280286	3.684683	-3.750885
C	3.318778	0.619580	-2.764168	H	0.584051	1.458353	2.462647
C	3.048221	1.692323	-3.600709	H	-1.168606	2.997700	3.370653
C	2.455679	2.845526	-3.086558	H	-1.691558	5.099412	2.147718
C	2.095020	2.960941	-1.745209	H	-0.484874	5.663281	0.084087
C	2.306193	1.842540	-0.933606	H	0.601683	6.100776	-1.622776
O	1.975396	1.827804	0.379263	H	0.049141	4.700952	-2.553985
C	1.021249	2.745479	0.816159	H	1.619192	5.477013	-2.898639
C	0.354371	2.404671	1.982074	H	2.581600	5.971226	-0.156119
C	-0.618549	3.264806	2.474957	H	3.392543	4.442815	0.195507
C	-0.913311	4.436805	1.785436	H	3.584603	5.192167	-1.404561
C	-0.224526	4.756922	0.619011	H	6.026086	2.703877	0.502023
C	0.767558	3.918309	0.107870	H	5.177942	1.803870	-0.756523
C	1.627722	4.264143	-1.103309	H	4.263199	2.611426	0.512206
C	0.921625	5.178093	-2.110898	H	6.743370	1.823074	2.383105
C	2.880671	5.010573	-0.585636	H	6.732881	0.446431	5.242759
C	4.458103	-0.319361	1.089576	H	7.661741	-0.932383	4.651516
C	5.242549	0.847732	1.217242	H	8.071311	0.710006	4.121681
C	5.175889	2.048769	0.306936	H	5.605216	-2.048253	3.780323
C	6.139135	0.925364	2.282977	H	4.150072	-3.342436	2.739811
C	6.288510	-0.096243	3.215486	H	3.835390	-3.157505	1.020387
C	7.247130	0.037229	4.367336	H	2.720654	-2.472503	2.216528
C	5.504468	-1.235890	3.065494	H	2.884047	-4.873833	-2.798705
C	4.586129	-1.374664	2.027047	H	6.369878	-5.128034	-4.112273
C	3.774873	-2.647923	1.986804	H	5.611924	-6.219703	-2.948193
C	3.972446	-2.037828	-1.291777	H	4.703697	-5.681226	-4.360916
C	3.073182	-3.041991	-1.715674	H	6.823372	-3.211818	-2.701209
C	3.573556	-4.100969	-2.469909	H	7.224112	-1.120038	-1.925361
C	4.919261	-4.191766	-2.819136	H	6.654179	-1.095813	-0.250028
C	5.430721	-5.366042	-3.609058	H	5.939068	-0.013799	-1.448841
C	5.776081	-3.171695	-2.412925	H	1.085041	-3.817605	-1.905137
C	5.334686	-2.087742	-1.655727	H	1.432766	-3.159806	-0.309985
C	6.338967	-1.020474	-1.294951	H	1.121912	-2.076404	-1.662470
C	1.606431	-3.016382	-1.380986				
H	-3.593968	-2.164740	2.739475				
H	-5.353510	-3.500503	3.930367				
H	-6.756954	-5.095126	2.639348				
H	-6.380678	-5.399347	0.227103				
H	-2.575171	0.566607	-3.172289				
H	-3.805288	-0.916509	-4.710613				
H	-4.698969	-3.075090	-3.905854				
H	-5.141488	-5.004400	-3.195265				
H	-6.372762	-4.209506	-2.191716				
H	-5.734384	-5.810220	-1.754078				
H	-2.769229	-5.236858	-2.385923				
				74			
				<b>22H<sub>2</sub></b>			
				B	1.090123	0.489113	-0.232543
				P	-2.024844	-1.616715	-1.210341
				O	-1.679613	0.836357	0.187290
				C	-0.961788	2.048972	0.193595
				C	0.418128	1.941599	0.039564
				C	1.095465	3.165661	0.045494
				C	0.425878	4.382011	0.163750
				C	-0.960274	4.421049	0.285358
				C	-1.688038	3.231172	0.306561



C	0.237803	-3.416804	-2.786667	C	-2.573931	3.476643	0.600044
C	-0.697915	-1.408486	-4.033206	C	-3.289317	2.456415	-0.276715
F	1.641279	-0.355943	-1.933449	C	-4.546431	2.632959	-0.849934
F	4.026696	-0.522995	-3.191249	C	-5.172011	1.591094	-1.530386
F	6.248401	0.550386	-2.038718	C	-4.546959	0.351503	-1.629807
F	6.067352	1.780823	0.376446	C	-3.274833	0.134191	-1.090855
F	3.670722	1.938318	1.634831	C	-2.661616	1.215160	-0.439026
F	1.590308	-2.001875	0.189966	C	-2.778941	3.054130	2.073393
F	0.901531	-3.905626	1.919110	C	-3.123226	4.889216	0.408549
F	-0.279909	-3.253172	4.279097	C	2.927580	0.238063	-0.650511
F	-0.817863	-0.655383	4.858172	C	3.486491	0.042084	-1.910100
F	-0.204933	1.264072	3.107920	C	4.857310	-0.041822	-2.136989
H	-0.273117	-1.062972	-0.963346	C	5.735541	0.079283	-1.072217
H	1.929054	3.542191	0.523265	C	5.230483	0.284470	0.202813
H	0.476810	5.533073	0.305507	C	3.854453	0.360344	0.381164
H	-1.955337	5.276368	0.044232	C	0.894517	-0.739650	0.783502
H	-5.388360	2.219556	-1.920680	C	0.647375	-2.076804	0.479711
H	-5.577338	0.144777	-3.229346	C	0.235132	-3.017172	1.417618
H	-3.867405	-1.628756	-3.018440	C	0.093110	-2.642287	2.744119
H	-4.994300	2.231113	1.395606	C	0.354497	-1.330036	3.104877
H	-3.786390	3.323887	2.109054	C	0.733374	-0.413399	2.128431
H	-3.381343	1.622469	1.828922	C	-3.053684	-2.324597	0.332781
H	-3.887179	4.367014	-1.494784	C	-2.847708	-1.440840	1.567430
H	-4.076011	4.913792	0.184920	C	-4.519465	-2.737926	0.221513
H	-5.278093	3.851205	-0.513604	C	-3.157922	-2.343353	-2.580797
H	-0.841279	-3.476694	0.145621	C	-2.610795	-3.774577	-2.603971
H	-3.434650	-1.994136	0.879797	C	-2.835453	-1.627860	-3.894619
H	-1.837905	-1.471795	1.438163	F	2.712935	-0.076656	-2.997129
H	-2.477239	-3.054488	1.927384	F	5.342146	-0.234445	-3.371729
H	-3.016398	-4.789544	0.086867	F	7.057244	0.003612	-1.272322
H	-2.281684	-4.656588	-1.512785	F	6.073720	0.409134	1.236674
H	-3.669053	-3.631578	-1.072354	F	3.432972	0.573975	1.637705
H	-1.845576	-3.098033	-3.304455	F	0.799557	-2.533990	-0.771381
H	0.502605	-3.878446	-3.740525	F	-0.050454	-4.277187	1.050887
H	0.046182	-4.219402	-2.069219	F	-0.313051	-3.530405	3.661011
H	1.098294	-2.835581	-2.442496	F	0.215798	-0.957737	4.385179
H	0.152795	-0.793392	-3.728297	F	0.932287	0.840225	2.559103
H	-1.561335	-0.760209	-4.196234	H	0.756469	-0.062533	-1.411358
H	-0.443800	-1.884066	-4.983444	H	2.709542	2.815429	-0.241929
				H	1.834854	5.097271	0.065661
				H	-0.581839	5.475841	0.408748
				H	-5.050742	3.589725	-0.759117
				H	-6.152545	1.742723	-1.971003
				H	-5.051121	-0.456817	-2.152634
				H	-3.845102	3.055962	2.326054
				H	-2.251631	3.748061	2.735718
				H	-2.378775	2.050511	2.243226
				H	-3.000866	5.229907	-0.624115
				H	-2.606526	5.589386	1.069874
				H	-4.184967	4.928032	0.669153
				H	-2.427325	-3.220215	0.446089

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[22H]<sup>-</sup>

B	1.307530	0.315341	-0.404858
P	-2.317665	-1.447162	-1.170241
O	-1.413250	1.017267	0.073067
C	-0.547637	2.109650	0.088114
C	0.810321	1.833015	-0.103860
C	1.641860	2.957486	-0.092133
C	1.152403	4.251842	0.077538
C	-0.207348	4.466698	0.269607
C	-1.084413	3.380847	0.289386

H -3.578146 -0.623476 1.572119  
H -1.851334 -0.993148 1.583749  
H -2.983401 -2.024989 2.484667  
H -4.862138 -3.172770 1.168043  
H -4.691946 -3.478450 -0.564969  
H -5.147057 -1.863589 0.012529  
H -4.246568 -2.384631 -2.449245  
H -2.998212 -4.322376 -3.470552  
H -2.882174 -4.333514 -1.702975  
H -1.517191 -3.762824 -2.667642  
H -1.751653 -1.569848 -4.038757  
H -3.227605 -0.607085 -3.906949  
H -3.263566 -2.171336 -4.744989

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**22**

P 1.936877 -1.516398 1.062094  
C 3.016965 -0.014771 1.085833  
C 4.220605 0.110129 1.786561  
C 4.963863 1.285188 1.736034  
C 4.528122 2.355675 0.960584  
C 3.348590 2.268195 0.223140  
C 2.613385 1.085899 0.320638  
O 1.426870 0.955744 -0.365684  
C 0.696191 2.082645 -0.630033  
C -0.692607 1.920119 -0.767359  
C -1.442409 3.090953 -0.970290  
C -0.840400 4.337880 -1.053953  
C 0.544077 4.443448 -0.942278  
C 1.339949 3.317132 -0.740705  
C 2.863913 3.322314 -0.764526  
C 3.448009 4.703487 -0.469734  
C 3.302602 2.877273 -2.179677  
B -1.416604 0.542904 -0.725148  
C -2.891766 0.507725 -0.166416  
C -3.896535 -0.254374 -0.764089  
F -3.624760 -0.980108 -1.851531  
C -5.197975 -0.293978 -0.288819  
F -6.129281 -1.020098 -0.900377  
C -5.525123 0.435712 0.847690  
F -6.763303 0.404534 1.321247  
C -4.554554 1.192659 1.489251  
C -3.265036 1.221981 0.974008  
F -2.366728 1.944370 1.646444  
F -4.865990 1.877299 2.586445  
C -0.762147 -0.793741 -1.225141  
C -1.069571 -2.028271 -0.646876  
F -1.982682 -2.113001 0.328100  
C -0.413103 -3.204177 -0.973218  
F -0.691017 -4.342608 -0.338286  
C 0.593738 -3.173788 -1.924357

F 1.269553 -4.279568 -2.210902  
C 0.917079 -1.978762 -2.552850  
C 0.239149 -0.823289 -2.199935  
F 0.588680 0.291996 -2.843570  
F 1.874366 -1.954660 -3.476798  
C 3.115136 -2.872453 1.564730  
C 4.066094 -3.140860 0.394824  
C 2.295449 -4.125149 1.891639  
C 0.925763 -1.239093 2.624997  
C 1.734769 -1.042801 3.904304  
C -0.047904 -0.079078 2.399738  
H 4.579169 -0.719011 2.388873  
H 5.888923 1.365910 2.296913  
H 5.123110 3.261605 0.922607  
H -2.521177 3.011496 -1.071828  
H -1.440866 5.226816 -1.212200  
H 1.008405 5.420719 -1.021286  
H 3.110026 5.429466 -1.213097  
H 4.538391 4.678098 -0.533956  
H 3.162586 5.058313 0.524851  
H 2.957672 3.602366 -2.923424  
H 4.393444 2.806048 -2.230153  
H 2.876693 1.901141 -2.428670  
H 3.698782 -2.597508 2.450971  
H 4.762298 -3.948373 0.643448  
H 4.650984 -2.253957 0.134019  
H 3.500719 -3.445822 -0.493177  
H 2.957948 -4.984764 2.034748  
H 1.605261 -4.367917 1.074629  
H 1.706284 -4.003346 2.805200  
H 0.330137 -2.158177 2.711489  
H 1.065057 -0.924112 4.762983  
H 2.391296 -1.893387 4.111787  
H 2.353548 -0.142299 3.836049  
H -0.667831 0.082018 3.287611  
H 0.479400 0.857831 2.188041  
H -0.720803 -0.294036 1.564134

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**22B**

B 0.846941 -0.236282 -0.356631  
O -1.957755 -0.037059 0.294729  
C -1.600787 -1.132689 -0.447026  
C -0.233029 -1.289033 -0.727355  
C 0.137327 -2.449885 -1.427538  
C -0.802795 -3.382149 -1.840048  
C -2.151591 -3.167098 -1.565431  
C -2.578947 -2.033774 -0.875619  
C -4.041411 -1.652959 -0.670648  
C -4.149728 -0.959468 0.680557  
C -5.256586 -1.023042 1.527361

C -5.315457 -0.263970 2.693306  
C -4.258904 0.576986 3.033020  
C -3.135547 0.642190 2.217526  
C -3.097197 -0.128135 1.062386  
C -4.405997 -0.621455 -1.764044  
C -4.980145 -2.853809 -0.781537  
C 2.315872 -0.734910 -0.075172  
C 2.576585 -1.905115 0.642838  
C 3.863882 -2.359397 0.899699  
C 4.947747 -1.635878 0.422594  
C 4.737883 -0.464056 -0.294390  
C 3.439898 -0.033566 -0.518628  
C 0.548677 1.307488 -0.325442  
C 1.232531 2.181694 0.523051  
C 0.973647 3.543271 0.580232  
C 0.006483 4.083633 -0.256043  
C -0.690846 3.259064 -1.129254  
C -0.414529 1.900570 -1.147587  
F 1.577424 -2.628667 1.147920  
F 4.065953 -3.473273 1.597616  
F 6.182409 -2.059300 0.652901  
F 5.777493 0.227805 -0.751211  
F 3.292236 1.101248 -1.206812  
F 2.174138 1.721663 1.351440  
F 1.641866 4.330343 1.419004  
F -0.249866 5.383633 -0.222535  
F -1.611826 3.778164 -1.936757  
F -1.111348 1.168224 -2.017640  
H 1.186508 -2.610912 -1.658964  
H -0.494391 -4.270302 -2.380213  
H -2.882009 -3.894999 -1.902412  
H -6.091214 -1.667337 1.273035  
H -6.189399 -0.326537 3.332544  
H -4.302114 1.173044 3.938312  
H -2.282546 1.267333 2.458394  
H -5.431172 -0.266957 -1.619838  
H -4.323409 -1.080597 -2.754149  
H -3.730650 0.237962 -1.727694  
H -4.755126 -3.612561 -0.026443  
H -4.906889 -3.309247 -1.772067  
H -6.018778 -2.536621 -0.661340

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[22BH]<sup>-</sup>

B 0.673857 -0.358020 0.670069  
O -2.138984 0.015224 0.491581  
C -1.720726 -1.209312 -0.017239  
C -0.342801 -1.446909 0.022026  
C 0.048202 -2.698310 -0.463138  
C -0.864808 -3.636511 -0.944033  
C -2.218938 -3.330567 -0.993596

C -2.668741 -2.088352 -0.540600  
C -4.099370 -1.583409 -0.699969  
C -4.422777 -0.726163 0.515256  
C -5.677207 -0.621246 1.115436  
C -5.908782 0.277847 2.154222  
C -4.873984 1.091936 2.609336  
C -3.609207 0.991186 2.043477  
C -3.393781 0.082438 1.010557  
C -4.129577 -0.668161 -1.946174  
C -5.106334 -2.716950 -0.889717  
C 2.239018 -0.800549 0.465635  
C 3.108671 -1.085686 1.511526  
C 4.446667 -1.421008 1.321548  
C 4.961236 -1.480360 0.036459  
C 4.133254 -1.203684 -1.042060  
C 2.806360 -0.869840 -0.803949  
C 0.550417 1.164132 0.060940  
C 1.182081 2.200851 0.744114  
C 1.154440 3.529948 0.341038  
C 0.473014 3.871101 -0.817159  
C -0.162010 2.876353 -1.542692  
C -0.101969 1.557834 -1.102693  
F 2.690872 -1.054234 2.783626  
F 5.246352 -1.689062 2.363490  
F 6.244890 -1.804792 -0.163696  
F 4.626276 -1.261367 -2.286787  
F 2.050158 -0.609956 -1.882522  
F 1.873104 1.938931 1.865935  
F 1.779070 4.483225 1.047711  
F 0.431213 5.145087 -1.229592  
F -0.817197 3.196820 -2.667565  
F -0.734219 0.664481 -1.880332  
H 0.442604 -0.277018 1.856050  
H 1.104710 -2.955059 -0.450210  
H -0.516693 -4.603101 -1.297658  
H -2.922423 -4.053490 -1.394225  
H -6.493094 -1.244397 0.762848  
H -6.895287 0.344391 2.601955  
H -5.046866 1.796749 3.416852  
H -2.769610 1.586147 2.386123  
H -5.121153 -0.217630 -2.066333  
H -3.890092 -1.253261 -2.840090  
H -3.385389 0.127425 -1.854298  
H -5.119011 -3.389932 -0.026913  
H -4.860564 -3.297995 -1.782073  
H -6.113322 -2.316383 -1.038738

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22P

P -4.858169 13.223008 8.998236  
O -5.265215 14.545798 11.569204

C	-4.972078	14.643503	12.909814	P	2.266527	0.536308	-0.034767
C	-5.037584	13.475835	13.659109	O	-0.596564	0.749447	0.353084
C	-4.745288	13.530943	15.016838	C	-1.878307	1.201680	0.036296
C	-4.377839	14.740417	15.601110	C	-2.025674	2.569844	-0.131763
C	-4.321717	15.899251	14.830628	C	-3.279530	3.070398	-0.462617
C	-4.631024	15.875310	13.470676	C	-4.349516	2.196467	-0.633238
C	-4.711640	17.100596	12.568905	C	-4.172523	0.827269	-0.454753
C	-4.237504	16.679036	11.181227	C	-2.929449	0.298599	-0.102617
C	-3.538908	17.504879	10.303015	C	-2.681169	-1.169305	0.230178
C	-3.246663	17.081407	9.010164	C	-1.253357	-1.505051	-0.186691
C	-3.653906	15.823546	8.578085	C	-0.827513	-2.761178	-0.612193
C	-4.334642	14.947335	9.430656	C	0.518489	-3.045315	-0.852707
C	-4.600788	15.407569	10.726296	C	1.476974	-2.060983	-0.672980
C	-6.198612	17.508143	12.454445	C	1.078266	-0.778418	-0.271560
C	-3.913040	18.280405	13.122030	C	-0.277058	-0.514755	-0.036387
C	-6.580849	13.567138	8.313298	C	-2.764921	-1.330523	1.766264
C	-7.486115	14.086206	9.433752	C	-3.703824	-2.095790	-0.429499
C	-6.631071	14.499902	7.105160	C	2.797103	0.657536	1.713209
C	-3.883551	12.911745	7.432605	C	1.579652	0.819131	2.630322
C	-4.433767	11.654090	6.753267	C	3.633240	-0.574788	2.077105
C	-2.405644	12.726158	7.786157	C	3.690218	0.350031	-1.164845
H	-5.300976	12.550096	13.159519	C	4.726183	1.443461	-0.873385
H	-4.790960	12.626337	15.614030	C	3.204521	0.386049	-2.619183
H	-4.137497	14.784632	16.657921	H	1.642223	1.741452	-0.381308
H	-4.039296	16.834764	15.301557	H	-1.165481	3.219006	-0.007950
H	-3.225373	18.492380	10.623565	H	-3.415675	4.137751	-0.595834
H	-2.707418	17.737445	8.334991	H	-5.327407	2.580289	-0.900971
H	-3.421014	15.515873	7.563742	H	-5.021045	0.165342	-0.585062
H	-6.303578	18.362247	11.778156	H	-1.558350	-3.550061	-0.750732
H	-6.590067	17.782416	13.438957	H	0.813223	-4.037323	-1.174002
H	-6.797126	16.680460	12.063430	H	2.524097	-2.282750	-0.857114
H	-2.850397	18.038455	13.215278	H	-2.557443	-2.366175	2.051670
H	-4.294113	18.571244	14.104011	H	-3.766748	-1.062047	2.112165
H	-4.019541	19.153596	12.473694	H	-2.044671	-0.678159	2.269101
H	-6.945527	12.574604	8.017540	H	-3.676952	-2.017686	-1.519749
H	-7.182416	15.094315	9.736618	H	-4.711108	-1.852978	-0.086012
H	-7.448195	13.447183	10.319318	H	-3.526364	-3.134928	-0.142985
H	-8.522359	14.141123	9.084601	H	3.417165	1.560975	1.762338
H	-7.670102	14.672840	6.803474	H	0.944043	-0.070701	2.591521
H	-6.100861	14.091518	6.240103	H	0.971380	1.686966	2.367181
H	-6.189068	15.471892	7.349716	H	1.929288	0.940537	3.658173
H	-3.985523	13.750082	6.734039	H	3.928930	-0.506450	3.126431
H	-3.816027	11.389648	5.888836	H	4.545727	-0.656445	1.480029
H	-5.459971	11.791123	6.400026	H	3.048751	-1.492522	1.956147
H	-4.424095	10.803601	7.443711	H	4.128647	-0.631058	-0.945553
H	-2.279947	11.875527	8.463891	H	5.550636	1.347912	-1.583541
H	-1.988100	13.609284	8.277591	H	5.145160	1.368190	0.132996
H	-1.818079	12.527836	6.883527	H	4.296332	2.442187	-1.001522
				H	2.759494	1.356820	-2.857887
				H	2.470666	-0.394645	-2.830901
				H	4.059261	0.240152	-3.283514



104				C	-2.635950	-1.140200	-2.489784
<b>22PHBH</b>				C	-1.436337	-0.984730	-3.180734
B	1.498477	0.679175	-0.090583	C	-0.260781	-1.508922	-2.661166
O	-1.259525	1.315024	-0.450923	C	-0.281920	-2.178243	-1.432898
C	-0.499457	1.658244	-1.545862	C	-1.482216	-2.234330	-0.717391
C	0.860345	1.327990	-1.435263	C	-4.341157	-3.538862	-0.701389
C	1.612160	1.497401	-2.600174	C	-5.115494	-1.164481	-0.929575
C	1.063150	2.006713	-3.777542	C	0.783369	-4.723802	-0.346790
C	-0.263334	2.414300	-3.793970	C	1.571822	-5.197622	0.879535
C	-1.077139	2.255253	-2.667063	C	0.968142	-5.643322	-1.554632
C	-2.506239	2.796110	-2.661871	C	2.641913	-2.705299	-1.761642
C	-3.213164	2.411006	-1.366870	C	3.909060	-3.266764	-1.099815
C	-4.539224	2.785603	-1.121335	C	2.516793	-3.257325	-3.193997
C	-5.169401	2.515459	0.088143	H	1.375521	-0.520460	-0.205157
C	-4.469879	1.847350	1.093773	H	2.670774	1.243262	-2.581879
C	-3.159596	1.449440	0.877112	H	1.680058	2.129266	-4.662494
C	-2.543910	1.735177	-0.344248	H	-0.672821	2.874475	-4.689299
C	-2.435816	4.336476	-2.742062	H	-5.085523	3.320748	-1.893690
C	-3.295268	2.272190	-3.874967	H	-6.194699	2.831396	0.247945
C	3.109619	0.947046	0.061072	H	-4.942567	1.631815	2.046946
C	3.930317	-0.031076	0.608869	H	-2.584419	0.917078	1.631958
C	5.304120	0.088386	0.763751	H	-3.439957	4.772382	-2.740825
C	5.918753	1.273581	0.388584	H	-1.926188	4.648078	-3.658712
C	5.143500	2.303429	-0.126173	H	-1.882225	4.734546	-1.888222
C	3.769676	2.129684	-0.266859	H	-2.827108	2.588058	-4.811070
C	0.797299	1.069942	1.335710	H	-4.318075	2.659588	-3.871897
C	0.580448	0.140797	2.342294	H	3.199503	-2.699605	-3.840277
C	0.002918	0.445363	3.570785	H	1.448521	-2.384579	0.541861
C	-0.409686	1.742426	3.823505	H	-0.929378	-2.339769	3.033976
C	-0.217590	2.713916	2.848082	H	-2.527132	-1.433416	4.715673
C	0.384145	2.363383	1.647213	H	-4.840312	-0.830369	4.012313
F	3.394744	-1.198643	1.041762	H	-5.511966	-1.066302	1.656442
F	6.026940	-0.918134	1.266546	H	-3.551624	-0.748407	-2.918295
F	7.236052	1.423085	0.524881	H	-1.408092	-0.431934	-4.113175
F	5.725975	3.451494	-0.475223	H	0.671484	-1.342144	-3.187087
F	3.089924	3.172129	-0.754315	H	-4.533062	-3.719947	-1.763528
F	0.923869	-1.161393	2.177692	H	-5.241951	-3.785792	-0.131745
F	-0.153452	-0.500736	4.508963	H	-3.536734	-4.204191	-0.374186
F	-0.970478	2.057173	4.992233	H	-4.869791	-0.103341	-0.823773
F	-0.608770	3.967502	3.082880	H	-6.018655	-1.378329	-0.353240
F	0.528029	3.339047	0.741556	H	-5.358695	-1.371859	-1.975419
P	1.164640	-2.955845	-0.699130	H	-0.278309	-4.694637	-0.080102
O	-1.431374	-2.758310	0.547663	H	1.285497	-6.225810	1.116666
C	-2.361316	-2.242419	1.446998	H	1.361587	-4.577159	1.754656
C	-1.949579	-2.096109	2.763231	H	2.650644	-5.185162	0.700920
C	-2.849051	-1.581401	3.691111	H	0.551062	-6.626506	-1.321464
C	-4.136583	-1.232562	3.291174	H	2.027119	-5.782492	-1.788674
C	-4.518321	-1.376510	1.960419	H	0.459327	-5.265646	-2.446044
C	-3.631722	-1.874814	1.006027	H	2.707247	-1.607625	-1.786959
C	-3.963253	-2.058260	-0.469842	H	4.770511	-2.977473	-1.708405
C	-2.685459	-1.771482	-1.249601	H	4.066898	-2.883241	-0.092279

H	3.881902	-4.360602	-1.074541
H	2.816539	-4.306501	-3.228309
H	1.515997	-3.182546	-3.620608
H	-3.343434	1.180758	-3.868077

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**Acetone**

C	1.28682	-0.61332	-0.00000
C	0.00000	0.18636	-0.00000
C	-1.28682	-0.61332	0.00000
O	0.00000	1.39554	0.00000
H	1.32677	-1.26237	0.88034
H	1.32674	-1.26245	-0.88028
H	2.14038	0.06348	-0.00004
H	-1.32675	-1.26243	-0.88030
H	-1.32676	-1.26240	0.88032
H	-2.14038	0.06348	-0.00001

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**Acetone + H<sup>+</sup>**

C	1.34546	-0.54117	-0.00766
C	0.00460	0.06297	-0.00148
C	-1.22857	-0.74587	0.00593
O	-0.03041	1.33437	-0.00438
H	1.35085	-1.46441	-0.59136
H	2.10099	0.16571	-0.34974
H	1.56873	-0.82107	1.03349
H	-2.11749	-0.17799	0.28596
H	-1.35951	-1.14101	-1.01233
H	-1.10257	-1.61351	0.65955
H	-0.92670	1.72178	0.02874

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**Isopropoxide**

C	-1.25821	-0.63731	-0.08637
C	-0.00000	0.19057	0.33582
C	1.25820	-0.63732	-0.08637
O	0.00001	1.41359	-0.15146
H	-1.30182	-1.65500	0.33607
H	-2.15510	-0.08813	0.22266
H	-1.27829	-0.70798	-1.18295
H	-0.00002	0.09784	1.48168
H	2.15510	-0.08818	0.22273
H	1.30179	-1.65504	0.33601
H	1.27832	-0.70791	-1.18296

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**Isopropanol**

C	-1.32151	-0.54826	-0.08875
C	-0.00131	0.04612	0.36870
C	1.18941	-0.78008	-0.10294

O	0.04859	1.35993	-0.16692
H	-1.45656	-1.55398	0.31742
H	-2.15221	0.08045	0.23866
H	-1.34077	-0.60308	-1.18111
H	0.00630	0.08904	1.47012
H	2.13403	-0.33287	0.22488
H	1.14574	-1.79805	0.29446
H	1.19391	-0.82898	-1.19574
H	0.88131	1.76133	0.10456

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**Benzaldehyde**

C	-1.73284	1.05573	-0.00001
C	-2.20743	-0.25357	-0.00001
C	-1.31729	-1.32922	0.00000
C	0.05084	-1.09584	0.00001
C	0.52841	0.21723	0.00002
C	-0.36136	1.29064	0.00000
C	1.98959	0.47127	0.00003
O	2.82879	-0.39792	-0.00003
H	-2.42902	1.88778	-0.00002
H	-3.27698	-0.43901	-0.00002
H	-1.69662	-2.34583	0.00000
H	0.77062	-1.90855	0.00002
H	0.02416	2.30758	0.00000
H	2.27805	1.54390	-0.00002

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**Benzaldehyde + H<sup>+</sup>**

C	-1.79450	1.05209	0.00000
C	-2.23653	-0.27547	-0.00000
C	-1.33893	-1.35476	-0.00000
C	0.01775	-1.11410	0.00000
C	0.47656	0.22915	0.00000
C	-0.43830	1.31186	0.00000
C	1.84360	0.53204	-0.00000
O	2.73203	-0.40019	0.00000
H	-2.51004	1.86582	0.00001
H	-3.30354	-0.47695	-0.00001
H	-1.71497	-2.37114	-0.00000
H	0.73487	-1.92856	0.00001
H	-0.07018	2.33418	-0.00000
H	2.18147	1.57017	-0.00001
H	3.64829	-0.07693	-0.00001

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**Benzylaldehyde + H<sup>-</sup>**

C	-1.83032	-0.99987	0.00001
C	-2.25198	0.33147	-0.00000
C	-1.29801	1.34878	0.00000

C	0.06044	1.03865	-0.00001
C	0.49207	-0.28609	-0.00001
C	-0.47018	-1.29898	0.00000
C	2.02443	-0.53877	-0.00001
O	2.76529	0.54416	0.00002
H	-2.56745	-1.80135	0.00002
H	-3.31344	0.56926	-0.00000
H	-1.62384	2.38813	0.00000
H	0.86394	1.77324	-0.00001
H	-0.13892	-2.33881	0.00001
H	2.14936	-1.25746	0.88032
H	2.14935	-1.25740	-0.88038

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**Benzyl Alcohol**

C	-1.87443	-0.99878	-0.02980
C	-2.29606	0.32947	-0.01593
C	-1.35159	1.34987	0.01670
C	0.00953	1.05114	0.03892
C	0.43381	-0.27505	0.02541
C	-0.51687	-1.29688	-0.01140
C	1.90132	-0.62681	0.07089
O	2.67480	0.53953	-0.10723
H	-2.60372	-1.80235	-0.05987
H	-3.35543	0.56476	-0.03322
H	-1.67385	2.38661	0.02471
H	0.75235	1.84011	0.06191
H	-0.18958	-2.33436	-0.02783
H	2.12158	-1.10338	1.03908
H	2.11401	-1.37162	-0.71135
H	3.60204	0.30616	-0.00429

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**Acetophenone**

C	-1.81509	1.27513	0.00001
C	-2.58147	0.11285	-0.00000
C	-1.95966	-1.13534	-0.00001
C	-0.57397	-1.21911	-0.00001
C	0.20188	-0.05611	0.00001
C	-0.42594	1.19146	0.00001
C	1.69501	-0.20504	0.00000
C	2.54601	1.04732	-0.00002
O	2.20482	-1.30602	0.00001
H	-2.29911	2.24634	0.00001
H	-3.66493	0.17918	-0.00001
H	-2.55852	-2.04029	-0.00001
H	-0.06166	-2.17562	-0.00002
H	0.16397	2.10277	0.00002
H	2.33309	1.65718	-0.88302
H	2.33311	1.65718	0.88300
H	3.59480	0.75451	-0.00002

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**Acetophenone + H<sup>+</sup>**

C	-1.86739	1.26648	-0.00001
C	-2.60117	0.07568	0.00000
C	-1.96344	-1.16901	0.00000
C	-0.58348	-1.23194	0.00000
C	0.16967	-0.03365	0.00000
C	-0.48667	1.21835	-0.00001
C	1.59303	-0.08907	0.00000
C	2.47464	1.11076	0.00001
O	2.12879	-1.26584	-0.00001
H	-2.37938	2.22163	-0.00001
H	-3.68581	0.11904	0.00000
H	-2.54951	-2.08058	0.00001
H	-0.07353	-2.18901	0.00001
H	0.08190	2.14235	-0.00001
H	3.53118	0.83827	0.00002
H	2.26680	1.72122	-0.88372
H	2.26679	1.72123	0.88373
H	3.10015	-1.25298	-0.00001

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**Acetophenone + H<sup>-</sup>**

C	1.97826	-1.14803	-0.15629
C	2.59646	0.06343	0.15484
C	1.81800	1.21443	0.27777
C	0.43878	1.15176	0.09511
C	-0.19217	-0.05434	-0.20688
C	0.59732	-1.20038	-0.33573
C	-1.74127	-0.01636	-0.38171
C	-2.33543	-0.94524	0.72978
O	-2.25054	1.19721	-0.35748
H	2.57760	-2.05100	-0.26037
H	3.67443	0.10844	0.29315
H	2.29782	2.16377	0.51133
H	-0.23344	2.00564	0.15709
H	0.11893	-2.14681	-0.58934
H	-1.89304	-0.61277	-1.34358
H	-3.42208	-0.97399	0.59643
H	-1.94770	-1.97498	0.72954
H	-2.12784	-0.48764	1.70429

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**Phenylethanol**

C	-2.04675	1.10112	-0.20714
C	-2.61872	-0.11886	0.14627
C	-1.80621	-1.23486	0.32231
C	-0.42754	-1.13621	0.15071
C	0.14870	0.08282	-0.20190
C	-0.67058	1.19828	-0.38163

C	1.64887	0.22531	-0.33815
C	2.24766	0.85195	0.92118
O	2.19708	-1.05929	-0.56965
H	-2.67362	1.97524	-0.35378
H	-3.69303	-0.19882	0.27870
H	-2.24745	-2.18948	0.59222
H	0.21334	-2.00191	0.27516
H	-0.22587	2.14959	-0.66688
H	1.85358	0.88517	-1.19675
H	3.33224	0.97225	0.81946
H	1.81307	1.83648	1.11177
H	2.04194	0.20722	1.77982
H	3.15658	-0.97869	-0.55243

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**N-Piperidino-Cyclohex-1-ene**

C	-1.43792	-1.25990	0.27567
C	-2.90088	-1.04263	0.65838
C	-3.56416	-0.09817	-0.34031
C	-2.89347	1.27305	-0.28352
C	-1.38946	1.18111	-0.22819
C	-0.71337	0.05122	0.03777
N	0.69061	-0.01352	0.19492
C	1.34647	-1.05748	-0.59742
C	2.78488	-1.27962	-0.14220
C	3.57644	0.02388	-0.21048
C	2.84972	1.09681	0.59651
C	1.40478	1.25306	0.12985
H	-1.39843	-1.88344	-0.62799
H	-0.90954	-1.80966	1.06263
H	-3.42243	-2.00421	0.69646
H	-2.95428	-0.60411	1.66276
H	-3.45632	-0.51689	-1.34903
H	-4.63665	-0.00574	-0.14219
H	-3.18950	1.87279	-1.15221
H	-3.25932	1.82352	0.59597
H	-0.85123	2.10805	-0.39608
H	0.78405	-1.98740	-0.49564
H	1.33828	-0.78457	-1.66993
H	2.77160	-1.64801	0.89048
H	3.24498	-2.05327	-0.76555
H	4.59692	-0.11749	0.15883
H	3.65327	0.34602	-1.25797
H	2.84507	0.81598	1.65622
H	3.35828	2.06276	0.51320
H	0.88526	1.96547	0.77665
H	1.38759	1.66686	-0.89744

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**N-Piperidino-Cyclohex-1-ene + H<sup>+</sup>**

C	1.48217	-1.24625	-0.73816
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C	2.19834	-1.25983	0.63666
C	3.03874	0.00000	0.83205
C	2.19833	1.25984	0.63667
C	1.48217	1.24624	-0.73816
C	0.64972	-0.00000	-0.81421
N	-0.64757	-0.00000	-0.81658
C	-1.49663	1.21635	-0.73410
C	-2.17045	1.25971	0.63881
C	-3.00419	0.00000	0.87775
C	-2.17045	-1.25971	0.63882
C	-1.49663	-1.21636	-0.73409
H	0.92816	-2.16827	-0.89166
H	2.23877	-1.17947	-1.52764
H	1.44604	-1.34077	1.43086
H	2.81677	-2.15875	0.68852
H	3.48397	0.00001	1.83038
H	3.86754	0.00001	0.11354
H	1.44602	1.34077	1.43086
H	2.81675	2.15876	0.68853
H	0.92816	2.16827	-0.89168
H	2.23878	1.17946	-1.52764
H	-0.90702	2.10572	-0.93025
H	-2.24193	1.12214	-1.52955
H	-1.39583	1.36071	1.40865
H	-2.79293	2.15692	0.68650
H	-3.40609	0.00000	1.89342
H	-3.86309	-0.00000	0.19560
H	-1.39583	-1.36071	1.40865
H	-2.79293	-2.15692	0.68651
H	-0.90703	-2.10573	-0.93024
H	-2.24193	-1.12214	-1.52954

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**N-Piperidino-Cyclohex-1-ene + H<sup>-</sup>**

C	1.41779	1.19233	-0.53521
C	2.90493	1.00169	-0.73550
C	3.51873	0.19180	0.41363
C	2.82101	-1.16677	0.50122
C	1.30821	-1.00489	0.65846
C	0.72928	-0.14194	-0.48706
N	-0.74576	0.02390	-0.37156
C	-1.52090	-1.19002	-0.44318
C	-2.98787	-0.85470	-0.72861
C	-3.53534	0.08843	0.34627
C	-2.61829	1.30498	0.51048
C	-1.17730	0.85121	0.73786
H	1.00259	1.75587	-1.38982
H	3.21167	0.44894	-1.67057
H	3.42122	1.97281	-0.80326
H	4.60257	0.04523	0.28047
H	3.35875	0.73951	1.35161

H	3.01723	-1.71176	-0.43594
H	3.23625	-1.78019	1.31445
H	0.83169	-1.99723	0.69292
H	1.09897	-0.49687	1.60892
H	0.83839	-0.78464	-1.40923
H	-1.10776	-1.82329	-1.23932
H	-1.48136	-1.78548	0.49732
H	-3.04181	-0.36209	-1.70716
H	-3.59051	-1.77143	-0.77811
H	-4.56575	0.38960	0.11477
H	-3.56921	-0.45468	1.30261
H	-2.64864	1.91378	-0.40147
H	-2.96238	1.93056	1.34462
H	-0.45116	1.67162	0.79219
H	-1.14186	0.29976	1.70579

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**N-Piperidino-Cyclohexane**

C	-1.47080	1.15158	0.64107
C	-2.96182	0.86864	0.84615
C	-3.54793	0.10559	-0.34430
C	-2.76721	-1.18304	-0.60894
C	-1.27718	-0.89285	-0.81134
C	-0.69580	-0.14777	0.40223
N	0.75097	0.08331	0.36804
C	1.53123	-1.12423	0.61119
C	2.99683	-0.77288	0.85798
C	3.56697	0.00262	-0.32974
C	2.68149	1.20988	-0.63638
C	1.23191	0.76898	-0.82708
H	-1.03970	1.66599	1.50556
H	-1.35824	1.81949	-0.22347
H	-3.09255	0.26841	1.75711
H	-3.50547	1.80562	1.00548
H	-4.60590	-0.11755	-0.17080
H	-3.50000	0.74321	-1.23776
H	-2.88859	-1.85978	0.24825
H	-3.17502	-1.70435	-1.48133
H	-0.72697	-1.82437	-0.98733
H	-1.15290	-0.27209	-1.70960
H	-0.86956	-0.78115	1.28613
H	1.11326	-1.63375	1.48635
H	1.47471	-1.83319	-0.23945
H	3.05653	-0.15671	1.76261
H	3.57038	-1.68822	1.03831
H	4.59807	0.31335	-0.13335
H	3.59144	-0.65525	-1.20943
H	2.72234	1.91894	0.19846
H	3.03004	1.72975	-1.53500
H	0.60047	1.64109	-1.01993
H	1.17464	0.11820	-1.72217

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**N-Benzylidene-tert-butylamine**

C	-3.02173	1.36362	0.00000
C	-3.94858	0.32000	0.00000
C	-3.50888	-0.99996	0.00000
C	-2.14398	-1.27511	0.00000
C	-1.21315	-0.23545	-0.00000
C	-1.66125	1.08956	-0.00000
C	0.23221	-0.54915	-0.00000
N	1.11159	0.36353	0.00000
C	2.54287	0.04848	0.00000
C	3.12172	0.71732	-1.25243
C	3.12172	0.71733	1.25242
C	2.89514	-1.44126	0.00000
H	-3.36623	2.39295	0.00000
H	-5.01194	0.53790	0.00000
H	-4.22637	-1.81424	0.00000
H	-1.79485	-2.30501	-0.00000
H	-0.92110	1.88304	-0.00000
H	0.47339	-1.62101	-0.00000
H	2.87013	1.78059	-1.25875
H	4.21045	0.60927	-1.27495
H	2.70714	0.26093	-2.15611
H	4.21045	0.60927	1.27494
H	2.70714	0.26095	2.15611
H	2.87013	1.78060	1.25875
H	2.50580	-1.94794	-0.88896
H	3.98231	-1.55635	0.00001
H	2.50580	-1.94794	0.88897

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**N-Benzylidene-tert-butylammonium**

C	3.51781	1.03622	0.00000
C	3.98657	-0.27502	0.00000
C	3.09516	-1.35352	0.00000
C	1.73150	-1.12318	-0.00000
C	1.24813	0.19836	-0.00000
C	2.15054	1.27444	-0.00000
C	-0.15628	0.52961	-0.00001
N	-1.13668	-0.31028	0.00000
C	-2.60816	-0.03072	0.00000
C	-3.17232	-0.68744	1.26230
C	-2.86326	1.47000	-0.00003
C	-3.17232	-0.68751	-1.26227
H	4.21393	1.86694	0.00001
H	5.05485	-0.46481	0.00001
H	3.47274	-2.36958	-0.00000
H	1.05750	-1.97547	-0.00001
H	1.77489	2.29382	-0.00000
H	-0.42687	1.58286	-0.00002

H	-0.90883	-1.30335	0.00002
H	-2.74885	-0.23869	2.16412
H	-4.25563	-0.54961	1.28231
H	-2.97424	-1.76365	1.27465
H	-2.46244	1.95477	-0.89529
H	-3.94326	1.62864	-0.00004
H	-2.46243	1.95481	0.89520
H	-2.74886	-0.23879	-2.16410
H	-4.25564	-0.54968	-1.28227
H	-2.97424	-1.76371	-1.27456

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**N-tert-butyl-benzylamide**

C	3.58222	0.89612	0.00821
C	3.92261	-0.45685	0.00683
C	2.90994	-1.41413	-0.00239
C	1.56984	-1.02950	-0.00971
C	1.22011	0.32174	-0.00815
C	2.24242	1.27441	0.00009
C	-0.24554	0.72769	-0.01608
N	-1.08577	-0.40123	-0.04237
C	-2.48226	-0.09733	-0.00076
C	-3.21789	-1.43964	-0.12070
C	-2.93896	0.56635	1.32899
C	-2.96968	0.80916	-1.16392
H	4.36312	1.65367	0.01551
H	4.96725	-0.75921	0.01258
H	3.17022	-2.47096	-0.00406
H	0.73513	-1.72466	-0.01629
H	1.97396	2.33062	-0.00028
H	-0.32900	1.44985	-0.88101
H	-0.34680	1.42399	0.86805
H	-2.88721	-2.09543	0.69162
H	-4.31115	-1.33314	-0.07821
H	-2.93722	-1.91636	-1.06583
H	-2.45548	1.54108	1.46354
H	-4.02629	0.72629	1.37745
H	-2.63734	-0.07380	2.16521
H	-2.52380	1.80835	-1.09345
H	-4.06224	0.93248	-1.17811
H	-2.64965	0.36774	-2.11470

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**N-tert-butyl-benzylamine**

C	3.57016	-0.92625	0.17200
C	3.94372	0.41416	0.14708
C	2.97082	1.39648	-0.02461
C	1.63399	1.04172	-0.17507
C	1.25192	-0.30155	-0.15517
C	2.23135	-1.27882	0.02527
C	-0.19597	-0.69474	-0.35614

N	-1.09136	0.27213	0.26327
C	-2.53603	0.07127	0.06320
C	-3.23456	1.08741	0.96828
C	-2.88604	0.37869	-1.39555
C	-3.00602	-1.34583	0.42492
H	4.32013	-1.69834	0.31298
H	4.98611	0.69225	0.26620
H	3.25543	2.44422	-0.04066
H	0.86559	1.79763	-0.30016
H	1.94094	-2.32637	0.05325
H	-0.33279	-1.72759	0.00611
H	-0.40943	-0.71513	-1.43232
H	-0.89706	0.29142	1.26279
H	-2.89082	2.09819	0.73297
H	-4.31941	1.04247	0.83840
H	-3.01327	0.88435	2.02243
H	-2.45528	-0.35561	-2.08234
H	-3.97110	0.35911	-1.53459
H	-2.51216	1.36913	-1.66817
H	-2.57064	-2.09505	-0.24326
H	-4.09476	-1.42398	0.34505
H	-2.72206	-1.59678	1.45310

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**N-Methylbenzylidene-tert-butylamine**

C	-2.96305	-1.55889	0.05974
C	-3.96622	-0.59409	-0.03162
C	-3.61986	0.75011	-0.09775
C	-2.27974	1.12982	-0.06794
C	-1.26639	0.17091	0.02230
C	-1.62835	-1.18071	0.08399
C	0.18921	0.55000	0.04444
N	1.02172	-0.40953	-0.01899
C	2.48657	-0.29233	-0.02706
C	2.99518	-1.73122	-0.19425
C	2.99551	0.52902	-1.22113
C	3.01524	0.24422	1.31132
C	0.47088	2.03710	0.13399
H	-3.22540	-2.61102	0.11236
H	-5.01015	-0.89096	-0.05130
H	-4.39168	1.50948	-0.17382
H	-2.03717	2.18559	-0.12357
H	-0.83542	-1.91696	0.15049
H	2.61756	-2.15430	-1.12902
H	4.08913	-1.76378	-0.20764
H	2.63308	-2.35314	0.62881
H	2.75714	1.59134	-1.14844
H	4.08345	0.43553	-1.29468
H	2.55766	0.14344	-2.14648
H	2.74732	1.28680	1.49160

H	4.10683	0.16915	1.33333	C	-3.21789	-1.43964	-0.12070
H	2.61459	-0.35592	2.13322	C	-2.93896	0.56635	1.32899
H	-0.09270	2.47122	0.96464	C	-2.96968	0.80916	-1.16392
H	1.52179	2.26165	0.28016	H	4.36312	1.65367	0.01551
H	0.13803	2.53496	-0.78294	H	4.96725	-0.75921	0.01258

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**N-Methylbenzylidene-tert-butylammonium**

C	-2.97362	-0.00269	1.05397
C	-3.27595	-0.98370	0.11138
C	-2.42189	-1.21193	-0.96574
C	-1.24566	-0.48147	-1.08832
C	-0.93750	0.49143	-0.13126
C	-1.81577	0.75519	0.92446
C	0.28454	1.30252	-0.28766
N	1.47792	0.80539	-0.24057
C	2.03028	-0.54280	0.16654
C	3.41460	-0.21108	0.73547
C	1.17225	-1.20217	1.24490
C	2.16823	-1.42351	-1.07590
C	0.11784	2.76254	-0.55374
H	-3.64454	0.17937	1.88613
H	-4.18764	-1.56316	0.20923
H	-2.67216	-1.95680	-1.71316
H	-0.59017	-0.63783	-1.93893
H	-1.58099	1.52017	1.65908
H	2.22283	1.46944	-0.44916
H	3.34011	0.44066	1.61041
H	3.90551	-1.13603	1.04258
H	4.05362	0.26457	-0.01675
H	0.22491	-1.58231	0.86326
H	1.73859	-2.04958	1.63868
H	0.97785	-0.51389	2.07233
H	1.19437	-1.74058	-1.45118
H	2.73092	-2.31999	-0.80441
H	2.71365	-0.91147	-1.87326
H	1.06542	3.30061	-0.61268
H	-0.49803	3.19518	0.24114
H	-0.44381	2.88994	-1.48399

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**N-tert-butyl-methylbenzylamide**

C	3.58222	0.89612	0.00821
C	3.92261	-0.45685	0.00683
C	2.90994	-1.41413	-0.00239
C	1.56984	-1.02950	-0.00971
C	1.22011	0.32174	-0.00815
C	2.24242	1.27441	0.00009
C	-0.24554	0.72769	-0.01608
N	-1.08577	-0.40123	-0.04237
C	-2.48226	-0.09733	-0.00076

C	-3.21789	-1.43964	-0.12070
C	-2.93896	0.56635	1.32899
C	-2.96968	0.80916	-1.16392
H	4.36312	1.65367	0.01551
H	4.96725	-0.75921	0.01258
H	3.17022	-2.47096	-0.00406
H	0.73513	-1.72466	-0.01629
H	1.97396	2.33062	-0.00028
H	-0.32900	1.44985	-0.88101
H	-0.34680	1.42399	0.86805
H	-2.88721	-2.09543	0.69162
H	-4.31115	-1.33314	-0.07821
H	-2.93722	-1.91636	-1.06583
H	-2.45548	1.54108	1.46354
H	-4.02629	0.72629	1.37745
H	-2.63734	-0.07380	2.16521
H	-2.52380	1.80835	-1.09345
H	-4.06224	0.93248	-1.17811
H	-2.64965	0.36774	-2.11470

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**N-tert-butyl-methylbenzylamine**

C	-2.79925	-0.74260	1.08829
C	-3.30501	-0.94314	-0.19156
C	-2.63929	-0.39819	-1.28915
C	-1.47348	0.33418	-1.10295
C	-0.94829	0.53261	0.17735
C	-1.62897	-0.00656	1.26778
C	0.34774	1.31096	0.37077
N	1.51961	0.79324	-0.32836
C	2.02790	-0.56040	-0.04295
C	3.41878	-0.61526	-0.68405
C	2.16415	-0.74260	1.46959
C	1.17260	-1.70083	-0.62360
C	0.16188	2.77139	-0.04477
H	-3.31212	-1.16193	1.94837
H	-4.21382	-1.51848	-0.33625
H	-3.03146	-0.54778	-2.29039
H	-0.95308	0.74435	-1.96634
H	-1.23163	0.14485	2.26925
H	0.58009	1.29865	1.44218
H	1.39102	0.89633	-1.33342
H	4.05830	0.16518	-0.26464
H	3.88718	-1.59065	-0.52134
H	3.34794	-0.45355	-1.76578
H	1.18587	-0.81367	1.95587
H	2.70629	-1.66812	1.68352
H	2.71675	0.09463	1.90717
H	0.19512	-1.77116	-0.14168
H	1.68624	-2.65930	-0.49279
H	1.01122	-1.55022	-1.69731

H	1.07816	3.33228	0.15081
H	-0.66962	3.22733	0.49807
H	-0.06234	2.84121	-1.11522

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**N-Benzylidene-phenylamine**

C	3.74781	1.21056	0.43250
C	4.60397	0.17446	0.05519
C	4.08023	-1.03560	-0.38994
C	2.70131	-1.20878	-0.45793
C	1.84037	-0.17571	-0.08161
C	2.37260	1.03901	0.36643
C	0.38580	-0.38299	-0.16252
N	-0.44986	0.52835	0.14262
C	-1.82621	0.23235	0.08414
C	-2.68649	1.21830	-0.41016
C	-4.05155	0.97714	-0.49284
C	-4.57945	-0.23654	-0.05447
C	-3.73045	-1.20741	0.46925
C	-2.35995	-0.97906	0.53928
H	4.15869	2.15278	0.78080
H	5.67917	0.31291	0.10937
H	4.74358	-1.84225	-0.68430
H	2.28586	-2.15093	-0.80694
H	1.68744	1.82912	0.65553
H	0.05921	-1.37283	-0.51551
H	-2.25843	2.16077	-0.73520
H	-4.70963	1.74259	-0.89166
H	-5.64791	-0.41754	-0.10677
H	-4.13639	-2.14548	0.83472
H	-1.70041	-1.72192	0.97783

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**N-Benzylidene-phenylammonium**

C	4.10269	-1.04845	0.39924
C	4.62982	0.17273	-0.01541
C	3.78913	1.21837	-0.41412
C	2.41745	1.04826	-0.39238
C	1.87421	-0.17949	0.03495
C	2.72764	-1.22838	0.42064
C	0.46234	-0.43157	0.10795
N	-0.47644	0.45105	-0.05929
C	-1.88537	0.20253	-0.04605
C	-2.71856	1.21856	0.41594
C	-4.08909	0.99390	0.45560
C	-4.60977	-0.22825	0.03508
C	-3.76264	-1.22771	-0.43998
C	-2.39004	-1.01690	-0.49285
H	4.76087	-1.85487	0.70110
H	5.70531	0.31446	-0.03776
H	4.21297	2.15821	-0.74898

H	1.78163	1.86172	-0.73150
H	2.30593	-2.17612	0.74332
H	0.12305	-1.43987	0.33859
H	-0.20339	1.42167	-0.19838
H	-2.30261	2.16166	0.75883
H	-4.74906	1.77349	0.81862
H	-5.68023	-0.39807	0.06495
H	-4.17133	-2.16823	-0.79168
H	-1.73487	-1.77300	-0.91378

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**N-Benzyl-anilide**

C	-4.20695	-0.93929	-0.00001
C	-4.58386	0.40302	-0.00000
C	-3.59826	1.38704	0.00001
C	-2.24885	1.03888	0.00001
C	-1.86180	-0.30168	0.00000
C	-2.85824	-1.28214	-0.00001
C	-0.39258	-0.68419	0.00000
N	0.45422	0.46028	-0.00000
C	1.76060	0.20434	0.00000
C	2.68324	1.30860	-0.00001
C	4.04977	1.13809	-0.00001
C	4.63236	-0.14153	-0.00001
C	3.76986	-1.23529	0.00001
C	2.38718	-1.08987	0.00001
H	-4.96590	-1.71806	-0.00002
H	-5.63579	0.67671	-0.00000
H	-3.88464	2.43631	0.00002
H	-1.44790	1.77124	0.00002
H	-2.56436	-2.33092	-0.00002
H	-0.23855	-1.35952	0.87464
H	-0.23855	-1.35953	-0.87462
H	2.24420	2.30357	-0.00001
H	4.69104	2.01969	-0.00002
H	5.71034	-0.27143	-0.00001
H	4.18656	-2.24334	0.00001
H	1.76912	-1.98256	0.00002

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**N-Benzyl-aniline**

C	-4.12355	-0.74437	-0.72535
C	-4.57038	0.40685	-0.08491
C	-3.67393	1.17965	0.65095
C	-2.33965	0.80030	0.74782
C	-1.88413	-0.35579	0.10793
C	-2.78566	-1.12028	-0.63100
C	-0.43752	-0.77075	0.23103
N	0.43914	0.35779	-0.01972
C	1.82062	0.18112	-0.03711
C	2.63459	1.19644	-0.56580



C	4.01440	1.06920	-0.56493
C	4.62427	-0.06805	-0.03463
C	3.82317	-1.07545	0.48814
C	2.43456	-0.96442	0.48594
H	-4.81378	-1.34889	-1.30520
H	-5.61168	0.70342	-0.15959
H	-4.01668	2.07933	1.15250
H	-1.63489	1.39857	1.31841
H	-2.43669	-2.01596	-1.13828
H	-0.25064	-1.12976	1.25182
H	-0.23247	-1.61770	-0.44446
H	0.09716	0.97050	-0.74871
H	2.16749	2.08988	-0.97208
H	4.62099	1.86753	-0.98171
H	5.70424	-0.16487	-0.03363
H	4.27749	-1.97119	0.90080
H	1.83469	-1.77203	0.88969

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**N-Methylbenzylidene-phenylamine**

C	4.19182	0.78085	0.13333
C	4.57861	-0.51376	-0.19431
C	3.60734	-1.49437	-0.39673
C	2.26168	-1.18054	-0.27242
C	1.86109	0.11927	0.06169
C	2.84142	1.09556	0.26253
C	0.40506	0.43410	0.18468
C	0.02926	1.81091	0.68246
N	-0.42083	-0.49295	-0.11513
C	-1.81293	-0.30224	-0.08900
C	-2.58772	-1.12400	0.73711
C	-3.97142	-0.99957	0.74661
C	-4.60398	-0.07900	-0.08667
C	-3.83744	0.72109	-0.92950
C	-2.45000	0.61580	-0.93148
H	4.94082	1.55052	0.28921
H	5.63131	-0.75951	-0.29217
H	3.90289	-2.50698	-0.65234
H	1.49339	-1.92940	-0.42846
H	2.56066	2.11264	0.51521
H	0.57813	2.03476	1.60127
H	0.29912	2.57498	-0.05390
H	-1.03918	1.88190	0.88029
H	-2.08470	-1.85036	1.36698
H	-4.56149	-1.63322	1.40141
H	-5.68533	0.00738	-0.08546
H	-4.31959	1.43386	-1.59142
H	-1.84703	1.22949	-1.59451

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**N-Methylbenzylidene-phenylammonium**

C	3.58212	-1.39739	0.69045
C	4.55718	-0.60257	0.08877
C	4.20168	0.58076	-0.55593
C	2.87250	0.97772	-0.60210
C	1.88150	0.17195	-0.02054
C	2.24991	-1.01764	0.63363
C	0.47074	0.55839	-0.08186
C	0.05659	1.98937	-0.05466
N	-0.42274	-0.39306	-0.14216
C	-1.85458	-0.27901	-0.06736
C	-2.61368	-0.89913	-1.05586
C	-3.99986	-0.82444	-0.97949
C	-4.60703	-0.14534	0.07528
C	-3.83237	0.45719	1.06401
C	-2.44485	0.38899	1.00275
H	3.86288	-2.30277	1.21655
H	5.59907	-0.90172	0.13143
H	4.96196	1.19582	-1.02393
H	2.61221	1.89098	-1.12475
H	1.50595	-1.61344	1.15604
H	-0.97557	2.12603	-0.37355
H	0.17617	2.37731	0.96265
H	0.72077	2.57537	-0.69126
H	-0.06390	-1.33792	-0.26682
H	-2.12807	-1.41791	-1.87676
H	-4.60427	-1.29690	-1.74556
H	-5.68870	-0.09248	0.13129
H	-4.30721	0.97047	1.89253
H	-1.83126	0.82547	1.78471

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**N-methylbenzyl-anilide**

C	3.52116	-1.55039	-0.03536
C	4.50940	-0.63789	0.32686
C	4.15864	0.69191	0.55312
C	2.83439	1.09518	0.40994
C	1.83526	0.18803	0.04448
C	2.19582	-1.14297	-0.17229
C	0.39147	0.64584	-0.13543
C	0.33032	1.58433	-1.36483
N	-0.47786	-0.48060	-0.28374
C	-1.77557	-0.27193	-0.06434
C	-2.68145	-1.38044	-0.22121
C	-4.03700	-1.27796	0.00034
C	-4.62986	-0.06743	0.39792
C	-3.78676	1.03004	0.55661
C	-2.41708	0.95377	0.33398
H	3.78551	-2.59116	-0.20798
H	5.54174	-0.95930	0.43765
H	4.91784	1.41317	0.84599
H	2.56240	2.13331	0.59406
H	1.39203	-1.82365	-0.43343

H	0.16058	1.26603	0.75805	C	0.943307	-0.387006	-0.229853
H	-0.69946	1.92005	-1.51593	C	2.182608	-1.219110	0.107948
H	0.98003	2.46340	-1.26557	B	3.587639	-0.516720	0.048638
H	0.63909	1.01792	-2.24878	C	4.920363	-1.312332	0.300859
H	-2.23535	-2.32485	-0.52396	C	3.648323	1.015712	-0.336732
H	-4.66075	-2.16173	-0.13618	C	-7.061810	-0.256292	-0.941749
H	-5.69900	0.00970	0.57003	C	-8.327119	-0.843452	-0.875455
H	-4.20899	1.98829	0.86185	C	-8.504527	-2.221246	-0.864482
H	-1.82299	1.85251	0.47152	C	-7.364187	-3.013478	-0.963619

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**N-methylbenzyl-aniline**

C	3.45429	-1.55931	0.59648	C	-4.315532	2.558425	2.751997
C	4.48886	-0.80135	0.04983	C	-4.745178	1.239763	2.840962
C	4.21860	0.46781	-0.44644	C	-4.761907	0.381294	1.736518
C	2.92255	0.98144	-0.39849	C	4.249923	1.451055	-1.511177
C	1.88150	0.23107	0.14630	C	4.237356	2.777463	-1.913463
C	2.16408	-1.04696	0.64181	C	3.613974	3.721417	-1.105090
C	0.45104	0.74716	0.23897	C	3.013873	3.330507	0.084654
C	0.22790	2.10409	-0.43083	C	3.038374	1.989339	0.442530
N	-0.43642	-0.28687	-0.28177	C	6.189104	-0.710737	0.286817
C	-1.81835	-0.22479	-0.13646	C	7.367413	-1.410951	0.500376
C	-2.62884	-1.00367	-0.97973	C	7.315141	-2.776626	0.743317
C	-4.00639	-1.01978	-0.82559	C	6.087861	-3.424029	0.772250
C	-4.62078	-0.25983	0.16879	C	4.929397	-2.692054	0.557223
C	-3.82497	0.51710	1.00290	C	-4.937886	-3.452192	-1.171167
C	-2.44082	0.54471	0.85765	C	-7.005793	1.253785	-0.980438
H	3.65427	-2.55191	0.98792	C	-9.874533	-2.837319	-0.753587
H	5.49749	-1.20013	0.01079	C	-5.289175	-1.016091	1.971463
H	5.01604	1.06549	-0.87682	C	-4.284943	3.456653	3.961100
H	2.73488	1.97463	-0.79256	C	-3.417024	2.799875	-0.926654
H	1.35166	-1.63670	1.05647	F	2.465221	1.641911	1.603153
H	0.22381	0.84730	1.30891	F	2.429960	4.235950	0.864132
H	-0.82757	2.37859	-0.36649	F	3.597982	4.997692	-1.468680
H	0.81656	2.89069	0.04928	F	4.815182	3.155343	-3.049851
H	0.50329	2.05812	-1.48923	F	4.873357	0.560987	-2.292784
H	-0.13159	-0.65923	-1.17229	F	6.331479	0.596174	0.075355
H	-2.15931	-1.60413	-1.75486	F	8.540554	-0.787643	0.478408
H	-4.60685	-1.63286	-1.49085	F	8.430449	-3.457503	0.949576
H	-5.69841	-0.27238	0.28741	F	6.032223	-4.730760	1.008008
H	-4.28256	1.11966	1.78184	F	3.792665	-3.386507	0.607444
H	-1.84875	1.16472	1.52167	H	-2.733053	-2.018786	-1.393112

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**S1**

C	-2.848095	-1.247330	-0.628277	H	-2.973106	-1.743564	0.339424
P	-4.298149	-0.149357	-1.077559	H	-1.678529	0.406304	0.141841
C	-1.573053	-0.397190	-0.598191	H	-1.433518	0.086345	-1.574212
C	-5.907169	-1.073440	-0.974107	H	-0.220613	-2.032627	-1.001297
C	-4.332253	0.864704	0.483239	H	-0.472380	-1.714698	0.709030
C	-0.333033	-1.225404	-0.264487	H	0.820931	0.416828	0.503976
				H	1.079380	0.101890	-1.203694
				H	2.242528	-2.077773	-0.579486
				H	2.065009	-1.700380	1.090376

H	-9.199753	-0.194386	-0.842201	C	5.992875	-0.294075	1.236135
H	-7.475033	-4.095314	-0.998039	C	7.276920	-0.803135	1.379612
H	-3.548122	4.050252	1.413983	C	7.546489	-2.091872	0.942434
H	-5.081787	0.857556	3.802540	C	6.527326	-2.836919	0.372262
H	-5.327580	-4.467811	-1.263935	C	5.257949	-2.281053	0.247249
H	-4.342445	-3.246663	-2.065037	C	-5.226478	-3.252927	-1.121230
H	-4.263691	-3.435983	-0.310918	C	-6.540882	1.732532	-1.044903
H	-6.252124	1.610655	-1.689848	C	-9.692725	-1.747997	-2.783597
H	-7.974315	1.653443	-1.288789	C	-5.467690	-1.735439	2.154269
H	-6.757756	1.678785	-0.003060	C	-4.678084	2.040106	5.356689
H	-10.646683	-2.151373	-1.109805	C	-3.318875	2.671553	0.585764
H	-9.941778	-3.760463	-1.334834	F	2.459209	2.498533	1.009560
H	-10.107888	-3.086666	0.286905	F	2.545874	4.492791	-0.755778
H	-6.344518	-1.090633	1.688539	F	3.632773	4.111034	-3.222689
H	-4.758579	-1.773329	1.392824	F	4.632956	1.666256	-3.894310
H	-5.202873	-1.272115	3.030072	F	4.549311	-0.354379	-2.139784
H	-4.664230	4.453575	3.721177	F	5.800629	0.961184	1.672388
H	-4.887991	3.047404	4.774585	F	8.254358	-0.072396	1.930001
H	-3.261549	3.576838	4.331053	F	8.773541	-2.608107	1.070499
H	-2.542550	2.273327	-1.319439	F	6.777208	-4.081201	-0.056497
H	-4.188645	2.742110	-1.699332	F	4.335828	-3.075606	-0.326866
H	-3.146384	3.848724	-0.787066	H	-2.813399	-1.698929	-1.465126
				H	-2.964601	-2.140203	0.244742
81				H	-3.935770	0.885552	-1.111583
<b>S1H<sub>2</sub></b>				H	-1.682672	-0.037032	0.871440
C	-2.852550	-1.301035	-0.446427	H	-1.478110	0.321377	-0.847240
P	-4.302329	-0.205128	-0.319792	H	-0.200622	-1.793591	-1.149979
C	-1.587811	-0.494828	-0.121367	H	-0.425439	-2.186203	0.554243
C	-5.873654	-0.751075	-1.043617	H	0.777485	-0.098513	1.209262
C	-4.440011	0.470715	1.352134	H	0.941270	0.348418	-0.478323
C	-0.323021	-1.351895	-0.152363	H	2.372794	-1.653391	-0.888764
C	0.906709	-0.516494	0.200895	H	2.180702	-2.148417	0.785811
C	2.232498	-1.267187	0.130488	H	3.213939	0.157908	1.698924
B	3.459072	-0.286347	0.594239	H	-8.752925	0.709522	-2.099676
C	4.929805	-1.001615	0.678841	H	-7.640378	-3.416926	-2.164027
C	3.545962	0.975666	-0.456667	H	-3.692918	3.251382	3.141881
C	-6.812370	0.272597	-1.317294	H	-5.502179	-0.393574	4.455117
C	-8.032899	-0.076314	-1.887550	H	-5.751153	-4.194584	-1.286315
C	-8.353606	-1.396772	-2.195727	H	-4.378649	-3.230192	-1.810927
C	-7.408808	-2.383015	-1.922943	H	-4.833934	-3.275437	-0.102956
C	-6.169005	-2.096599	-1.352985	H	-5.761784	2.123630	-1.709813
C	-3.956593	1.773918	1.621060	H	-7.440913	2.320938	-1.225371
C	-4.064202	2.253717	2.924081	H	-6.229879	1.912909	-0.011349
C	-4.616805	1.496026	3.956106	H	-10.055385	-0.954751	-3.440581
C	-5.075694	0.214120	3.661676	H	-9.643719	-2.676953	-3.354666
C	-4.993698	-0.321499	2.379170	H	-10.432493	-1.883433	-1.988171
C	4.069005	0.835161	-1.738829	H	-6.215890	-1.802348	1.359378
C	4.118198	1.862139	-2.674293	H	-4.629747	-2.393006	1.897315
C	3.609397	3.107959	-2.337623	H	-5.914205	-2.134500	3.065772
C	3.061131	3.297410	-1.078592	H	-4.911441	3.107045	5.355260
C	3.039311	2.239922	-0.175076	H	-5.429134	1.519380	5.953413

H -3.709867 1.915111 5.851561  
H -2.422094 2.222702 0.149812  
H -4.008009 2.921207 -0.227837  
H -3.013189 3.609787 1.049034

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**S2**

C 2.905918 -2.051429 -0.397196  
P 3.851300 -1.148780 0.947055  
C 1.413280 -1.871790 -0.106127  
C 5.688679 -1.257460 0.697551  
C 3.477383 0.580688 0.366637  
C 0.502082 -2.379274 -1.222686  
C -0.964121 -2.348111 -0.788266  
C -1.960536 -2.324309 -1.944930  
B -3.854271 -0.888500 -0.742006  
C -5.254549 -0.767210 -0.031465  
C -2.876710 0.358791 -0.757767  
C 6.443490 -0.335572 1.460070  
C 7.837290 -0.334722 1.368936  
C 8.526904 -1.233064 0.564877  
C 7.775360 -2.174310 -0.133800  
C 6.382504 -2.211292 -0.079057  
C 2.551252 1.327458 1.128126  
C 2.221698 2.628103 0.738613  
C 2.797396 3.227364 -0.377494  
C 3.704273 2.478718 -1.122232  
C 4.053002 1.170597 -0.781404  
C -2.474958 0.941826 -1.950523  
C -1.583030 2.005833 -2.003874  
C -1.060065 2.505853 -0.819547  
C -1.420537 1.935594 0.396846  
C -2.323506 0.884852 0.404330  
C -6.169818 -1.831755 0.002110  
C -7.404814 -1.763691 0.630010  
C -7.783031 -0.587016 1.260711  
C -6.924194 0.503074 1.251578  
C -5.696521 0.400060 0.613508  
C 5.699207 -3.304041 -0.866115  
C 5.812183 0.672193 2.392856  
C 10.028399 -1.196517 0.450273  
C 5.070239 0.486844 -1.666766  
C 2.457571 4.638719 -0.780452  
C 1.903810 0.782780 2.382541  
F -2.666339 0.353941 1.583896  
F -0.918519 2.417314 1.532672  
F -0.231926 3.542844 -0.847673  
F -1.241651 2.554219 -3.166233  
F -2.971756 0.482237 -3.107567  
F -5.895732 -2.992923 -0.592302  
F -8.226322 -2.808286 0.626276

F -8.958231 -0.502847 1.862018  
F -7.285557 1.635045 1.846067  
F -4.950339 1.502580 0.640552  
C -3.409738 -2.218316 -1.459681  
H 3.141228 -3.116950 -0.372046  
H 3.135163 -1.672255 -1.398839  
H 1.188001 -0.808190 0.045368  
H 1.165868 -2.381841 0.834303  
H 0.786850 -3.395630 -1.523063  
H 0.639253 -1.743528 -2.107539  
H -1.120207 -1.460156 -0.161786  
H -1.173812 -3.209232 -0.139979  
H -1.840218 -3.235823 -2.542826  
H -1.722374 -1.491092 -2.615491  
H 8.395912 0.390175 1.957337  
H 8.290886 -2.912783 -0.744392  
H 1.498321 3.186611 1.327297  
H 4.160017 2.926769 -2.003450  
H 6.445355 -3.936162 -1.351578  
H 5.094828 -3.947055 -0.220020  
H 5.044754 -2.907378 -1.646808  
H 4.996051 0.226960 2.971349  
H 6.558632 1.047808 3.096031  
H 5.395509 1.526169 1.849969  
H 10.477580 -0.680977 1.302249  
H 10.446206 -2.205485 0.401654  
H 10.338601 -0.669208 -0.457958  
H 6.075202 0.551819 -1.237022  
H 4.861797 -0.574321 -1.810734  
H 5.088895 0.966825 -2.648007  
H 1.792890 5.108727 -0.052907  
H 3.362215 5.247927 -0.864084  
H 1.955629 4.656493 -1.752338  
H 1.332056 -0.129695 2.190903  
H 2.653198 0.526225 3.137162  
H 1.223503 1.523496 2.806778  
H -4.112809 -2.367504 -2.294775  
H -3.630555 -3.060460 -0.791041

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**S2H<sub>2</sub>**

C 3.164698 -2.072170 -0.632249  
P 4.102959 -0.754853 0.217205  
C 1.696829 -1.941063 -0.205828  
C 5.914883 -0.845310 0.230119  
C 3.411202 0.851693 -0.221401  
C 0.720497 -2.811292 -0.997046  
C -0.698339 -2.402899 -0.609672  
C -1.834017 -3.118437 -1.330924  
B -3.605027 -1.146898 -0.954809  
C -5.173547 -0.819774 -0.572272

C	-2.727398	-0.060952	-0.055961	C	-3.198156	-2.721088	-0.750881
C	6.556987	-0.076578	1.229890	H	3.585867	-3.043391	-0.357248
C	7.946911	-0.104053	1.302752	H	3.265093	-1.944779	-1.713172
C	8.717559	-0.862558	0.424751	H	3.752798	-0.942795	1.556490
C	8.059371	-1.615352	-0.545194	H	1.376645	-0.899027	-0.328603
C	6.670981	-1.628637	-0.668353	H	1.605041	-2.179517	0.861478
C	2.484550	1.470998	0.653142	H	0.900959	-3.874749	-0.796697
C	1.896070	2.664769	0.242061	H	0.872101	-2.654140	-2.073146
C	2.183988	3.250870	-0.990268	H	-0.793538	-1.328571	-0.796072
C	3.109731	2.623087	-1.823116	H	-0.828216	-2.534414	0.475474
C	3.725925	1.426953	-1.471096	H	-1.674106	-4.205290	-1.257883
C	-2.172580	1.095879	-0.602474	H	-1.791628	-2.863126	-2.398636
C	-1.462394	2.031889	0.144231	H	-3.442574	-0.847160	-2.121372
C	-1.275101	1.825134	1.500353	H	8.440210	0.485384	2.070989
C	-1.786774	0.681159	2.092367	H	8.645818	-2.217424	-1.233996
C	-2.512522	-0.212379	1.312179	H	1.168925	3.136520	0.894825
C	-6.040803	-1.634062	0.148507	H	3.345594	3.068282	-2.786205
C	-7.358963	-1.291806	0.440231	H	6.868571	-2.876124	-2.396420
C	-7.859770	-0.072065	0.017272	H	5.544565	-3.354303	-1.343194
C	-7.032286	0.786964	-0.691581	H	5.382055	-1.938776	-2.391193
C	-5.726871	0.399782	-0.960588	H	5.243064	0.121680	2.938268
C	6.075372	-2.491662	-1.754245	H	6.498424	1.349402	2.830840
C	5.802138	0.754538	2.239077	H	5.096137	1.444084	1.766108
C	10.219544	-0.847674	0.505032	H	10.558842	-0.706723	1.533257
C	4.666643	0.779685	-2.457184	H	10.646099	-1.776930	0.122496
C	1.479929	4.502708	-1.430598	H	10.623210	-0.024559	-0.093197
C	2.071776	0.909327	1.995585	H	5.633307	0.527626	-2.012102
F	-2.995362	-1.287422	1.954619	H	4.229094	-0.134078	-2.875782
F	-1.576074	0.467310	3.397734	H	4.852777	1.450951	-3.296559
F	-0.588547	2.720937	2.238856	H	1.142099	5.088140	-0.574018
F	-0.953121	3.139151	-0.426502	H	2.127121	5.122428	-2.055142
F	-2.269854	1.364968	-1.909152	H	0.591914	4.236935	-2.011391
F	-5.646327	-2.831420	0.613826	H	1.578991	-0.062999	1.898699
F	-8.145280	-2.125668	1.131526	H	2.921182	0.796673	2.678017
F	-9.121029	0.275757	0.290729	H	1.353652	1.579528	2.468184
F	-7.500891	1.973017	-1.098504	H	-3.965505	-3.320881	-1.257331
F	-4.974752	1.288403	-1.631728	H	-3.229085	-3.039645	0.297880