

*Supplemental Information for*

**Proton affinity and gas phase basicity of diamondoid molecules: diamantane  
to C<sub>131</sub>H<sub>116</sub>**

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**XYZ files [last column corresponds to the Bader charges (e)]**

**References.**

### Discussion S1. Benchmarking: adamantane, dodecahedrane, cyclohexane

**Adamantane:** We have found one structure with stoichiometry  $C_{10}H_{17}^+$  where the added proton is closer to the secondary carbon and farther from the tertiary as well as two isomers with stoichiometry  $C_{10}H_{15}^+$  and a  $H_2$  molecule, been the tertiary isomer the most favorable according to its GPB.

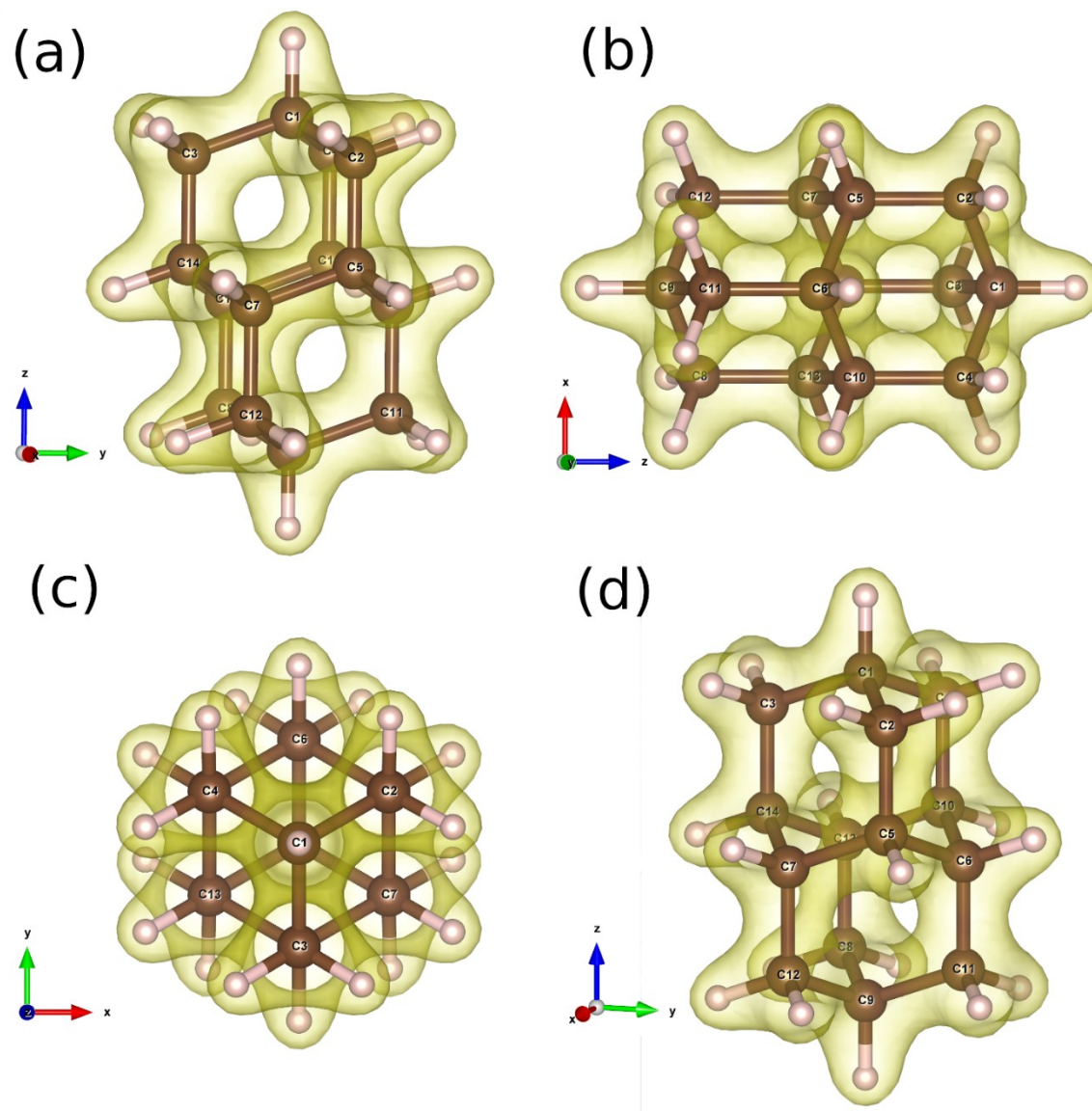
**Table S1.** Adamantane monoprotonated (N=1) molecules. Our calculated values, and experimental values and values from other theoretical studies.

	$C_{10}H_{17}^+$	$C_{10}H_{15}^+ + H_2$ tertiary	$C_{10}H_{15}^+ + H_2$ secondary
GPB <sub>0-1</sub> (eV)	7.3	7.89	7.41
PA <sub>0-1</sub> (eV)	7.54	7.73	7.28
PA <sub>0-1</sub> (eV) experimental		7.43 <sup>[2,3]</sup>	7.01 <sup>[2,4]</sup>
GPB <sub>0-1</sub> (eV) <sup>[5]</sup>		7.54	7.12
PA <sub>0-1</sub> (eV) <sup>[5]</sup>		7.44	6.9
PA <sub>0-1</sub> (eV) <sup>[6]</sup>	7.21	7.62	7.11

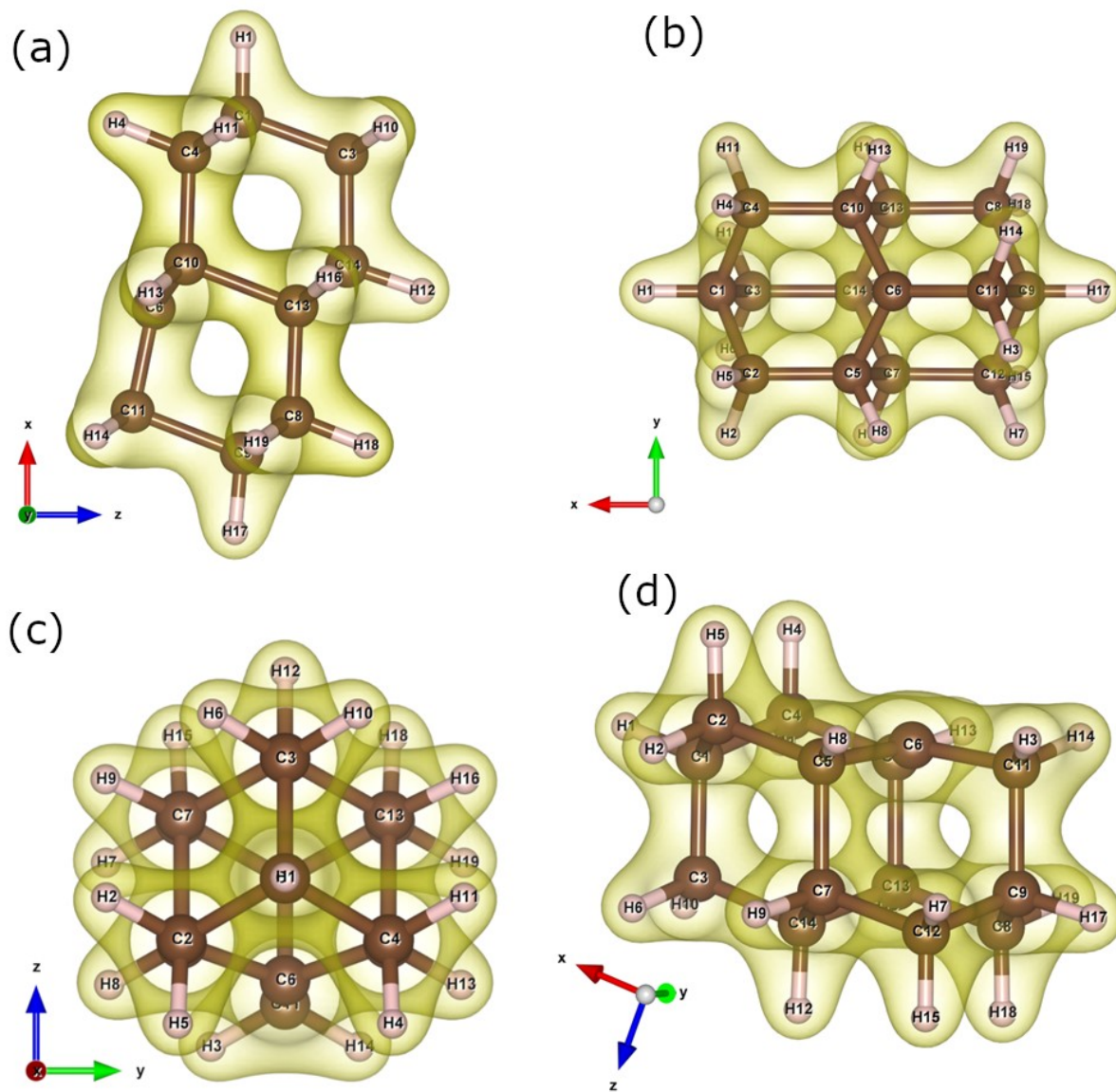
**Dodecahedrane:** The reported experimental values according to ref <sup>[7]</sup> are 8.47 eV for GPB and 8.74 eV for PA. Chen et al. <sup>[8]</sup> reported a theoretical value of 8.03 eV for PA. We calculated values of 8.02 eV for GPB and 8.33 eV for PA.

**Cyclohexane:** The reported experimental values according to ref <sup>[9]</sup> are 6.91 eV for GPB and 7.12 eV for PA. To the best of our knowledge, theoretical values for PA and/or GPB for cyclohexane have not been reported. We calculated values of 6.81 eV for GPB and 7.08 eV for PA .

Diamantane ( $C_{14}H_{20}$ )



**Figure S1.** Diamantane  $C_{14}H_{20}$  electron density viewed (a) to (d) in different directions at an 0.080  $eV/Bohr^3$  isosurface.



**Figure S2.**  $C_{14}H_{19}^+$ . electron density viewed (a) to (d) in different directions at an  $0.080 \text{ eV/Bohr}^3$  (A.U.) isosurface.

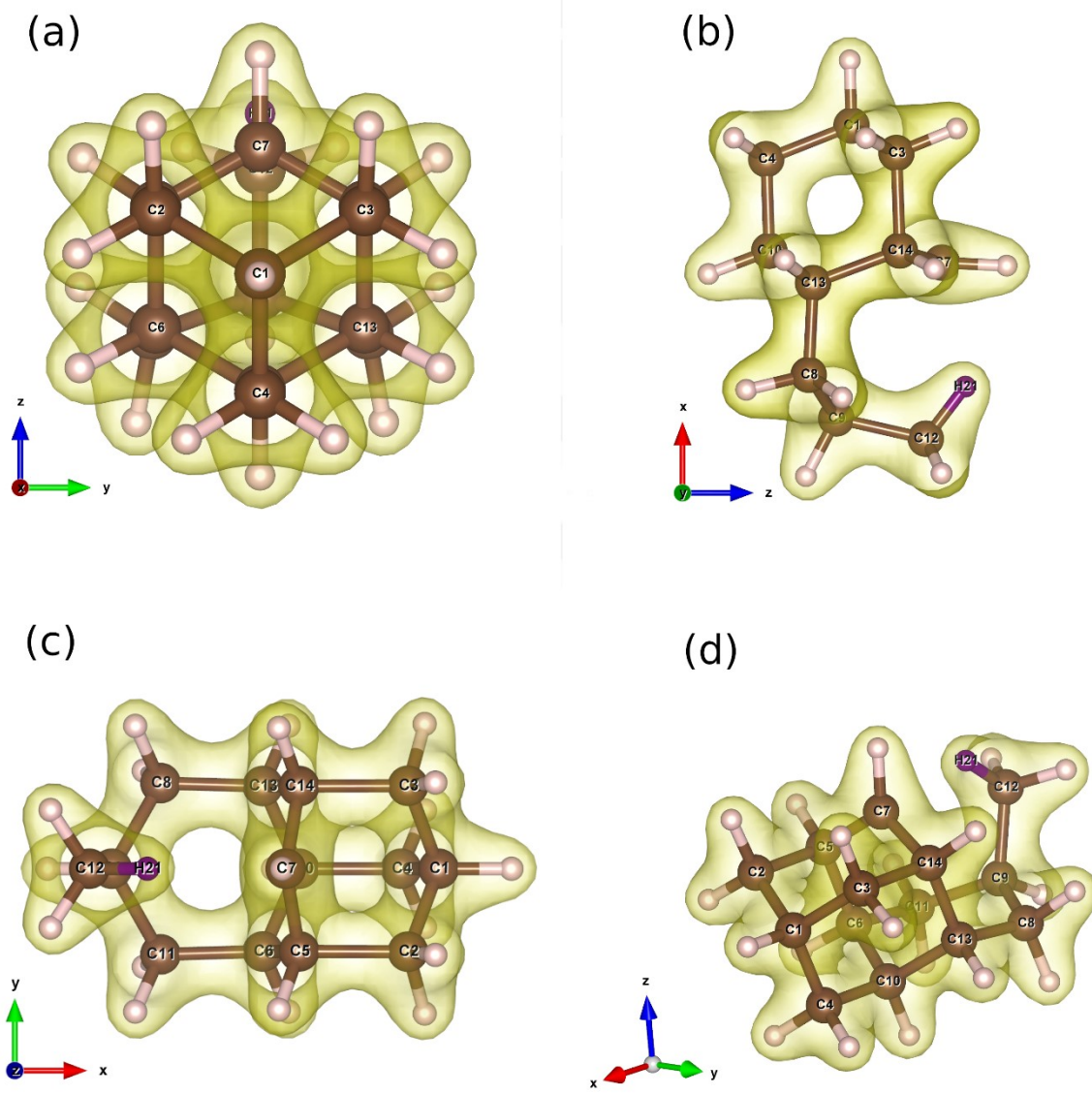
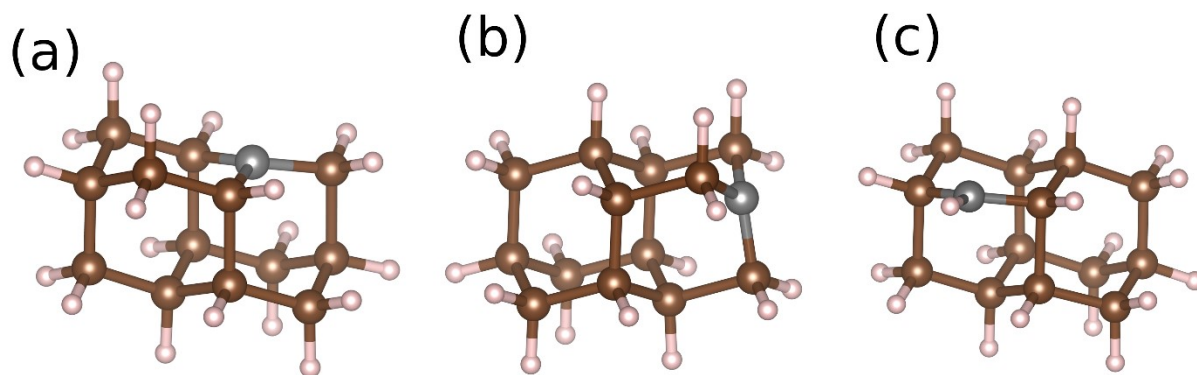


Figure S3.  $C_{14}H_{21}^+$  Electron density viewed (a) to (d) in different directions at an isosurface of 0.080 A.U.

### Discussion S2. Three isomers of $C_{14}H_{19}^+$

We found 3 isomers of  $C_{14}H_{19}^+$  (see **figure S31**): **(a)** corresponds to the structure proposed by Olah and Lukas [1]. The most stable structure according to our calculations is **(a)**. Structure **(c)** is 0.47 eV less stable than **(a)** and structure **(b)** is 0.14 eV less stable than **(a)**.



**Figure S4**  $C_{14}H_{19}^+$  structures. H atoms are pink, C atoms brown, and the gray C atom had its H atom “abstracted” by the proton to form  $H_2(g)$ .

We calculated (see supplementary file  $C_{14}H_{19}^+.xyz$  fourth column for the Bader charge analysis) that the positive charge is delocalized around all the H centers, while the C centers are almost neutral or with a slightly negative charge.

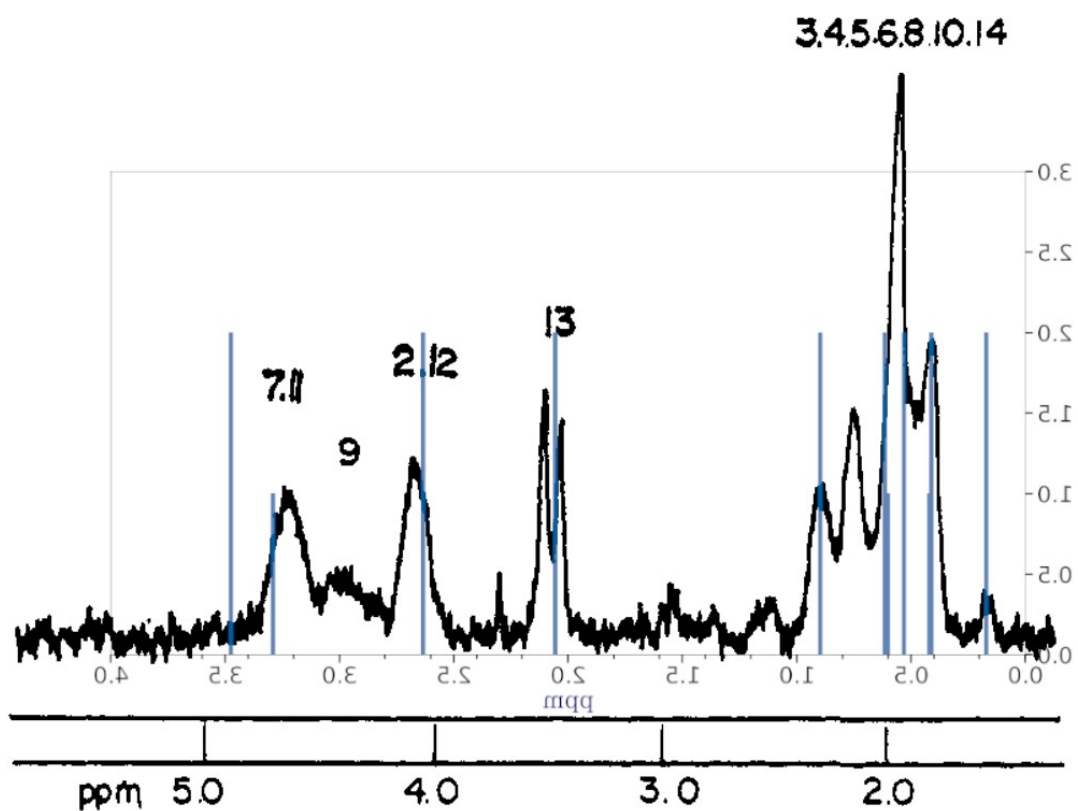
We calculated the NMR spectra for the three structures **(a-c)** using the recommended scaling factors of Tantillo et al [10] at the level of B3LYP/6-311+G(2d,p). The results are shown in **tables S2, S3, and S4** and **figures S5, S6, S7, and S8**. Our calculated NMR spectra for the 3 different  $C_{14}H_{19}^+$  isomers ('structures'), show that **(a)** and **(c)** are reasonably good matches with the experimental NMR spectrum published by Olah and Lukas in 1968 [1]. Their published spectrum is a solution phase NMR spectrum and counteranions and/or solvent molecules might play some role in both chemical shifts and peak intensities; in this regard we suggest it is perhaps interesting that the calculated spectra of **(a)** and **(c)** agree as well as they do. Given that the calculated *GPB* values are reasonably close, we suggest the *possibility* that the "hydride abstraction reaction" as proposed by Olah and Lukas, could have happened at several different locations on the diamondane molecule in the magic acid solution and under the conditions used. Or perhaps on the time scale relevant to the NMR spectrum acquired and published by Olah and Lukas [1] there is no interconversion between some or all 3 of the ‘inequivalent isomers’ we have calculated, if indeed interconversion is happening,.

We note that Olah and Lukas referred to the cation  $C_{14}H_{19}^+$  as a "carbonium ion" [1] but according to our calculated structures and Bader charges showing extensive charge delocalization, the IUPAC guideline [11] causes us to refer to such products as a "monocation", and more specifically, as  $C_{14}H_{19}^+$ . Indeed, we have referred to all the positively charged ions that are products of calculated protonation reactions as "cations," and indicated whether there is uptake of an additional H atom, or "subtraction" of an H atom to form  $H_2(g)$  as in the case of diamantane:  $C_{14}H_{21}^+$  *or*  $C_{14}H_{19}^+ + H_2(g)$ .

**Table S2. NMR  $C_{14}H_{19}^+$  structure (a)**

	<b>atom</b>	<b>ppm</b>		<b>atom</b>	<b>ppm</b>
	3 H	0.171		1 C	24.638
	7 H	0.171		3 C	32.742
	15 H	0.412		4 C	32.742
	16 H	0.412		12 C	36.088
	8 H	0.421		11 C	36.088
	2 H	0.533		2 C	36.401
	5 H	0.533		5 C	40.771
	1 H	0.601		8 C	64.305
	4 H	0.615		14 C	74.479
	6 H	0.615		10 C	74.479
	11 H	0.899		9 C	91.739
	12 H	0.899		7 C	105.755
	18 H	2.056		6 C	105.755
	19 H	2.056		13 C	307.016
	13 H	2.636			
	14 H	2.636			
	17 H	3.292			
	9 H	3.476			
	10 H	3.476			

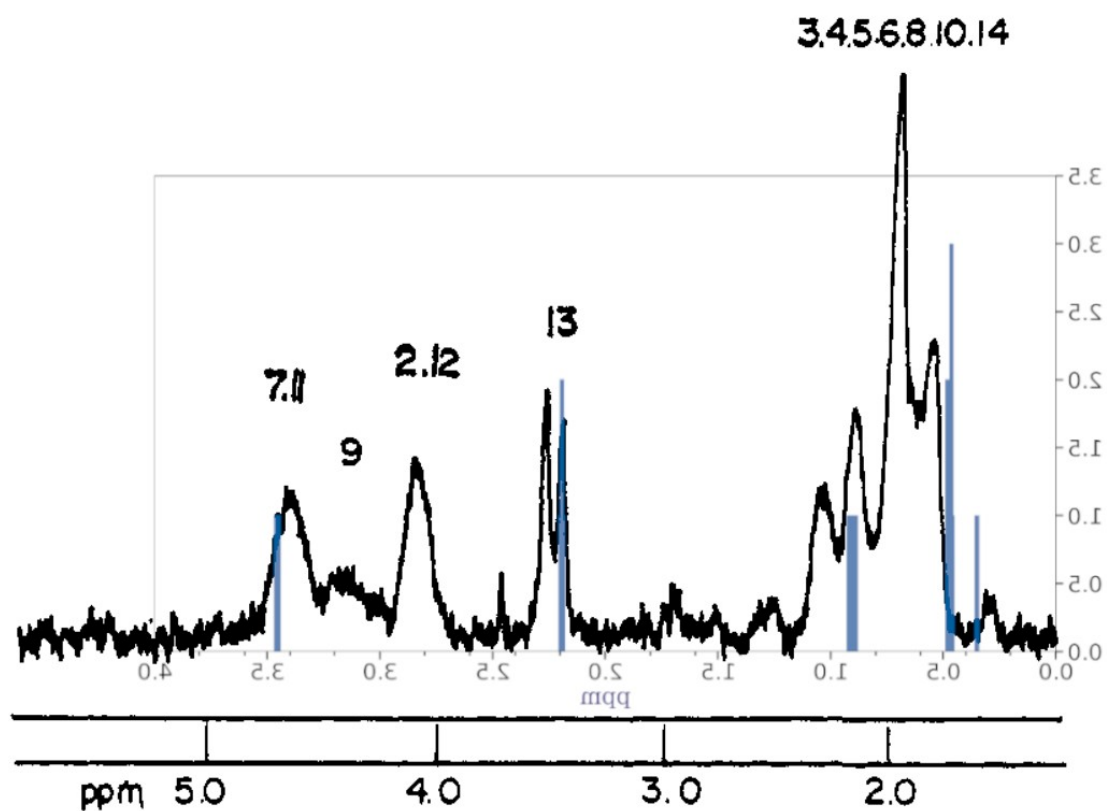




**Figure S5.** Proton NMR spectra for  $C_{14}H_{19}^+$  **structure (a)** shown in blue; in reasonable agreement with the NMR spectrum in Figure 5 of reference [1] that is reproduced here in black color.

**Table S3. NMR C<sub>14</sub>H<sub>19</sub><sup>+</sup> structure (b)**

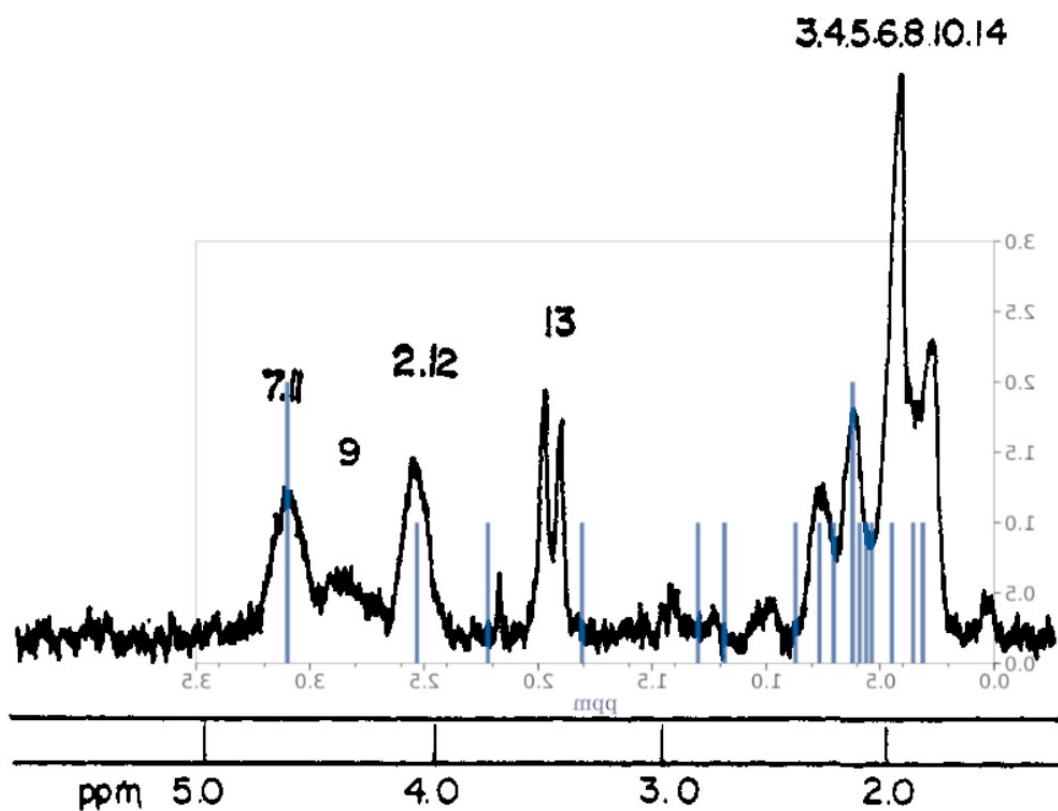
	<b>atom</b>	<b>ppm</b>		<b>atom</b>	<b>ppm</b>
	1 H	0.352		1 C	23.306
	12 H	0.460		4 C	31.790
	11 H	0.464		2 C	32.028
	5 H	0.464		3 C	32.241
	4 H	0.465		14 C	42.679
	6 H	0.481		10 C	42.842
	2 H	0.482		5 C	42.918
	14 H	0.891		12 C	64.474
	8 H	0.912		8 C	64.531
	13 H	0.919		11 C	64.702
	15 H	2.188		7 C	105.514
	3 H	2.193		6 C	105.751
	19 H	2.193		13 C	105.793
	16 H	2.195		9 C	309.230
	7 H	2.197			
	18 H	2.198			
	17 H	3.450			
	10 H	3.454			
	9 H	3.462			



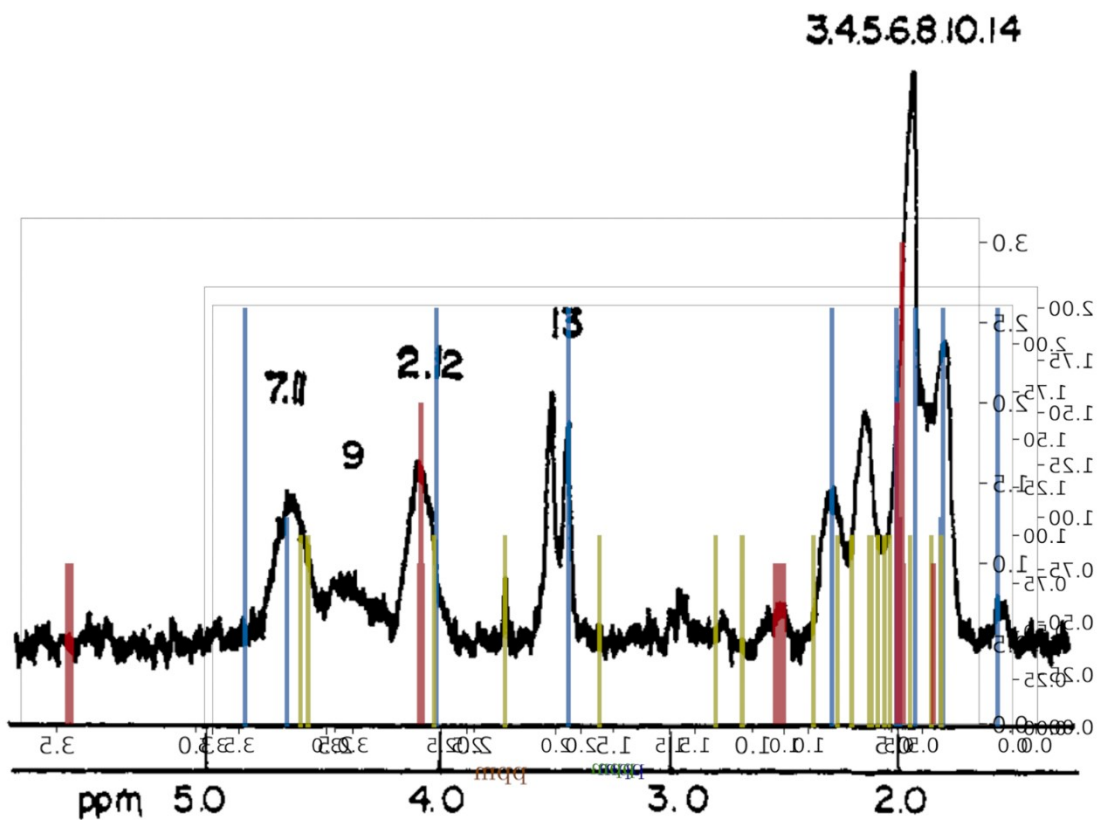
**Figure S6.** Proton NMR spectra for  $C_{14}H_{19}^+$  **structure (b)** in blue. We find this to have a relatively poor agreement with the NMR spectrum in Figure 5 of reference [1] that is reproduced here in black.

**Table S4. NMR  $C_{14}H_{19}^+$  structure (c)**

	<b>atom</b>	<b>ppm</b>		<b>atom</b>	<b>ppm</b>
12	H	0.314	1	C	23.705
10	H	0.357	4	C	32.091
2	H	0.449	2	C	32.953
5	H	0.537	11	C	34.771
4	H	0.562	6	C	37.140
9	H	0.591	5	C	38.626
11	H	0.618	7	C	40.670
8	H	0.628	10	C	40.990
1	H	0.705	3	C	41.114
3	H	0.767	9	C	60.725
15	H	0.873	12	C	72.259
6	H	1.184	13	C	89.492
14	H	1.301	14	C	102.386
16	H	1.808	8	C	282.223
7	H	2.222			
18	H	2.532			
13	H	3.083			
17	H	3.115			
19	H	10.903			



**Figure S7.** Proton NMR spectra for  $C_{14}H_{19}^+$  **structure c**, in relatively good agreement with the NMR spectrum in Figure 5 of reference [1] that is reproduced here.



**Figure S8.** Proton NMR spectra for  $C_{14}H_{19}^+$  **structure (a)** in blue, **structure (b)** in red and **structure (c)** in yellow. The NMR spectrum in Figure 5 of reference [1] is reproduced here. The concept of this figure is to show the possibility that 2 or even all 3 of the  $C_{14}H_{19}^+$  isomers might have been produced by Olah and Lukas, although the authors assigned this NMR spectrum as being due to only structure (a).

XYZ files. The last column corresponds to the Bader charges (e units)

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diamantane C14H20

C	4.709485	4.904885	8.127558	#	0.064
C	5.971390	5.633203	7.605239	#	-0.032
C	4.709275	3.447884	7.605239	#	-0.027
C	3.447790	5.633568	7.605239	#	-0.034
C	5.972570	5.634127	6.059451	#	0.069
C	4.709486	6.363369	5.514507	#	0.010
C	5.972569	4.175642	5.514507	#	0.021
C	3.447580	4.176567	3.968718	#	-0.003
C	4.709485	4.904885	3.446400	#	0.047
C	3.446401	5.634128	6.059451	#	0.057
C	4.709695	6.361886	3.968718	#	-0.002
C	5.971179	4.176202	3.968718	#	-0.002
C	3.446400	4.175642	5.514507	#	0.016
C	4.709485	3.446400	6.059451	#	0.056
H	4.709485	4.904885	9.226847	#	-0.029
H	6.877380	5.134434	7.980271	#	-0.007
H	5.594637	6.897111	3.593686	#	-0.007
H	3.426742	6.667562	7.980271	#	-0.007
H	5.992685	6.666996	7.980890	#	-0.007
H	5.593918	2.912545	7.980890	#	-0.008
H	6.877118	4.674657	3.593068	#	-0.007
H	6.872125	6.153397	5.693079	#	-0.022
H	4.709562	7.402042	5.880879	#	-0.009
H	6.872048	3.656240	5.880879	#	-0.016
H	3.824333	2.912658	7.980271	#	-0.012
H	2.541852	5.135113	7.980890	#	-0.010
H	4.709408	2.407728	5.693079	#	-0.016
H	2.546922	6.153530	5.693079	#	-0.016
H	3.825052	6.897224	3.593068	#	-0.011
H	5.992228	3.142207	3.593686	#	-0.003
H	2.546845	3.656373	5.880879	#	-0.015
H	4.709485	4.904885	2.347111	#	-0.016
H	3.426285	3.142774	3.593068	#	-0.003
H	2.541590	4.675335	3.593686	#	-0.011

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Diamantane C14H19 +

C	8.142756	4.714597	4.973487	#	0.030
C	7.637531	3.456811	4.233491	#	0.047
C	7.610477	4.714597	6.425700	#	-0.031
C	7.637531	5.972383	4.233491	#	0.051
C	6.094857	3.462814	4.184742	#	-0.124
C	5.475199	4.714597	3.738629	#	0.078

C	5.496958	3.458849	5.728947	# -0.007
C	3.959680	5.982794	5.673142	# -0.017
C	3.446400	4.714597	4.965842	# 0.044
C	6.094857	5.966380	4.184742	# -0.125
C	4.039102	4.714597	3.446400	# -0.044
C	3.959680	3.446400	5.673142	# -0.007
C	5.496958	5.970345	5.728947	# -0.013
C	6.062216	4.714597	6.432929	# 0.026
H	9.238915	4.714597	4.985373	# 0.057
H	7.972201	2.545828	4.743466	# 0.044
H	3.687558	3.815990	2.935058	# 0.085
H	8.038694	6.014258	3.213367	# 0.050
H	8.038694	3.414936	3.213367	# 0.051
H	7.980914	3.833344	6.964812	# 0.032
H	3.600633	2.544218	5.163105	# 0.048
H	5.679138	2.583489	3.684135	# 0.088
H	5.892087	2.538070	6.173997	# 0.069
H	7.980914	5.595850	6.964812	# 0.028
H	7.972201	6.883367	4.743466	# 0.040
H	5.711408	4.714597	7.475084	# 0.061
H	5.679138	6.845705	3.684135	# 0.095
H	3.687558	5.613204	2.935058	# 0.079
H	3.557276	3.407933	6.693822	# 0.058
H	5.892087	6.891124	6.173997	# 0.074
H	2.356023	4.714597	4.868890	# 0.035
H	3.557276	6.021262	6.693822	# 0.058
H	3.600633	6.884976	5.163105	# 0.048

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Diamantane C<sub>14</sub>H<sub>21</sub> +

C	8.722116	4.739603	4.882843	# 0.057
C	8.259361	3.487226	5.639741	# -0.006
C	8.259363	5.991991	5.639726	# -0.006
C	8.155086	4.739595	3.446400	# 0.008
C	6.616751	3.491676	5.697117	# -0.033
C	6.068573	3.490407	4.234591	# 0.035
C	6.412660	4.739611	6.406619	# 0.045
C	4.522872	6.032804	4.161005	# 0.012
C	3.787983	4.739605	4.626101	# 0.052
C	6.613090	4.739597	3.497028	# 0.027
C	4.522869	3.446401	4.161014	# 0.010
C	3.446400	4.739611	6.133270	# -0.040
C	6.068576	5.988795	4.234579	# 0.034
C	6.616757	5.987539	5.697105	# -0.032
H	9.821998	4.739601	4.852257	# 0.050
H	8.672405	3.438507	6.652944	# 0.045



H	4.140883	2.583062	4.722418	# 0.020
H	8.515259	3.858131	2.901032	# 0.024
H	8.510939	2.553626	5.124753	# 0.074
H	8.672410	6.040719	6.652928	# 0.046
H	2.862405	3.851320	6.399674	# 0.043
H	6.310121	2.613466	6.272213	# 0.072
H	6.457210	2.581470	3.755833	# 0.022
H	6.361050	4.739616	7.497172	# 0.119
H	8.510943	6.925582	5.124726	# 0.073
H	8.515261	5.621053	2.901022	# 0.024
H	6.310127	6.865755	6.272193	# 0.072
H	6.222082	4.739592	2.471050	# 0.031
H	4.269273	3.258617	3.108999	# 0.026
H	2.862416	5.627909	6.399670	# 0.044
H	6.457214	6.897727	3.755813	# 0.022
H	2.815881	4.739604	4.115282	# 0.026
H	4.140888	6.896146	4.722401	# 0.018
H	4.269276	6.220578	3.108988	# 0.025
H	4.323973	4.739606	6.801900	# -0.042

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Diamantane C<sub>14</sub>H<sub>22</sub> 2+

C	7.105021	7.954766	4.744715	# 0.034
C	6.440365	7.631758	6.043030	# -0.025
C	6.440365	7.631758	3.446400	# -0.028
C	8.559055	5.897762	4.744715	# -0.017
C	5.565089	6.347895	6.003155	# 0.025
C	6.440365	5.053270	6.003155	# 0.041
C	4.648195	6.442955	4.744715	# 0.036
C	5.565089	3.769406	3.446400	# -0.015
C	4.900434	3.446400	4.744715	# 0.026
C	7.357259	4.958210	4.744715	# 0.025
C	5.565089	3.769406	6.043030	# -0.017
C	3.446400	5.503403	4.744715	# -0.021
C	6.440365	5.053270	3.486275	# 0.038
C	5.565089	6.347895	3.486275	# 0.025
H	7.821475	8.784350	4.744715	# 0.160
H	5.794129	8.511374	6.243486	# 0.118
H	4.846567	3.767160	6.871505	# 0.100
H	9.174066	5.825256	5.648027	# 0.111
H	7.158886	7.634004	6.871505	# 0.095
H	5.794129	8.511374	3.245944	# 0.116
H	2.831388	5.575911	5.648027	# 0.113
H	4.951912	6.345956	6.912986	# 0.050
H	7.053542	5.055209	6.912987	# 0.044
H	4.186523	7.444516	4.744715	# 0.044

H	7.158886	7.634004	2.617925	#	0.096
H	9.174066	5.825256	3.841403	#	0.114
H	4.951912	6.345956	2.576444	#	0.049
H	7.818932	3.956649	4.744715	#	0.050
H	6.211325	2.889790	6.243486	#	0.115
H	2.831388	5.575911	3.841403	#	0.110
H	7.053542	5.055209	2.576443	#	0.047
H	4.183980	2.616815	4.744715	#	0.159
H	4.846567	3.767160	2.617925	#	0.099
H	6.211325	2.889790	3.245944	#	0.116
H	3.735637	4.382416	4.744715	#	-0.027
H	8.269816	7.018749	4.744715	#	-0.032

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Triamantane C<sub>18</sub>H<sub>24</sub>

C	8.535240	5.970504	6.137191	#	0.002
C	3.448126	3.446419	6.137191	#	-0.001
C	7.275936	5.969513	5.241726	#	0.023
C	4.707430	3.447410	5.241726	#	0.026
C	5.991683	5.969077	6.114844	#	0.015
C	5.991683	3.447847	6.114844	#	0.002
C	5.991683	4.708462	7.043570	#	0.037
C	7.268035	4.708460	7.916656	#	-0.006
C	4.715331	4.708463	7.916656	#	-0.013
C	8.536966	4.708457	7.032888	#	0.047
C	3.446400	4.708466	7.032888	#	0.046
C	8.535231	3.446400	6.137192	#	0.000
C	3.448135	5.970523	6.137192	#	0.000
C	7.275930	3.447398	5.241729	#	0.024
C	4.707436	5.969525	5.241729	#	0.026
C	7.255158	4.708451	4.332309	#	0.028
C	4.728208	4.708472	4.332309	#	0.032
C	5.991683	4.708462	3.446400	#	0.002
H	8.551440	6.876248	6.761271	#	-0.008
H	3.431925	2.540675	6.761271	#	-0.007
H	9.440729	5.991800	5.513079	#	-0.010
H	2.542637	3.425124	5.513079	#	-0.007
H	7.274961	6.869476	4.606604	#	-0.019
H	4.708405	2.547447	4.606604	#	-0.017
H	5.991690	6.869857	6.751443	#	-0.026
H	5.991676	2.547066	6.751443	#	-0.019
H	7.263266	5.593190	8.572204	#	-0.006
H	4.720100	3.823733	8.572204	#	-0.015
H	7.263263	3.823731	8.572195	#	-0.015
H	4.720103	5.593192	8.572195	#	-0.005
H	9.431851	4.708453	7.671521	#	-0.012
H	2.551515	4.708471	7.671521	#	-0.012

H	9.440725	3.425104	5.513083	#	-0.008
H	2.542642	5.991819	5.513083	#	-0.008
H	8.551432	2.540663	6.761280	#	-0.008
H	3.431934	6.876260	6.761280	#	-0.008
H	7.274946	2.547434	4.606609	#	-0.017
H	4.708420	6.869490	4.606609	#	-0.019
H	8.153111	4.708451	3.694901	#	-0.013
H	3.830256	4.708472	3.694901	#	-0.015
H	5.991676	3.824135	2.791513	#	-0.008
H	5.991690	5.592789	2.791513	#	-0.013

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Triamantane C16H23 +

C	3.453524	5.224739	8.533951	#	0.020
C	5.981977	5.229164	3.446400	#	0.008
C	3.446400	6.097093	7.261736	#	-0.010
C	6.003109	6.134439	4.701641	#	0.025
C	3.692648	5.383152	5.997928	#	0.006
C	6.027126	5.296543	5.997928	#	-0.007
C	4.682034	4.295434	5.997928	#	-0.003
C	4.714218	3.446400	7.289580	#	0.005
C	4.714218	3.446400	4.706275	#	0.005
C	4.717734	4.339354	8.546534	#	0.053
C	4.717734	4.339354	3.449322	#	0.053
C	5.981977	5.229164	8.549456	#	0.007
C	3.453524	5.224739	3.461905	#	0.020
C	6.003109	6.134439	7.294214	#	0.025
C	3.446400	6.097093	4.734119	#	-0.010
C	4.771546	7.067307	7.256594	#	0.012
C	4.771546	7.067307	4.739262	#	0.013
C	4.744120	7.945946	5.997928	#	0.000
H	2.546211	4.608947	8.568430	#	0.033
H	6.884287	4.604500	3.425838	#	0.025
H	3.427150	5.878296	9.413813	#	0.026
H	6.005159	5.852044	2.543182	#	0.022
H	2.570804	6.751298	7.202638	#	0.053
H	6.909885	6.756300	4.677150	#	0.032
H	6.866020	4.588100	5.997928	#	0.043
H	3.848565	2.770615	7.294785	#	0.026
H	5.608620	2.811414	4.731766	#	0.029
H	5.608620	2.811414	7.264090	#	0.029
H	3.848565	2.770615	4.701070	#	0.025
H	4.712741	3.707214	9.442410	#	0.032
H	4.712741	3.707214	2.553445	#	0.032
H	6.005159	5.852044	9.452673	#	0.023
H	3.427150	5.878296	2.582043	#	0.026

H	6.884287	4.604500	8.570019	# 0.025
H	2.546211	4.608947	3.427426	# 0.033
H	6.909885	6.756300	7.318706	# 0.032
H	2.570804	6.751298	4.793218	# 0.054
H	4.696089	7.668366	8.170377	# 0.051
H	4.696089	7.668366	3.825479	# 0.051
H	5.615552	8.614154	5.997928	# 0.045
H	3.857763	8.592552	5.997928	# 0.038

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Triamantane C<sub>16</sub>H<sub>25</sub> +

C	3.891318	5.697365	3.446400	# -0.004
C	9.058430	5.099933	6.010640	# -0.007
C	5.294887	6.352849	3.493290	# 0.042
C	7.911892	6.127454	5.996350	# 0.007
C	6.462751	5.331959	3.492590	# -0.020
C	6.462751	5.331959	5.987816	# -0.021
C	6.655619	4.586361	4.740203	# 0.039
C	3.813363	3.448133	4.740203	# -0.033
C	7.584869	3.446400	4.740203	# -0.028
C	3.446400	4.949737	4.740203	# 0.069
C	9.001925	4.230040	4.740203	# 0.044
C	3.891318	5.697365	6.034006	# -0.004
C	9.058430	5.099933	3.469766	# -0.008
C	5.294887	6.352849	5.987116	# 0.043
C	7.911892	6.127454	3.484056	# 0.007
C	5.427518	7.260532	4.740203	# 0.040
C	7.945274	7.027675	4.740203	# 0.028
C	6.765841	8.022703	4.740203	# -0.003
H	3.820526	5.017148	2.586553	# 0.014
H	9.005383	4.474278	6.910108	# 0.034
H	3.177825	6.508934	3.249541	# 0.018
H	10.019694	5.628270	6.053749	# 0.051
H	5.408025	6.962967	2.586258	# 0.016
H	7.896473	6.725710	6.915061	# 0.053
H	6.452601	4.683604	2.610580	# 0.051
H	6.452601	4.683603	6.869826	# 0.052
H	3.402444	2.951038	3.853722	# 0.032
H	7.522505	2.827135	5.637827	# 0.066
H	3.402442	2.951037	5.626683	# 0.032
H	7.522505	2.827135	3.842578	# 0.066
H	2.347908	4.972323	4.740203	# 0.008
H	9.783528	3.463311	4.740203	# 0.057
H	3.177824	6.508934	6.230865	# 0.018
H	10.019694	5.628270	3.426657	# 0.051
H	3.820526	5.017148	6.893853	# 0.014

H	9.005383	4.474279	2.570298	#	0.034
H	5.408025	6.962966	6.894147	#	0.016
H	7.896473	6.725710	2.565345	#	0.053
H	4.601689	7.983738	4.740203	#	0.020
H	8.891071	7.588336	4.740203	#	0.037
H	6.829706	8.673996	5.621768	#	0.027
H	6.829706	8.673996	3.858638	#	0.026
H	4.893997	3.250957	4.740203	#	-0.033

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Triamantane C<sub>16</sub>H<sub>26</sub> +2

C	8.690180	4.818025	6.168753	#	-0.011
C	3.446400	5.843572	3.446400	#	-0.012
C	7.424393	5.515772	6.616445	#	0.009
C	4.748201	6.471868	3.915717	#	0.029
C	6.097910	4.904857	6.180841	#	0.007
C	6.021074	5.598000	3.713291	#	0.009
C	6.097901	4.383665	4.703557	#	0.056
C	7.387440	3.577741	4.407486	#	-0.003
C	4.865203	3.446400	4.550697	#	-0.014
C	8.633971	4.451404	4.663564	#	0.054
C	3.578976	3.999982	5.082965	#	0.017
C	8.605684	5.698105	3.745637	#	-0.002
C	3.591645	4.861012	6.310969	#	-0.010
C	7.283877	6.512065	3.853815	#	0.028
C	4.832352	5.791438	6.406723	#	0.033
C	7.227708	7.391710	5.096929	#	0.003
C	4.736577	6.974526	5.390166	#	0.038
C	5.905889	7.978374	5.542346	#	-0.002
H	8.779417	3.901477	6.776896	#	0.082
H	3.475197	5.435752	2.430623	#	0.115
H	9.572525	5.421148	6.411808	#	0.077
H	2.559829	6.464946	3.611377	#	0.116
H	7.426394	5.900547	7.645008	#	0.114
H	4.849974	7.356429	3.263270	#	0.052
H	6.012090	4.025229	6.846541	#	0.044
H	6.029603	5.194742	2.691185	#	0.038
H	7.421316	2.679137	5.039587	#	0.029
H	4.749281	3.084365	3.521709	#	0.082
H	7.374266	3.229013	3.366575	#	0.036
H	5.037595	2.528364	5.148520	#	0.095
H	9.535217	3.876271	4.425256	#	0.061
H	2.678922	3.395851	4.917525	#	0.160
H	9.466784	6.347244	3.949998	#	0.040
H	2.649067	5.408857	6.424377	#	0.092
H	8.713684	5.367239	2.706144	#	0.051

H	3.599480	4.142987	7.154373	#	0.106
H	7.266533	7.233766	3.017393	#	0.067
H	4.846334	6.211355	7.420959	#	0.047
H	8.098536	8.047865	5.223328	#	0.127
H	3.805826	7.519557	5.594229	#	0.039
H	5.720608	8.856599	4.901106	#	0.088
H	5.977504	8.375650	6.561885	#	0.074
H	7.533213	6.637372	6.073609	#	-0.034
H	3.151505	4.885089	4.063282	#	-0.029

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Triamantane C<sub>16</sub>H<sub>26</sub> +3

C	8.763284	4.993583	6.225890	#	-0.008
C	3.468827	6.118845	3.446400	#	-0.005
C	7.447388	5.672966	6.615902	#	0.009
C	4.808490	6.674086	3.908675	#	0.023
C	6.103912	5.051245	6.184180	#	0.015
C	6.053208	5.741510	3.718091	#	0.019
C	6.016716	4.518431	4.709130	#	0.062
C	7.060820	3.446400	4.358035	#	-0.044
C	4.670023	3.704157	4.573329	#	-0.033
C	9.032323	4.865414	4.753374	#	0.029
C	3.446400	4.361198	5.141163	#	0.022
C	8.705803	5.929945	3.747087	#	-0.006
C	3.574908	5.192265	6.378514	#	-0.007
C	7.334612	6.656180	3.878225	#	0.011
C	4.884290	6.023010	6.417124	#	0.036
C	7.276126	7.598287	5.061829	#	0.006
C	4.810470	7.194793	5.379856	#	0.023
C	5.986999	8.187181	5.519702	#	-0.011
H	8.847346	4.017840	6.726269	#	0.137
H	3.473558	5.613302	2.475516	#	0.128
H	9.621657	5.564232	6.631921	#	0.150
H	2.645265	6.838370	3.522224	#	0.152
H	7.435636	5.922530	7.685948	#	0.139
H	4.952054	7.542376	3.243411	#	0.064
H	5.974370	4.193800	6.866331	#	0.058
H	6.064470	5.358423	2.688851	#	0.056
H	7.126749	2.624005	5.078914	#	0.129
H	4.499733	3.381674	3.539295	#	0.100
H	6.985519	3.069441	3.330551	#	0.142
H	4.757910	2.761498	5.147147	#	0.113
H	9.906796	4.249848	4.501774	#	0.187
H	2.506073	3.811429	5.004572	#	0.192
H	9.535826	6.660955	3.829908	#	0.134
H	2.685990	5.811974	6.545542	#	0.113

H	8.818486	5.527146	2.733253	#	0.122
H	3.556334	4.463322	7.213381	#	0.123
H	7.306120	7.357474	3.019551	#	0.118
H	4.960306	6.458278	7.421369	#	0.063
H	8.183082	8.186956	5.253837	#	0.165
H	3.889598	7.755800	5.579067	#	0.076
H	5.818770	9.070510	4.867988	#	0.137
H	6.076813	8.616552	6.525527	#	0.114
H	7.539166	6.764678	6.187833	#	-0.025
H	3.044183	5.272398	4.156777	#	-0.019
H	8.170294	3.821019	4.343741	#	-0.016

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Tetramantane "globular" C<sub>22</sub>H<sub>28</sub>

C	6.444273	4.674736	5.672897	#	0.020
C	5.598691	3.456643	6.137483	#	-0.003
C	4.201076	3.464055	5.472204	#	0.044
C	3.446400	4.743757	5.890060	#	0.029
C	4.254686	5.973892	5.433078	#	0.026
C	5.666667	5.974274	6.081386	#	0.014
C	6.458058	7.236481	5.661892	#	0.019
C	6.592875	7.236699	4.115327	#	0.035
C	5.204607	7.230181	3.446400	#	-0.004
C	4.427680	5.974899	3.888046	#	0.032
C	5.178015	4.675479	3.471465	#	0.040
C	4.355429	3.446512	3.931782	#	-0.001
C	6.606886	4.674861	4.103967	#	0.022
C	7.452503	3.456959	3.639276	#	0.013
C	8.850280	3.464316	4.304548	#	0.049
C	8.695854	3.446400	5.844892	#	0.002
C	7.873062	4.675230	6.305450	#	0.033
C	8.623213	5.974770	5.889089	#	0.036
C	7.846313	7.229988	6.330894	#	0.022
C	7.384351	5.974637	3.695639	#	0.024
C	8.796234	5.974139	4.343906	#	0.030
C	9.604704	4.744196	3.886772	#	0.001
H	6.106090	2.512748	5.911174	#	-0.004
H	5.490391	3.499080	7.232011	#	-0.022
H	3.638184	2.577279	5.795659	#	-0.014
H	3.310163	4.765103	6.980810	#	-0.027
H	2.443974	4.759965	5.438694	#	-0.016
H	3.728937	6.893390	5.733177	#	-0.017
H	5.555179	5.971993	7.178226	#	-0.023
H	5.898298	8.130555	5.976437	#	-0.018
H	4.644263	8.134901	3.723373	#	-0.013
H	5.315669	7.241848	2.352448	#	-0.010
H	3.433579	5.973064	3.415579	#	-0.017
H	5.281950	4.657708	2.374818	#	-0.031

H	3.363473	3.475206	3.458230	#	-0.009
H	4.829750	2.512554	3.606102	#	-0.011
H	7.560931	3.499664	2.544767	#	-0.028
H	6.945369	2.512856	3.865348	#	-0.015
H	8.221741	2.512335	6.170493	#	-0.010
H	7.769077	4.657163	7.402092	#	-0.023
H	7.735169	7.241425	7.424839	#	-0.027
H	7.495775	5.972618	2.598793	#	-0.031
H	9.321838	6.893781	4.044015	#	-0.019
H	9.741049	4.765802	2.796007	#	-0.007
H	7.152528	8.130892	3.800986	#	-0.016
H	9.413118	2.577651	3.980765	#	-0.013
H	9.687776	3.475210	6.318498	#	-0.007
H	9.617327	5.972913	6.361527	#	-0.019
H	8.406571	8.134814	6.054066	#	-0.012
H	10.607156	4.760537	4.338165	#	-0.013

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Tetramantane "globular" C<sub>22</sub>H<sub>27</sub> +

C	6.696809	4.716953	4.023267	#	-0.043
C	7.541802	3.482501	3.626323	#	-0.008
C	8.912934	3.498931	4.344026	#	0.060
C	9.675313	4.786329	3.966494	#	-0.006
C	8.858161	6.009849	4.426525	#	0.044
C	7.473326	6.041101	3.725201	#	0.029
C	6.650738	7.275604	4.158872	#	0.040
C	6.474789	7.253525	5.701012	#	0.029
C	7.844709	7.233137	6.406641	#	0.018
C	8.634746	5.987245	5.962523	#	0.025
C	7.885274	4.677602	6.339941	#	0.025
C	8.707589	3.452173	5.875209	#	-0.004
C	6.438594	4.690200	5.756160	#	-0.011
C	5.602074	3.446400	6.123498	#	-0.015
C	4.225614	3.465956	5.434586	#	0.040
C	4.474636	3.490338	3.841413	#	-0.021
C	5.279388	4.721790	3.704314	#	0.030
C	4.523666	5.988602	3.838330	#	-0.007
C	5.287803	7.263262	3.446400	#	0.011
C	5.665007	5.992750	6.103977	#	0.002
C	4.269203	5.976793	5.443503	#	0.022
C	3.446400	4.734898	5.822106	#	0.000
H	7.025130	2.543675	3.841901	#	0.010
H	7.697059	3.517077	2.538803	#	0.034
H	9.483239	2.618320	4.023849	#	0.025
H	9.843561	4.827445	2.881547	#	0.011
H	10.663939	4.793541	4.443038	#	0.022



H	9.393309	6.931408	4.158622	# 0.012
H	7.637373	6.078911	2.637302	# 0.001
H	7.202383	8.181963	3.875973	# 0.020
H	8.408912	8.141850	6.159427	# 0.014
H	7.707681	7.231567	7.496893	# -0.001
H	9.611166	5.975924	6.465202	# 0.015
H	7.766260	4.638976	7.434768	# 0.021
H	9.682170	3.474746	6.379219	# 0.025
H	8.230945	2.511206	6.175176	# 0.005
H	5.462913	3.442850	7.213516	# 0.044
H	6.132174	2.522098	5.882663	# 0.029
H	4.981980	2.575035	3.537333	# 0.057
H	5.419852	7.305134	2.357827	# 0.028
H	5.529761	6.005754	7.196579	# 0.034
H	3.721726	6.900512	5.668011	# 0.044
H	3.253420	4.733248	6.902660	# 0.044
H	5.909799	8.143553	6.011865	# 0.015
H	3.655331	2.557949	5.658040	# 0.052
H	3.507751	3.560343	3.337132	# 0.064
H	3.544645	5.923700	3.352900	# 0.052
H	4.690197	8.139037	3.727530	# 0.028
H	2.467128	4.757077	5.328512	# 0.027

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Tetramantane "globular" C22H29 +

C	6.572287	4.677332	4.263023	# 0.031
C	7.430883	3.469217	3.786810	# 0.010
C	8.844452	3.503251	4.417448	# 0.053
C	9.577421	4.804101	4.015305	# -0.001
C	8.751916	6.024320	4.491307	# 0.028
C	7.359528	5.954291	3.788549	# -0.008
C	6.570474	7.243203	3.843760	# -0.007
C	6.453346	7.243203	6.256859	# 0.000
C	7.908349	7.195614	6.654217	# 0.010
C	8.622394	5.969877	6.044511	# 0.043
C	7.887379	4.661022	6.448697	# 0.034
C	8.710006	3.446401	5.956725	# -0.001
C	6.451533	4.677332	5.837595	# 0.031
C	5.592937	3.469217	6.313807	# 0.008
C	4.179368	3.503250	5.683169	# 0.051
C	4.313814	3.446401	4.143892	# -0.009
C	5.136441	4.661022	3.651921	# 0.034
C	4.401427	5.969877	4.056108	# 0.040
C	5.115471	7.195614	3.446400	# 0.005
C	5.664292	5.954291	6.312069	# 0.006
C	4.271904	6.024321	5.609311	# 0.020

C	3.446400	4.804102	6.085312	#	-0.009
H	6.945221	2.521739	4.036231	#	0.011
H	7.503280	3.502943	2.689469	#	-0.008
H	9.418417	2.637444	4.064462	#	0.019
H	9.713145	4.848095	2.926055	#	0.010
H	10.578730	4.830215	4.463726	#	0.017
H	9.263938	6.954131	4.199328	#	0.002
H	7.546515	5.826570	2.703896	#	0.041
H	7.130125	8.132145	3.522894	#	0.097
H	8.416183	8.135808	6.404835	#	0.041
H	7.928822	7.122267	7.754979	#	0.052
H	9.639886	5.946265	6.456576	#	0.016
H	7.801681	4.621407	7.545930	#	-0.015
H	9.702998	3.468832	6.425313	#	0.014
H	8.242060	2.505221	6.266747	#	0.015
H	5.520540	3.502944	7.411149	#	-0.009
H	6.078600	2.521739	6.064387	#	0.012
H	4.781760	2.505221	3.833871	#	0.015
H	5.222139	4.621407	2.554687	#	-0.013
H	5.094998	7.122267	2.345639	#	0.052
H	5.477305	5.826570	7.396723	#	0.040
H	3.759882	6.954131	5.901290	#	0.004
H	3.310675	4.848096	7.174562	#	0.008
H	5.893695	8.132145	6.577725	#	0.097
H	3.605403	2.637445	6.036156	#	0.020
H	3.320822	3.468832	3.675305	#	0.015
H	3.383934	5.946265	3.644043	#	0.021
H	4.607637	8.135809	3.695783	#	0.042
H	2.445091	4.830215	5.636892	#	0.021
H	6.511909	7.593868	5.050309	#	-0.036

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Tetramantane "globular" C<sub>22</sub>H<sub>30</sub> 2+

C	6.462988	4.676380	5.742301	#	0.038
C	5.639166	3.458986	6.277153	#	-0.020
C	4.170107	3.508129	6.017076	#	0.028
C	3.446400	4.799485	6.041782	#	-0.029
C	4.281993	5.981504	5.494804	#	0.032
C	5.688563	5.986107	6.143804	#	0.022
C	6.488412	7.247474	5.726439	#	0.041
C	6.604593	7.247475	4.181500	#	0.032
C	5.208157	7.249482	3.527812	#	0.013
C	4.437061	5.977198	3.948331	#	0.040
C	5.230958	4.730116	3.446400	#	0.031
C	4.402521	3.446400	3.475650	#	-0.034

C	6.630017	4.676380	4.165637	#	0.031
C	7.453838	3.458986	3.630784	#	-0.014
C	8.922896	3.508129	3.890862	#	0.036
C	8.690488	3.446400	6.432289	#	-0.030
C	7.862048	4.730115	6.461538	#	0.027
C	8.655943	5.977198	5.959606	#	0.022
C	7.884850	7.249481	6.380127	#	0.008
C	7.404442	5.986107	3.764134	#	0.004
C	8.811012	5.981503	4.413133	#	0.041
C	9.646605	4.799485	3.866154	#	-0.026
H	6.038490	2.482004	5.986181	#	0.050
H	5.701209	3.466428	7.386222	#	0.097
H	3.597998	2.596255	6.221191	#	0.157
H	3.238934	4.967808	7.121302	#	0.113
H	2.453223	4.716490	5.584080	#	0.092
H	3.757402	6.902725	5.775466	#	0.048
H	5.580689	5.986826	7.240097	#	-0.008
H	5.934424	8.137820	6.051124	#	0.029
H	4.653672	8.145932	3.830249	#	0.043
H	5.294424	7.287856	2.434090	#	0.019
H	3.444838	5.980923	3.477371	#	0.026
H	5.442035	4.895152	2.375363	#	0.032
H	3.427651	3.565306	2.991766	#	0.108
H	4.903830	2.548433	3.101669	#	0.079
H	7.391796	3.466430	2.521715	#	0.089
H	7.054514	2.482005	3.921756	#	0.050
H	8.189178	2.548433	6.806270	#	0.084
H	7.650971	4.895151	7.532575	#	0.035
H	7.798582	7.287854	7.473849	#	0.030
H	7.512315	5.986827	2.667841	#	0.013
H	9.335604	6.902724	4.132472	#	0.047
H	9.854068	4.967808	2.786633	#	0.112
H	7.158581	8.137822	3.856814	#	0.031
H	9.495007	2.596256	3.686745	#	0.147
H	9.665357	3.565307	6.916171	#	0.098
H	9.648168	5.980922	6.430566	#	0.031
H	8.439335	8.145931	6.077691	#	0.037
H	10.639782	4.716490	4.323855	#	0.095
H	8.989683	3.133190	5.362910	#	-0.033
H	4.103322	3.133189	4.545028	#	-0.034

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Tetramantane "globular" C<sub>22</sub>H<sub>31</sub> 3+

C	5.186859	7.134748	4.704544	#	0.040
C	5.203214	8.131591	3.497416	#	-0.037
C	6.213982	9.239129	3.576765	#	0.024

C	6.570894	9.844873	4.890306	#	-0.014
C	6.570894	8.823153	6.056253	#	0.037
C	5.223470	8.037096	5.998892	#	0.007
C	4.833436	7.331130	7.291471	#	-0.001
C	6.792816	5.960143	7.291471	#	0.003
C	7.913624	6.971729	7.242298	#	-0.005
C	7.811310	7.877582	5.992741	#	0.031
C	7.789562	6.963657	4.726622	#	0.031
C	8.179852	7.701303	3.446400	#	-0.028
C	6.439394	6.156525	4.704544	#	0.043
C	6.423038	5.159682	3.497416	#	-0.023
C	5.412271	4.052144	3.576765	#	0.022
C	3.446400	5.589970	3.446400	#	-0.026
C	3.836691	6.327616	4.726622	#	0.029
C	3.814943	5.413692	5.992741	#	0.027
C	3.712629	6.319544	7.242298	#	0.007
C	6.402782	5.254178	5.998892	#	-0.012
C	5.055358	4.468121	6.056253	#	0.046
C	5.055358	3.446400	4.890306	#	-0.030
H	5.267207	7.639083	2.522408	#	0.070
H	4.231591	8.666308	3.467431	#	0.116
H	6.302979	9.879619	2.690470	#	0.185
H	5.791856	10.618040	5.060256	#	0.127
H	7.501641	10.422020	4.830753	#	0.117
H	6.624904	9.396245	6.990258	#	0.065
H	4.412127	8.781470	5.889468	#	0.054
H	4.838590	7.986670	8.173248	#	0.154
H	7.960510	7.552547	8.171011	#	0.096
H	8.858402	6.401864	7.216199	#	0.110
H	8.711826	8.503295	5.969111	#	0.064
H	8.596970	6.220479	4.849241	#	0.046
H	9.128565	8.241186	3.539607	#	0.140
H	8.167933	7.108806	2.526789	#	0.112
H	7.394662	4.624966	3.467431	#	0.111
H	6.359046	5.652190	2.522408	#	0.068
H	3.458319	6.182467	2.526789	#	0.105
H	3.029283	7.070795	4.849241	#	0.050
H	2.767851	6.889409	7.216199	#	0.104
H	7.214125	4.509803	5.889468	#	0.062
H	5.001348	3.895028	6.990258	#	0.063
H	5.834397	2.673233	5.060256	#	0.136
H	6.787663	5.304604	8.173248	#	0.147
H	5.323273	3.411654	2.690470	#	0.179
H	2.497688	5.050087	3.539607	#	0.137
H	2.914426	4.787979	5.969111	#	0.065
H	3.665743	5.738726	8.171011	#	0.093
H	4.124612	2.869252	4.830753	#	0.124
H	4.171799	4.718120	3.178203	#	-0.021

H	7.454453	8.573153	3.178203	#	-0.024
H	5.813126	6.645637	7.681468	#	-0.025

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Tetramantane "planar" C<sub>22</sub>H<sub>28</sub>

C	5.658696	6.052935	5.964785	#	0.040
C	4.176053	8.141594	5.967910	#	0.002
C	5.631146	7.601279	5.964785	#	-0.008
C	6.387721	8.139654	4.707803	#	0.016
C	5.631146	7.601279	3.450822	#	-0.010
C	4.176053	8.141594	3.447696	#	-0.001
C	3.446400	7.597157	4.707803	#	0.001
C	3.455420	6.054625	4.707803	#	0.013
C	4.902121	5.514559	4.707803	#	0.038
C	4.928473	3.968378	4.707803	#	-0.004
C	6.384299	3.446400	4.707803	#	0.048
C	7.113789	3.967310	5.969207	#	0.006
C	7.113789	5.512620	5.967910	#	0.025
C	7.843442	6.057056	4.707803	#	0.050
C	7.834422	7.599589	4.707803	#	-0.025
C	5.658696	6.052935	3.450822	#	0.035
C	7.113789	5.512620	3.447696	#	0.020
C	7.113789	3.967310	3.446400	#	-0.006
C	4.176053	9.686904	5.969207	#	0.041
C	6.361369	9.685836	4.707803	#	0.029
C	4.176053	9.686904	3.446400	#	0.036
C	4.905542	10.207813	4.707803	#	0.068
H	6.150395	7.966186	6.867189	#	-0.022
H	3.660963	7.772626	2.546813	#	-0.016
H	2.406563	7.959397	4.707803	#	-0.014
H	4.392448	3.592665	3.822702	#	-0.013
H	4.392448	3.592665	5.592905	#	-0.008
H	6.614796	3.593168	6.875361	#	-0.016
H	7.628879	5.881587	6.868793	#	-0.015
H	8.367658	7.979666	5.592954	#	-0.010
H	5.139447	5.688027	2.548418	#	-0.018
H	7.628879	5.881587	2.546813	#	-0.015
H	6.614796	3.593168	2.540246	#	-0.010
H	6.150395	7.966186	2.548418	#	-0.020
H	6.382519	2.347146	4.707803	#	-0.016
H	8.147345	3.591408	5.990829	#	-0.004
H	8.883279	5.694817	4.707803	#	-0.016
H	8.367658	7.979666	3.822654	#	-0.013
H	8.147345	3.591408	3.424777	#	-0.004
H	4.675046	10.061046	6.875361	#	-0.014
H	3.142497	10.062805	5.990829	#	-0.014

H	6.897394	10.061549	3.822702	#	-0.013
H	6.897394	10.061549	5.592905	#	-0.014
H	4.907323	11.307068	4.707803	#	-0.030
H	3.142497	10.062805	3.424777	#	-0.014
H	4.675046	10.061046	2.540246	#	-0.012
H	5.139447	5.688027	6.867189	#	-0.026
H	2.922184	5.674548	3.822654	#	-0.003
H	2.922184	5.674548	5.592954	#	-0.009
H	3.660963	7.772626	6.868793	#	-0.016

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Tetramantane "planar" C<sub>22</sub>H<sub>27</sub> +

C	6.065332	7.434138	5.965288	#	0.012
C	6.633745	4.947990	5.963060	#	0.012
C	5.492660	5.981826	5.968733	#	0.003
C	4.607325	5.806347	4.707591	#	0.025
C	5.492660	5.981826	3.446449	#	0.004
C	6.633745	4.947990	3.452121	#	0.020
C	7.512869	5.146410	4.707591	#	0.030
C	8.098701	6.586933	4.707591	#	0.009
C	6.966371	7.635397	4.707591	#	0.034
C	7.532104	9.078076	4.707591	#	0.000
C	6.379404	10.109509	4.707591	#	0.045
C	5.507466	9.907261	5.968782	#	0.009
C	4.916156	8.477762	5.968561	#	0.029
C	4.039804	8.248375	4.707591	#	0.029
C	3.446400	6.814244	4.707591	#	0.003
C	6.065332	7.434138	3.449894	#	0.015
C	4.916156	8.477762	3.446621	#	0.035
C	5.507466	9.907261	3.446400	#	0.006
C	5.993152	3.446400	5.956140	#	-0.037
C	3.992796	4.269591	4.707591	#	-0.036
C	5.993152	3.446400	3.459042	#	-0.023
C	5.231496	3.506633	4.707591	#	0.059
H	4.874595	5.851352	6.868929	#	0.018
H	7.231357	5.008488	2.535206	#	0.048
H	8.337007	4.421040	4.707591	#	0.017
H	8.169960	9.221513	3.823891	#	0.006
H	8.169960	9.221513	5.591291	#	0.005
H	6.107177	10.062820	6.876061	#	0.010
H	4.302069	8.334657	6.870033	#	0.007
H	2.815190	6.665805	5.593737	#	0.017
H	6.678207	7.570171	2.546449	#	0.004
H	4.302069	8.334657	2.545149	#	0.000
H	6.107177	10.062820	2.539120	#	0.008
H	4.874595	5.851352	2.546253	#	0.014

H	6.799055	11.123299	4.707591	#	0.019
H	4.695529	10.646004	5.992154	#	0.008
H	3.205923	8.963464	4.707591	#	0.021
H	2.815190	6.665805	3.821445	#	0.017
H	4.695529	10.646004	3.423028	#	0.008
H	5.380451	3.329028	6.852135	#	0.077
H	6.810703	2.722916	5.948699	#	0.063
H	3.386977	4.159038	3.806435	#	0.072
H	3.386977	4.159038	5.608747	#	0.067
H	6.810703	2.722916	3.466483	#	0.063
H	5.380451	3.329028	2.563047	#	0.071
H	6.678207	7.570171	6.868733	#	0.011
H	8.738685	6.723859	3.825634	#	0.018
H	8.738685	6.723859	5.589548	#	0.021
H	7.231357	5.008488	6.879976	#	0.054

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Tetramantane "planar" C<sub>22</sub>H<sub>29</sub> +

C	7.631364	5.472700	5.973806	#	0.021
C	5.055987	4.920812	5.992164	#	-0.003
C	6.211094	6.100273	5.980040	#	-0.007
C	5.800832	6.757446	4.734459	#	0.034
C	6.211094	6.100273	3.488878	#	-0.007
C	5.055987	4.920812	3.476754	#	-0.005
C	5.280229	4.051176	4.734459	#	0.028
C	6.690889	3.446400	4.734459	#	0.019
C	7.781534	4.538565	4.734459	#	0.039
C	9.166912	3.849774	4.734459	#	-0.003
C	10.288424	4.901677	4.734459	#	0.053
C	10.144406	5.753673	6.022518	#	0.004
C	8.791989	6.521287	5.996191	#	0.026
C	8.842097	7.438568	4.734459	#	0.039
C	7.937013	8.684596	4.734459	#	-0.019
C	7.631364	5.472700	3.495111	#	0.021
C	8.791989	6.521289	3.472727	#	0.028
C	10.144406	5.753673	3.446400	#	0.004
C	3.654214	5.557462	6.007854	#	-0.002
C	4.561473	7.560317	4.734459	#	-0.016
C	3.654214	5.557462	3.461065	#	-0.005
C	3.446400	6.401943	4.734459	#	0.032
H	6.033879	6.723498	6.862913	#	0.053
H	5.248329	4.350106	2.560399	#	0.054
H	4.536089	3.241670	4.734459	#	0.034
H	9.246093	3.200290	3.851152	#	0.002
H	9.246093	3.200290	5.617766	#	0.004
H	10.201757	5.098239	6.902379	#	0.002

H	8.701826	7.138753	6.901911	#	0.002
H	8.137477	9.296957	5.622144	#	0.033
H	7.715602	4.868200	2.579737	#	0.011
H	8.701826	7.138753	2.567007	#	0.001
H	10.201758	5.098239	2.566539	#	0.004
H	6.033879	6.723498	2.606005	#	0.050
H	11.265937	4.403122	4.734459	#	0.024
H	10.967298	6.474298	6.107971	#	0.014
H	9.855325	7.866439	4.734459	#	0.007
H	8.137478	9.296958	3.846775	#	0.032
H	10.967298	6.474299	3.360948	#	0.013
H	3.517752	6.174378	6.904805	#	0.026
H	2.897281	4.763960	6.055734	#	0.048
H	4.442020	8.172868	3.837789	#	0.066
H	4.442020	8.172868	5.631130	#	0.066
H	2.469321	6.896260	4.734459	#	0.057
H	2.897281	4.763960	3.413184	#	0.048
H	3.517752	6.174379	2.564112	#	0.032
H	7.715602	4.868199	6.889180	#	0.015
H	6.820029	2.803554	3.852769	#	0.014
H	6.820029	2.803553	5.616148	#	0.014
H	5.248329	4.350105	6.908518	#	0.052
H	6.857183	8.493115	4.734457	#	-0.043

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Tetramantane "planar" C<sub>22</sub>H<sub>30</sub> 2+

C	6.163723	5.719150	6.249031	#	0.018
C	8.669066	6.292247	6.361981	#	0.032
C	7.616947	5.178901	6.126564	#	0.012
C	7.833578	4.557420	4.708802	#	0.055
C	7.634735	5.697738	3.655059	#	0.004
C	8.614767	6.891618	3.860283	#	0.034
C	8.451890	7.421637	5.316401	#	0.043
C	7.012887	7.970488	5.465245	#	-0.008
C	5.964881	6.859468	5.195289	#	0.048
C	4.543391	7.483838	5.266480	#	-0.020
C	3.446400	6.602794	4.757296	#	0.020
C	3.749573	4.809017	6.457689	#	-0.013
C	5.183693	4.525270	6.043806	#	0.032
C	5.346570	3.995251	4.587689	#	0.035
C	6.785573	3.446400	4.438845	#	-0.008
C	6.181512	6.237987	3.777526	#	0.021
C	5.129393	5.124641	3.542109	#	0.041
C	3.702781	5.729752	3.570997	#	-0.025
C	10.095678	5.687135	6.333094	#	-0.010
C	9.255069	3.933052	4.637609	#	-0.033



C	10.048886	6.607870	3.446400	#	-0.022
C	10.352059	4.814094	5.146794	#	0.022
H	7.749996	4.391647	6.884971	#	0.009
H	8.298781	7.697788	3.175666	#	0.048
H	9.165545	8.236142	5.498910	#	0.025
H	4.506680	8.370698	4.601276	#	0.094
H	4.311670	7.873679	6.265539	#	0.078
H	3.637254	5.214190	7.468864	#	0.099
H	5.499678	3.719100	6.728424	#	0.041
H	6.934539	2.616486	5.143724	#	0.024
H	6.048462	7.025241	3.019119	#	0.004
H	5.274642	4.692793	2.543607	#	0.033
H	3.571274	6.404220	2.701379	#	0.097
H	7.770314	5.279426	2.646242	#	0.017
H	2.418669	6.953062	4.907136	#	0.141
H	3.050791	3.988150	6.266544	#	0.113
H	4.632915	3.180746	4.405179	#	0.024
H	6.929216	3.034282	3.430844	#	0.029
H	2.921311	4.969467	3.456308	#	0.082
H	10.227183	5.012667	7.202712	#	0.095
H	10.877149	6.447420	6.447785	#	0.085
H	9.486790	3.543211	3.638550	#	0.078
H	9.291780	3.046190	5.302813	#	0.098
H	11.379790	4.463827	4.996954	#	0.143
H	10.747667	7.428740	3.637540	#	0.104
H	10.161203	6.202692	2.435228	#	0.107
H	6.028144	6.137463	7.257848	#	0.015
H	6.863920	8.800402	4.760366	#	0.023
H	6.869243	8.382606	6.473246	#	0.030
H	8.523816	6.724096	7.360483	#	0.039
H	10.533391	5.748935	4.085652	#	-0.034
H	3.265071	5.667959	5.818443	#	-0.034

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Tetramantane "planar" C<sub>22</sub>H<sub>31</sub> 3+

C	9.177765	7.256814	6.201585	#	-0.008
C	6.916556	8.627794	6.276483	#	0.036
C	7.890963	7.876126	5.390068	#	-0.023
C	7.481420	6.675930	4.610034	#	0.035
C	6.902771	5.494445	5.291328	#	-0.022
C	5.815750	5.632476	6.403008	#	0.056
C	6.295347	6.572026	7.514655	#	0.006
C	7.679900	6.292624	8.076728	#	-0.014
C	8.775521	5.992765	7.016015	#	0.028
C	10.066751	5.449419	7.729829	#	-0.002
C	11.146511	5.102027	6.681083	#	0.051

C	11.533786	6.359948	5.881912	#	0.013
C	10.257277	6.912628	5.153179	#	0.021
C	9.710451	5.837262	4.205248	#	0.009
C	8.292850	6.407309	3.446400	#	-0.047
C	8.275382	4.913202	6.023969	#	-0.009
C	9.342836	4.567144	4.976707	#	0.021
C	10.620766	4.020693	5.718199	#	0.003
C	5.799295	9.423528	5.669885	#	-0.041
C	3.544826	3.446400	5.720973	#	-0.095
C	4.384992	5.943602	5.878304	#	-0.063
C	3.446400	4.866042	5.520775	#	0.093
H	8.299229	8.646229	4.717593	#	0.114
H	5.779569	4.651381	6.904358	#	0.071
H	5.546324	6.813463	8.281020	#	0.129
H	9.804198	4.562887	8.320950	#	0.043
H	10.436615	6.204282	8.434939	#	0.050
H	11.942662	7.141248	6.532322	#	0.057
H	10.542289	7.814834	4.597555	#	0.056
H	8.592772	7.281801	2.867039	#	0.117
H	7.948891	4.009695	6.555438	#	0.057
H	8.977511	3.787262	4.297525	#	0.052
H	10.360673	3.098773	6.250499	#	0.056
H	6.597898	4.738770	4.561386	#	0.068
H	12.033530	4.718651	7.201661	#	0.084
H	12.305184	6.131804	5.138850	#	0.061
H	10.376528	5.645802	3.358224	#	0.101
H	7.953726	5.596560	2.800826	#	0.104
H	11.378981	3.754226	4.974555	#	0.065
H	6.264304	10.350951	5.281950	#	0.153
H	5.066813	9.762743	6.408951	#	0.115
H	2.668511	3.117867	6.332884	#	0.219
H	3.281496	2.922929	4.773129	#	0.209
H	2.510839	5.221303	5.071404	#	0.184
H	4.380319	6.666057	5.041927	#	0.126
H	3.793897	6.506584	6.643489	#	0.153
H	9.523645	8.057189	6.868179	#	0.070
H	7.564579	5.411323	8.732324	#	0.097
H	7.989718	7.101555	8.750145	#	0.085
H	7.397236	9.118965	7.130881	#	0.137
H	6.321948	7.696960	6.984663	#	-0.033
H	4.466106	3.052140	6.143250	#	0.108
H	5.305286	8.939912	4.823670	#	0.062

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Pentamantane "globular" C26H32

C	6.043062	3.609011	7.609264	#	-0.003
C	4.197527	5.282589	7.995405	#	-0.008
C	6.520254	4.391542	6.364536	#	0.053
C	4.644256	6.092530	6.756749	#	0.050
C	5.309951	5.134719	5.721366	#	0.004
C	5.765667	5.929460	4.459229	#	0.051
C	6.417694	4.960218	3.446400	#	-0.008
C	4.550185	6.654067	3.837720	#	-0.005
C	7.629684	4.245254	4.085115	#	0.048
C	3.911732	7.618111	4.863517	#	0.044
C	8.673141	5.298019	4.523067	#	0.001
C	4.959743	8.666833	5.299739	#	0.007
C	8.057840	6.273043	5.552652	#	0.048
C	6.181932	7.974541	5.944522	#	0.046
C	7.558909	5.472818	6.794814	#	-0.006
C	5.717898	7.142099	7.179075	#	-0.007
C	6.936081	6.436756	7.850023	#	0.042
C	7.159013	3.446400	5.321536	#	-0.003
C	3.446400	6.814923	6.099034	#	-0.001
C	6.818945	6.981506	4.924377	#	-0.001
C	9.087939	7.334376	6.002750	#	-0.010
C	7.242062	9.008840	6.387995	#	-0.003
C	8.455164	8.299355	7.030272	#	0.054
C	5.407137	4.568863	8.639732	#	0.051
C	6.452467	5.622060	9.071560	#	-0.004
C	7.983539	7.496089	8.263391	#	-0.013
H	2.975223	7.486796	6.832911	#	-0.010
H	5.073462	3.998056	9.518163	#	-0.009
H	6.017457	6.303563	9.818624	#	-0.007
H	7.313565	5.128343	9.547640	#	-0.012
H	7.545207	8.173410	9.012266	#	-0.012
H	8.840800	6.997612	8.741466	#	-0.008
H	5.313280	2.843430	7.303750	#	-0.016
H	3.437114	4.544718	7.696659	#	-0.008
H	4.563105	4.383018	5.410708	#	-0.030
H	5.672677	4.220786	3.114798	#	-0.009
H	3.809714	5.910435	3.505573	#	-0.014
H	6.735369	5.521045	2.553972	#	-0.009
H	4.871580	7.210904	2.944200	#	-0.014
H	8.080929	3.560225	3.353053	#	-0.010
H	9.550286	4.801228	4.965411	#	-0.015
H	9.029929	5.864507	3.649268	#	-0.011
H	5.288280	9.258606	4.431537	#	-0.016
H	8.424485	4.963189	7.253497	#	-0.022
H	5.264349	7.830135	7.914094	#	-0.023
H	6.425793	2.681985	5.021523	#	-0.012

H	2.686762	6.074111	5.805916	#	-0.011
H	8.009349	2.916101	5.777064	#	-0.011
H	7.154021	7.554841	4.042188	#	-0.022
H	9.963723	6.832951	6.442596	#	-0.011
H	6.792139	9.712464	7.105268	#	-0.009
H	9.444522	7.895582	5.125418	#	-0.010
H	7.565739	9.599649	5.517341	#	-0.012
H	9.198946	9.047445	7.340169	#	-0.016
H	6.896395	3.078989	8.059587	#	-0.012
H	3.723075	5.957280	8.724403	#	-0.012
H	3.049953	8.125557	4.406783	#	-0.009
H	4.515524	9.371249	6.019741	#	-0.013

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Pentamantane "globular" C26H31 +

C	3.446400	5.099179	5.517015	#	0.020
C	4.490761	4.079373	3.448582	#	0.000
C	4.852910	5.495168	6.003406	#	0.012
C	5.908793	4.457541	3.935339	#	0.054
C	5.913410	4.485887	5.506295	#	-0.023
C	7.326233	4.864680	6.007210	#	0.014
C	7.300669	4.888310	7.650352	#	-0.031
C	8.373130	3.843701	5.523998	#	0.018
C	6.268962	5.894774	7.883121	#	0.048
C	8.374151	3.843808	3.970369	#	0.032
C	6.625202	7.290859	7.648256	#	-0.019
C	8.737360	5.253450	3.453305	#	-0.012
C	6.635576	7.321991	6.004791	#	0.016
C	7.700030	6.293420	3.936460	#	0.064
C	5.232347	6.908370	5.503778	#	-0.012
C	6.275026	5.892148	3.448335	#	-0.001
C	5.214363	6.926691	3.932846	#	0.056
C	4.882160	5.504709	7.646726	#	-0.018
C	6.974157	3.446400	3.452252	#	-0.004
C	7.670848	6.286795	5.507389	#	-0.026
C	6.997183	8.738075	5.519497	#	0.016
C	8.043721	7.720644	3.451180	#	0.003
C	6.998780	8.735382	3.965950	#	0.026
C	3.450113	5.098453	3.963498	#	0.030
C	3.807040	6.509598	3.446400	#	0.000
C	5.597044	8.344034	3.447559	#	0.001
H	3.179534	4.104254	5.897170	#	0.018
H	4.238202	3.066715	3.793837	#	0.007
H	5.656036	3.478495	5.867467	#	0.007
H	7.040781	3.884892	7.993767	#	0.065

H	8.130428	2.842619	5.904088	#	0.012
H	8.297006	5.172532	7.995046	#	0.069
H	9.367643	4.110784	5.905027	#	0.014
H	5.880280	8.012277	7.990176	#	0.065
H	7.623597	7.568116	7.992738	#	0.065
H	9.740015	5.541772	3.799798	#	0.012
H	4.487456	7.634642	5.863276	#	0.002
H	6.276258	5.891587	2.347691	#	0.003
H	4.629046	4.499441	7.989769	#	0.064
H	6.710310	2.436700	3.797885	#	0.013
H	4.142386	6.231366	7.988719	#	0.065
H	8.671345	6.568341	5.869690	#	0.009
H	2.699851	5.809791	5.895550	#	0.017
H	6.268281	9.466685	5.898276	#	0.017
H	8.071143	7.734433	2.353167	#	0.013
H	7.984980	9.028845	5.900677	#	0.017
H	9.049494	7.997540	3.798053	#	0.007
H	7.256064	9.742733	3.615175	#	0.027
H	4.478616	4.053047	2.350501	#	0.011
H	9.118758	3.117388	3.621260	#	0.025
H	8.768092	5.254312	2.355268	#	0.015
H	6.974688	3.416425	2.354191	#	0.014
H	2.449645	4.816782	3.611773	#	0.030
H	3.782830	6.524483	2.348319	#	0.009
H	3.063844	7.242825	3.790870	#	0.011
H	5.582307	8.368655	2.349485	#	0.011
H	4.845585	9.068738	3.791996	#	0.009

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Pentamantane "globular" C26H33 +

C	3.446400	7.264140	7.805402	#	-0.008
C	5.431372	5.998163	8.778726	#	-0.049
C	4.105231	7.276801	6.410264	#	0.027
C	5.860326	5.998167	7.367998	#	0.039
C	5.761694	7.245948	6.615702	#	-0.041
C	6.462360	7.269128	5.224942	#	0.063
C	6.006697	8.537025	4.459609	#	-0.009
C	8.010117	7.287355	5.356766	#	0.008
C	4.480713	8.539749	4.239512	#	0.059
C	8.689871	5.998171	5.902514	#	0.037
C	4.067227	7.278624	3.446406	#	-0.005
C	8.010119	4.708987	5.356761	#	0.007
C	4.469411	5.998173	4.214190	#	0.051
C	6.462362	4.727216	5.224936	#	0.063

C	3.758385	5.998170	5.606798	#	-0.024
C	5.761695	4.750389	6.615697	#	-0.042
C	4.105232	4.719535	6.410258	#	0.026
C	3.770973	8.549939	5.609176	#	0.014
C	8.908456	5.998166	7.433691	#	-0.020
C	6.010984	5.998173	4.454730	#	-0.013
C	4.067228	4.717726	3.446400	#	-0.006
C	6.006698	3.459322	4.459598	#	-0.010
C	4.480714	3.456597	4.239501	#	0.063
C	3.834285	5.998163	8.588408	#	0.025
C	3.446402	4.732191	7.805397	#	-0.010
C	3.770973	3.446400	5.609165	#	0.017
H	6.010075	8.125499	7.219784	#	0.042
H	6.316292	9.436246	5.012048	#	0.009
H	8.315884	8.151093	5.964444	#	0.007
H	6.524947	8.567565	3.492308	#	0.016
H	8.397642	7.477161	4.345920	#	0.009
H	2.982193	7.278258	3.269135	#	0.011
H	4.550100	7.279954	2.459683	#	0.010
H	8.397644	4.519187	4.345913	#	0.009
H	4.193604	9.438165	3.679421	#	0.024
H	2.671037	5.998170	5.431483	#	0.030
H	6.010076	3.870836	7.219775	#	0.043
H	4.055945	9.439284	6.187274	#	0.015
H	9.478211	6.884219	7.737883	#	0.025
H	2.680667	8.591238	5.474038	#	0.009
H	6.509539	5.998176	3.473378	#	0.009
H	2.982194	4.718093	3.269130	#	0.012
H	6.316294	2.560099	5.012032	#	0.010
H	4.550101	4.716400	2.459677	#	0.010
H	6.524947	3.428787	3.492296	#	0.016
H	4.193606	2.558185	3.679405	#	0.021
H	2.355895	7.300370	7.682180	#	0.038
H	5.728921	5.101185	9.326800	#	0.067
H	9.705277	5.998173	5.481498	#	0.016
H	8.315884	3.845247	5.964434	#	0.008
H	9.478225	5.112119	7.737875	#	0.026
H	3.728405	8.166770	8.363235	#	0.026
H	5.728920	6.895140	9.326804	#	0.067
H	3.394956	5.998162	9.591925	#	0.059
H	3.728405	3.829557	8.363226	#	0.027
H	2.355896	4.695961	7.682173	#	0.038
H	4.055947	2.557052	6.187259	#	0.014
H	2.680668	3.405102	5.474027	#	0.008
H	7.983912	5.998157	8.023892	#	-0.032

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Pentamantane "globular" C26H34 2+

C	3.955897	7.291727	7.821135	# 0.007
C	6.096671	6.017128	8.377851	# -0.020
C	4.309043	7.305961	6.316263	# 0.029
C	6.223781	6.017645	6.917103	# 0.041
C	5.968577	7.260172	6.186326	# -0.021
C	6.461752	7.305276	4.706948	# 0.074
C	5.776918	8.492396	3.965260	# -0.013
C	8.029705	7.348006	4.627058	# -0.026
C	4.222589	8.535076	4.113253	# 0.050
C	8.774438	6.018236	5.027336	# 0.038
C	3.446486	7.350435	3.447279	# -0.017
C	8.029659	4.688747	4.626081	# -0.027
C	3.738172	6.018585	4.119900	# 0.008
C	6.461697	4.731481	4.706028	# 0.073
C	3.721136	6.018062	5.649566	# -0.010
C	5.968568	4.775594	6.185458	# -0.021
C	4.309021	4.729717	6.315418	# 0.027
C	3.846737	8.589748	5.605237	# 0.005
C	9.258103	6.017661	6.496175	# -0.017
C	6.139428	6.018623	3.991687	# 0.011
C	3.446400	4.687217	3.446400	# -0.020
C	5.776814	3.544887	3.963554	# -0.012
C	4.222479	3.502098	4.111571	# 0.049
C	4.481783	6.017101	8.504971	# 0.029
C	3.955913	4.742937	7.820300	# 0.008
C	3.846678	3.446401	5.603518	# 0.004
H	4.361599	8.186638	8.308228	# 0.055
H	6.490057	6.914359	8.859847	# 0.085
H	6.320508	8.144215	6.726743	# 0.071
H	6.176579	9.436660	4.357277	# 0.049
H	8.399690	8.177380	5.243672	# 0.047
H	6.057452	8.460274	2.904400	# 0.041
H	8.284161	7.602798	3.590074	# 0.036
H	3.878104	9.450953	3.620612	# 0.061
H	2.363698	7.536975	3.544869	# 0.087
H	3.648444	7.282779	2.372185	# 0.069
H	8.284085	4.434682	3.588915	# 0.036
H	2.640455	6.017994	5.883316	# 0.076
H	6.320539	3.891196	6.725262	# 0.071
H	4.298491	9.464254	6.088361	# 0.040
H	9.873019	6.901483	6.698275	# 0.048
H	2.759485	8.692341	5.726073	# 0.048
H	6.463715	6.018983	2.942046	# 0.095
H	2.363615	4.500629	3.543919	# 0.087

H	6.176468	2.600352	4.354917	#	0.050
H	3.648332	4.755567	2.371345	#	0.070
H	6.057289	3.577713	2.902701	#	0.040
H	3.877996	2.586565	3.618286	#	0.061
H	2.865409	7.349317	7.933880	#	0.043
H	6.490039	5.119535	8.859190	#	0.086
H	9.694312	6.018459	4.428823	#	0.044
H	8.399582	3.858925	5.242119	#	0.047
H	9.873263	5.133820	6.697460	#	0.049
H	4.258568	6.016740	9.576678	#	0.088
H	4.361622	3.847708	8.306804	#	0.053
H	2.865426	4.685294	7.933029	#	0.043
H	4.298440	2.571576	6.086061	#	0.040
H	2.759430	3.343755	5.724349	#	0.048
H	8.449697	6.017177	7.239452	#	-0.036
H	4.989697	6.018696	3.797449	#	-0.054

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Pentamantane "globular" C26H35 3+

C	3.446400	8.551035	4.454035	#	-0.018
C	5.628867	9.091749	5.641457	#	-0.017
C	4.504519	6.260584	4.624068	#	0.008
C	6.168897	7.678296	5.831985	#	0.016
C	5.990820	6.659653	4.692247	#	-0.011
C	6.808536	5.285652	4.926466	#	0.048
C	6.354465	4.232785	3.869861	#	-0.012
C	8.359957	5.529156	4.941031	#	-0.007
C	4.810992	4.027176	3.789529	#	0.043
C	8.851147	6.365051	6.174585	#	0.036
C	4.097773	3.446400	5.049017	#	-0.024
C	8.215616	5.946177	7.548424	#	-0.008
C	4.166317	4.376540	6.250387	#	0.027
C	6.662413	5.717521	7.469189	#	0.057
C	3.876121	5.886973	5.978250	#	0.002
C	5.879339	7.048665	7.175280	#	-0.013
C	4.284227	6.862412	7.154827	#	0.046
C	4.133615	5.413118	3.446400	#	0.005
C	8.664899	7.837545	5.917286	#	-0.008
C	6.551280	4.749671	6.316868	#	-0.026
C	3.929457	3.900486	7.666838	#	-0.006
C	6.069888	5.043296	8.748496	#	-0.021
C	4.514377	4.889272	8.730941	#	0.062
C	4.062003	9.057266	5.739451	#	0.053
C	3.618799	8.260216	6.988423	#	0.005
C	3.859555	6.261586	8.517157	#	-0.006



H	3.783824	9.029431	3.528469	#	0.135
H	5.942896	9.519506	4.683252	#	0.084
H	6.304415	7.074249	3.728168	#	0.086
H	6.708976	4.531978	2.875496	#	0.072
H	8.677293	6.002295	4.002987	#	0.066
H	6.846560	3.276365	4.087842	#	0.069
H	8.841030	4.543889	4.961173	#	0.077
H	4.601398	3.357035	2.948066	#	0.110
H	3.031140	3.281511	4.817521	#	0.112
H	4.495095	2.459879	5.315085	#	0.105
H	8.679868	5.013259	7.888823	#	0.069
H	2.777189	5.915995	5.881532	#	0.084
H	6.090931	7.756495	7.985507	#	0.069
H	4.533533	5.803533	2.506262	#	0.095
H	8.998687	8.225787	4.949584	#	0.143
H	3.051677	5.284467	3.343548	#	0.079
H	7.077247	3.802949	6.504348	#	0.119
H	2.836950	3.831183	7.814865	#	0.102
H	6.331591	5.648026	9.626023	#	0.071
H	4.315228	2.881575	7.787981	#	0.093
H	6.550664	4.068219	8.899458	#	0.055
H	4.221496	4.495776	9.710113	#	0.083
H	2.364122	8.386453	4.469104	#	0.125
H	6.009823	9.738963	6.438448	#	0.091
H	9.942587	6.219916	6.255152	#	0.111
H	8.443887	6.695566	8.317236	#	0.065
H	8.858696	8.523008	6.748161	#	0.141
H	3.726492	10.101884	5.846953	#	0.119
H	3.860054	8.848447	7.881758	#	0.067
H	2.526918	8.146567	6.994492	#	0.053
H	4.146690	6.954315	9.316876	#	0.061
H	2.764748	6.182402	8.558240	#	0.059
H	7.441533	7.976752	5.801006	#	-0.040
H	5.467778	4.324307	6.337545	#	-0.043
H	3.860691	7.424715	4.292358	#	-0.024

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Pentamantane "planar" C<sub>26</sub>H<sub>32</sub>

C	5.963612	7.268611	5.240783	#	0.002
C	5.968810	4.706588	5.241820	#	0.022
C	5.965964	5.990698	6.114141	#	0.011
C	4.708043	5.990902	7.041893	#	0.043
C	3.450121	5.990698	6.114141	#	0.015
C	3.447275	4.706588	5.241820	#	0.022
C	4.708043	4.728527	4.332468	#	0.030
C	4.708043	5.991086	3.446400	#	-0.009

C	4.708043	7.268611	4.313427	# 0.038
C	4.708043	8.546136	3.446400	# -0.007
C	4.708043	9.808695	4.332468	# 0.033
C	5.968810	9.830633	5.241820	# 0.021
C	5.965964	8.546523	6.114141	# 0.007
C	4.708043	8.546319	7.041893	# 0.048
C	4.708043	7.268611	7.907531	# -0.009
C	3.452473	7.268611	5.240783	# 0.006
C	3.450121	8.546523	6.114141	# 0.011
C	3.447275	9.830633	5.241820	# 0.020
C	5.969686	3.447492	6.137609	# -0.004
C	4.708043	11.090821	7.033767	# 0.048
C	4.708043	4.715875	7.917293	# -0.001
C	3.446400	3.447492	6.137609	# -0.002
C	5.969686	11.089730	6.137609	# 0.011
C	4.708043	9.821346	7.917293	# -0.003
C	3.446400	11.089730	6.137609	# 0.001
C	4.708043	3.446400	7.033767	# 0.049
H	6.867754	5.994742	6.749329	# -0.017
H	2.547057	4.708230	4.607372	# -0.013
H	4.708043	3.831325	3.693932	# -0.016
H	3.823386	8.545485	2.790748	# -0.015
H	5.592699	8.545485	2.790748	# -0.005
H	6.869029	9.828992	4.607372	# -0.012
H	6.867754	8.542480	6.749329	# -0.017
H	5.593049	7.268611	8.564236	# -0.014
H	2.549861	7.268611	4.606444	# -0.017
H	2.548332	8.542480	6.749329	# -0.020
H	2.547057	9.828992	4.607372	# -0.013
H	2.548332	5.994742	6.749329	# -0.020
H	4.708043	10.705896	3.693932	# -0.019
H	3.823037	7.268611	8.564236	# -0.008
H	6.875741	3.431164	6.761008	# -0.005
H	5.990274	2.541967	5.513603	# -0.010
H	3.823356	4.721142	8.572584	# -0.010
H	5.592730	4.721142	8.572584	# -0.014
H	4.708043	2.552009	7.672845	# -0.010
H	3.425811	2.541967	5.513603	# -0.011
H	2.540344	3.431164	6.761008	# -0.010
H	6.866225	7.268611	4.606444	# -0.014
H	3.823386	5.991736	2.790748	# -0.014
H	5.592699	5.991736	2.790748	# -0.005
H	6.869029	4.708230	4.607372	# -0.012
H	5.990274	11.995255	5.513603	# -0.008
H	6.875741	11.106057	6.761008	# -0.019
H	5.592730	9.816080	8.572584	# -0.013
H	3.823356	9.816080	8.572584	# -0.009
H	2.540344	11.106057	6.761008	# -0.009

H 3.425811 11.995255 5.513603 # -0.010  
H 4.708043 11.985212 7.672845 # -0.009

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Pentamantane "planar" C26H31 +

C 6.126089 6.022192 7.280519 # -0.006  
C 6.159361 5.976645 9.857102 # 0.046  
C 5.282615 6.023603 8.571785 # 0.001  
C 4.298864 4.820682 8.557810 # 0.031  
C 5.264939 3.464686 8.539849 # -0.037  
C 6.121787 3.451016 9.833772 # 0.038  
C 7.042280 4.698768 9.821662 # 0.035  
C 7.930153 4.680810 8.567841 # 0.007  
C 7.079921 4.677434 7.280519 # 0.009  
C 7.930153 4.680810 5.993198 # 0.005  
C 7.042280 4.698768 4.739376 # 0.034  
C 6.159361 5.976645 4.703936 # 0.038  
C 5.282615 6.023603 5.989253 # 0.004  
C 4.298864 4.820682 6.003228 # 0.031  
C 3.446400 4.808745 7.280519 # -0.016  
C 5.973945 3.700196 7.280519 # 0.019  
C 5.264939 3.464686 6.021188 # -0.034  
C 6.121787 3.451016 4.727266 # 0.042  
C 5.260310 5.974813 11.114637 # 0.001  
C 4.344722 4.726926 3.458332 # 0.056  
C 3.450117 4.760480 9.844463 # -0.002  
C 5.208872 3.446400 11.078068 # 0.001  
C 5.260310 5.974813 3.446400 # 0.001  
C 3.450117 4.760480 4.716574 # -0.006  
C 5.208872 3.446400 3.482970 # -0.010  
C 4.344722 4.726926 11.102707 # 0.055  
H 4.686119 6.948344 8.591408 # 0.027  
H 6.737268 2.540533 9.833308 # 0.014  
H 7.678860 4.679666 10.716280 # 0.020  
H 8.585232 3.799027 5.990452 # 0.025  
H 8.586977 5.560029 6.014592 # 0.020  
H 6.810003 6.862623 4.691194 # 0.002  
H 4.686119 6.948344 5.969630 # 0.029  
H 2.797442 5.695533 7.280519 # 0.036  
H 4.585002 2.607485 6.079682 # 0.045  
H 6.737268 2.540533 4.727730 # 0.014  
H 4.585002 2.607485 8.481357 # 0.045  
H 7.678860 4.679666 3.844757 # 0.020  
H 2.778264 3.936136 7.280519 # 0.022  
H 4.654239 6.890535 11.147161 # 0.012  
H 5.885164 5.974809 12.017032 # 0.019  
H 2.792304 3.881210 9.812990 # 0.015  
H 2.798364 5.645799 9.866237 # 0.024

H	3.709099	4.725430	11.996400	#	0.022
H	5.829947	3.389869	11.980962	#	0.016
H	4.568762	2.553098	11.077085	#	0.015
H	6.842617	6.855500	7.280519	#	0.039
H	8.585232	3.799027	8.570585	#	0.025
H	8.586977	5.560029	8.546446	#	0.021
H	6.810003	6.862623	9.869843	#	0.002
H	5.885164	5.974809	2.544005	#	0.019
H	4.654239	6.890535	3.413878	#	0.013
H	2.798364	5.645799	4.694801	#	0.025
H	2.792304	3.881210	4.748048	#	0.016
H	4.568762	2.553098	3.483952	#	0.014
H	5.829947	3.389869	2.580076	#	0.021
H	3.709099	4.725430	2.564638	#	0.023

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Pentamantane "planar" C<sub>26</sub>H<sub>33</sub> +

C	7.274828	6.232312	3.464938	#	0.019
C	4.709934	6.224297	3.513548	#	0.032
C	5.990891	5.356465	3.465317	#	0.008
C	5.997345	4.310765	4.632213	#	0.048
C	5.957517	5.051412	6.007097	#	0.026
C	4.745096	6.036743	6.037333	#	0.013
C	4.752460	7.038240	4.832524	#	0.028
C	5.954285	8.026097	4.782795	#	-0.006
C	7.274917	7.321223	4.534808	#	-0.014
C	8.595457	8.025947	4.782946	#	-0.007
C	9.797266	7.038256	4.832489	#	0.026
C	9.839738	6.224274	3.513489	#	0.028
C	8.558842	5.356412	3.465245	#	0.010
C	8.552354	4.310811	4.632164	#	0.047
C	7.274839	3.446400	4.544471	#	-0.016
C	7.274907	5.721088	6.354148	#	-0.017
C	8.592142	5.051512	6.007039	#	0.020
C	9.804650	6.036747	6.037313	#	0.013
C	3.446400	5.341213	3.446401	#	-0.001
C	11.101982	4.359612	4.639268	#	0.038
C	4.704644	3.458610	4.544114	#	-0.002
C	3.457026	5.174445	5.957756	#	0.008
C	11.103300	5.341208	3.446400	#	0.000
C	9.845015	3.458612	4.544151	#	-0.002
C	11.092648	5.174428	5.957779	#	0.008
C	3.447703	4.359621	4.639251	#	0.038
H	6.000581	4.787940	2.523908	#	0.015
H	4.753143	6.601341	6.982072	#	0.006
H	3.844162	7.649785	4.915044	#	0.025

H	8.531990	8.645307	5.686356	#	0.041
H	8.745906	8.721183	3.939356	#	0.061
H	9.837621	6.918081	2.658921	#	0.001
H	8.549090	4.787899	2.523820	#	0.014
H	7.274853	2.883704	3.599928	#	0.015
H	7.274868	6.210311	7.339691	#	0.078
H	8.758053	4.291947	6.791346	#	0.028
H	9.796556	6.601416	6.982013	#	0.005
H	5.791570	4.291855	6.791392	#	0.027
H	10.705639	7.649700	4.914927	#	0.026
H	7.274912	2.701457	5.354751	#	0.003
H	3.426039	4.789671	2.496822	#	0.011
H	2.548059	5.972244	3.469653	#	0.015
H	4.707057	2.715043	5.354012	#	0.003
H	4.693027	2.899569	3.598180	#	0.010
H	2.547825	3.733067	4.606159	#	0.021
H	2.568509	5.817186	6.005958	#	0.017
H	3.412722	4.502788	6.825547	#	0.011
H	7.274853	6.820085	2.525803	#	0.042
H	6.017650	8.645470	5.686198	#	0.040
H	5.803652	8.721112	3.939113	#	0.061
H	4.712048	6.918102	2.658968	#	0.001
H	12.001632	5.972250	3.469690	#	0.015
H	11.123710	4.789630	2.496846	#	0.011
H	9.856606	2.899530	3.598246	#	0.011
H	9.842587	2.715096	5.354094	#	0.004
H	11.136925	4.502735	6.825545	#	0.011
H	11.981179	5.817148	6.006014	#	0.017
H	12.001864	3.733072	4.606128	#	0.023
H	7.274373	6.697880	5.695411	#	-0.043

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Pentamantane "planar" C<sub>26</sub>H<sub>34</sub> 2+

C	7.273917	6.022206	6.379520	#	0.013
C	9.850663	5.986788	6.406733	#	0.035
C	8.555724	5.143924	6.276055	#	0.022
C	8.572180	4.390725	4.906723	#	0.049
C	8.603284	5.469123	3.771973	#	0.007
C	9.847318	6.402302	3.865730	#	0.037
C	9.873813	7.056776	5.279459	#	0.024
C	8.616548	7.942910	5.413289	#	-0.002
C	7.321758	7.106240	5.247285	#	0.042
C	6.109480	8.069510	5.277774	#	-0.001
C	4.798462	7.392787	4.961767	#	0.007
C	4.709145	5.687405	6.683353	#	0.003
C	6.038717	5.074016	6.276587	#	0.001

C	6.010163	4.394610	4.866178	#	0.046
C	7.290792	3.538718	4.742413	#	-0.015
C	7.323383	6.346375	3.885005	#	0.008
C	6.031163	5.501439	3.765727	#	0.026
C	4.751605	6.388662	3.821804	#	0.019
C	11.091526	5.059522	6.402180	#	-0.011
C	3.478315	4.392041	4.887097	#	0.052
C	9.806061	3.446400	4.856343	#	-0.018
C	11.155951	5.757235	3.446400	#	-0.012
C	3.446400	4.926857	6.341687	#	-0.006
C	4.742729	3.525285	4.704513	#	0.000
C	3.455891	5.528076	3.831317	#	-0.001
C	11.097060	4.076648	5.274809	#	0.027
H	8.526805	4.402862	7.090572	#	-0.001
H	9.706314	7.211854	3.128488	#	0.043
H	10.769915	7.683244	5.383792	#	0.026
H	6.249040	8.844587	4.503706	#	0.070
H	6.050524	8.612799	6.229696	#	0.056
H	4.717064	6.189072	7.660354	#	0.108
H	6.179258	4.273250	7.028043	#	0.046
H	7.270878	2.747449	5.506872	#	0.015
H	7.343851	7.083093	3.067021	#	0.003
H	6.027560	4.994817	2.790117	#	0.023
H	4.732502	7.019142	2.914406	#	0.061
H	8.597997	4.959370	2.796534	#	0.017
H	3.906953	8.028104	5.042855	#	0.115
H	7.300944	3.034144	3.765811	#	0.030
H	11.086469	4.430901	7.314740	#	0.100
H	12.032933	5.619239	6.451771	#	0.073
H	9.902152	2.945085	3.885278	#	0.067
H	9.658190	2.625527	5.587086	#	0.089
H	12.006952	3.481311	5.136586	#	0.147
H	12.034688	6.402135	3.550441	#	0.107
H	11.130226	5.251811	2.475357	#	0.102
H	7.270089	6.525826	7.358456	#	0.015
H	8.642603	8.734002	4.651332	#	0.024
H	8.611454	8.445986	6.389723	#	0.025
H	9.845906	6.512885	7.370034	#	0.039
H	2.558547	5.540206	6.535740	#	0.059
H	3.387950	4.081691	7.048840	#	0.078
H	4.749887	2.705314	5.436193	#	0.014
H	4.743685	3.060658	3.709944	#	0.034
H	3.343538	5.074085	2.839756	#	0.049
H	2.576573	6.169713	3.976312	#	0.029
H	2.584404	3.776116	4.738541	#	0.055
H	4.562576	6.748878	6.019740	#	-0.035
H	11.459288	4.863514	4.153009	#	-0.033

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Pentamantane "planar" C<sub>26</sub>H<sub>35</sub> 3+

C	7.251437	4.912105	3.446400	# -0.037
C	10.771279	5.147798	3.846652	# 0.032
C	10.331153	6.624842	3.774460	# -0.066
C	9.494164	7.250255	4.725815	# 0.026
C	9.252188	6.585386	6.068165	# 0.019
C	10.188737	5.341827	6.274204	# 0.017
C	10.170507	4.377012	5.056375	# 0.021
C	8.868111	3.446400	4.805413	# -0.064
C	7.515428	3.997029	4.590225	# 0.060
C	6.348544	3.492787	5.370622	# -0.057
C	5.102683	4.428814	5.439476	# 0.030
C	4.727424	4.920062	4.022666	# 0.013
C	6.004408	5.817394	3.547357	# -0.005
C	5.961610	6.900152	4.564646	# 0.030
C	8.912876	8.605598	4.453906	# -0.056
C	7.784879	6.104520	6.415597	# 0.015
C	6.447941	6.721066	5.942275	# -0.028
C	5.205585	5.653695	6.400744	# -0.018
C	12.317609	5.225582	4.091602	# 0.019
C	3.585638	6.946127	4.962403	# 0.040
C	11.700415	7.488024	4.672219	# -0.064
C	11.684373	5.749756	6.512779	# -0.001
C	3.446401	5.763191	3.998318	# 0.001
C	4.867837	7.857612	4.413875	# -0.039
C	3.905133	6.477445	6.388741	# 0.003
C	12.395026	6.260064	5.232173	# 0.042
H	10.357024	7.068566	2.779635	# 0.105
H	9.855194	4.824274	7.182730	# 0.048
H	10.884915	3.579998	5.292074	# 0.078
H	6.655432	3.117569	6.353868	# 0.105
H	6.038054	2.573397	4.822764	# 0.147
H	4.653661	4.089406	3.309530	# 0.072
H	5.772607	6.210908	2.553817	# 0.097
H	9.447110	9.136801	3.660623	# 0.102
H	6.261969	7.632423	6.515747	# 0.081
H	5.484012	5.351847	7.417615	# 0.093
H	9.507383	7.340719	6.825915	# 0.072
H	4.282691	3.809631	5.827031	# 0.092
H	8.882178	9.234009	5.350049	# 0.101
H	12.836966	5.584207	3.195774	# 0.062
H	12.745806	4.253350	4.350379	# 0.068
H	11.416832	8.247095	5.404556	# 0.098
H	12.158250	7.972514	3.806167	# 0.130

H	13.434230	6.531637	5.470075	#	0.113
H	12.226431	4.877065	6.893495	#	0.069
H	11.727921	6.509091	7.303663	#	0.053
H	7.076869	4.226077	2.589858	#	0.142
H	8.845675	2.708630	5.612750	#	0.094
H	9.129439	2.905068	3.875575	#	0.129
H	10.555272	4.657103	2.891088	#	0.058
H	2.592690	5.141066	4.300352	#	0.095
H	3.224458	6.099946	2.979388	#	0.070
H	4.634104	8.135090	3.384422	#	0.101
H	4.941438	8.740572	5.050907	#	0.101
H	3.982252	7.321777	7.082617	#	0.064
H	3.073188	5.863106	6.760582	#	0.097
H	2.725599	7.621588	4.928601	#	0.113
H	7.875280	8.501926	4.102842	#	0.065
H	7.782209	5.033103	6.227237	#	-0.007
H	7.736310	6.156187	7.510692	#	0.086
H	8.147524	5.464331	3.15454	#	0.078



## References

1. G. A. Olah and J. Lukas, *J Am Chem Soc*, 1968, **90**, 933-&.
2. R. H. Boyd, S. N. Sanwal, Sharyteh.S and D. Mcnally, *J Phys Chem-Us*, 1971, **75**, 1264-&.
3. Y. Li and T. Baer, *J Phys Chem A*, 2002, **106**, 272-278.
4. J. L. Abboud, O. Castano, J. Z. Davalos, P. Jimenez, R. Gomperts, P. Muller and M. V. Roux, *J Org Chem*, 2002, **67**, 1057-1060.
5. J. Z. Davalos, R. Herrero, E. Quintanilla, P. Jimenez, J. F. Gal, P. C. Maria and J. L. M. Abboud, *Chem-Eur J*, 2006, **12**, 5505-5513.
6. P. M. Esteves, G. G. P. Alberto, A. Ramirez-Solis and C. J. A. Mota, *J Phys Chem A*, 2001, **105**, 4308-4311.
7. I. Santos, D. W. Balogh, C. W. Doecke, A. G. Marshall and L. A. Paquette, *J Am Chem Soc*, 1986, **108**, 8183-8185.
8. Z. F. Chen, H. J. Jiao, D. Moran, A. Hirsch, W. Thiel and P. V. Schleyer, *J Phys Chem A*, 2003, **107**, 2075-2079.
9. P. Ausloos, R. E. Rebbert, F. P. Schwarz and S. G. Lias, *Radiat Phys Chem*, 1983, **21**, 27-43.
10. M. W. Lodewyk, M. R. Siebert and D. J. Tantillo, *Chemical Reviews*, 2012, **112**, 1839-1862.
11. A. D. M. a. A. W. Blackwell, *IUPAC. Compendium of Chemical Terminology*, Blackwell Scientific Publications,, Oxford, 1997.