

Supporting Information

Free-Base Porphyrins with Localized NH Protons. Can Substituents Alone Stabilize the Elusive *Cis* Tautomer?

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Optimized BP86-D3/STO-TZ2P Cartesian coordinates (Å)

1.	H ₂ [<i>opp</i> -Br ₄ TPP]; trans1; saddled	3
2.	H ₂ [<i>opp</i> -Br ₄ TPP]; trans2; saddled	4
3.	H ₂ [<i>opp</i> -Br ₄ TPP]; trans1; waved	6
4.	H ₂ [<i>opp</i> -(CN) ₄ TPP]; trans1; saddled	7
5.	H ₂ [<i>opp</i> -(CN) ₄ TPP]; trans2; saddled	9
6.	H ₂ [<i>opp</i> -(CF ₃) ₄ TPP]; trans1; saddled	11
7.	H ₂ [<i>opp</i> -(CF ₃) ₄ TPP]; trans2; saddled	13
8.	H ₂ [<i>opp</i> -(CF ₃) ₄ TPP]; trans1; waved	14
9.	H ₂ [<i>opp</i> -(CH ₃) ₄ TPP]; trans1; saddled	16
10.	H ₂ [<i>opp</i> -(CH ₃) ₄ TPP]; trans2; saddled	18
11.	H ₂ [<i>opp</i> -(CH ₃) ₄ TPP]; trans1; waved	20
12.	H ₂ [<i>opp</i> -Br ₄ (CH ₃) ₄ TPP]; trans1; saddled	22
13.	H ₂ [<i>opp</i> -Br ₄ (CH ₃) ₄ TPP]; trans2; saddled	24
14.	H ₂ [<i>opp</i> -(CF ₃) ₄ (CH ₃) ₄ TPP]; trans1; saddled	25

15.	$H_2[opp-(CF_3)_4(CH_3)_4TPP]; trans2; saddled$	28
16.	$H_2[adj-Br_4TPP]; trans; saddled$	30
17.	$H_2[adj-Br_4TPP]; cis1; saddled$	31
18.	$H_2[adj-(CN)_4TPP]; trans; saddled$	33
19.	$H_2[adj-(CN)_4TPP]; cis1; saddled$	35
20.	$H_2[adj-(CF_3)_4TPP]; trans; saddled$	36
21.	$H_2[adj-(CF_3)_4TPP]; cis1; saddled$	38
22.	$H_2[adj-(CH_3)_4TPP]; trans; saddled$	40
23.	$H_2[adj-(CH_3)_4TPP]; cis1; saddled$	42
24.	$H_2[adj-Br_4(CH_3)_4TPP]; trans; saddled$	44
25.	$H_2[adj-Br_4(CH_3)_4TPP]; cis1; saddled$	45
26.	$H_2[adj-(CF_3)_4(CH_3)_4TPP]; trans; saddled$	47
27.	$H_2[adj-(CF_3)_4(CH_3)_4TPP]; cis1; saddled$	49
28.	$H_2[adj-(CF_3)_4Ph_4TPP]; trans; saddled$	51
29.	$H_2[adj-(CF_3)_4Ph_4TPP]; cis1; saddled$	54

1. H₂[*opp*-Br₄TPP]; *trans*1; *saddled*

N	2.064980000	0.000000000	-0.583932000
N	0.000000000	2.088550000	-0.641395000
C	2.829680000	-1.103572000	-0.304229000
C	4.096193000	-0.684493000	0.291059000
C	4.096193000	0.684493000	0.291059000
C	2.829680000	1.103572000	-0.304229000
C	2.454806000	2.434679000	-0.607328000
C	1.132333000	2.846208000	-0.838310000
C	0.686172000	4.151363000	-1.233234000
C	-0.686172000	4.151363000	-1.233234000
C	-1.132333000	2.846208000	-0.838310000
C	-2.454806000	2.434679000	-0.607328000
C	-3.504656000	3.480699000	-0.726440000
C	-4.524457000	3.339081000	-1.680702000
C	-5.528350000	4.299040000	-1.791256000
C	-5.531713000	5.410504000	-0.944375000
C	-4.515851000	5.565237000	0.002767000
C	-3.505012000	4.611119000	0.106267000
C	3.504656000	3.480699000	-0.726440000
C	3.505012000	4.611119000	0.106267000
C	4.515851000	5.565237000	0.002767000
C	5.531713000	5.410504000	-0.944375000
C	5.528350000	4.299040000	-1.791256000
C	4.524457000	3.339081000	-1.680702000
H	0.000000000	1.085138000	-0.467773000
H	1.344826000	4.973501000	-1.485540000
H	-1.344826000	4.973501000	-1.485540000
H	-4.526769000	2.460192000	-2.325434000
H	-6.315549000	4.175973000	-2.535263000
H	-6.324431000	6.155000000	-1.021824000
H	-4.516929000	6.427137000	0.670544000
H	-2.724275000	4.715877000	0.859653000
H	2.724275000	4.715877000	0.859653000
H	4.516929000	6.427137000	0.670544000
H	6.324431000	6.155000000	-1.021824000
H	6.315549000	4.175973000	-2.535263000
H	4.526769000	2.460192000	-2.325434000
N	-2.064980000	0.000000000	-0.583932000
N	0.000000000	-2.088550000	-0.641395000
C	-2.829680000	1.103572000	-0.304229000
C	-4.096193000	0.684493000	0.291059000
C	-4.096193000	-0.684493000	0.291059000
C	-2.829680000	-1.103572000	-0.304229000
C	-2.454806000	-2.434679000	-0.607328000
C	-1.132333000	-2.846208000	-0.838310000
C	-0.686172000	-4.151363000	-1.233234000
C	0.686172000	-4.151363000	-1.233234000
C	1.132333000	-2.846208000	-0.838310000

C	2.454806000	-2.434679000	-0.607328000
C	3.504656000	-3.480699000	-0.726440000
C	4.524457000	-3.339081000	-1.680702000
C	5.528350000	-4.299040000	-1.791256000
C	5.531713000	-5.410504000	-0.944375000
C	4.515851000	-5.565237000	0.002767000
C	3.505012000	-4.611119000	0.106267000
C	-3.504656000	-3.480699000	-0.726440000
C	-3.505012000	-4.611119000	0.106267000
C	-4.515851000	-5.565237000	0.002767000
C	-5.531713000	-5.410504000	-0.944375000
C	-5.528350000	-4.299040000	-1.791256000
C	-4.524457000	-3.339081000	-1.680702000
H	0.000000000	-1.085138000	-0.467773000
H	-1.344826000	-4.973501000	-1.485540000
H	1.344826000	-4.973501000	-1.485540000
H	4.526769000	-2.460192000	-2.325434000
H	6.315549000	-4.175973000	-2.535263000
H	6.324431000	-6.155000000	-1.021824000
H	4.516929000	-6.427137000	0.670544000
H	2.724275000	-4.715877000	0.859653000
H	-2.724275000	-4.715877000	0.859653000
H	-4.516929000	-6.427137000	0.670544000
H	-6.324431000	-6.155000000	-1.021824000
H	-6.315549000	-4.175973000	-2.535263000
H	-4.526769000	-2.460192000	-2.325434000
Br	-5.402557000	1.739941000	1.146902000
Br	-5.402557000	-1.739941000	1.146902000
Br	5.402557000	1.739941000	1.146902000
Br	5.402557000	-1.739941000	1.146902000

2. H₂[*opp*-Br₄TPP]; *trans*2; *saddled*

N	0.000000000	-2.158674000	-0.418796000
N	1.980946000	0.000000000	-0.507268000
C	-1.144368000	-2.908355000	-0.242168000
C	-0.691078000	-4.216839000	0.156046000
C	0.691078000	-4.216839000	0.156046000
C	1.144368000	-2.908355000	-0.242168000
C	2.451548000	-2.440648000	-0.462745000
C	2.803544000	-1.087995000	-0.652778000
C	4.169198000	-0.677711000	-0.969102000
C	4.169198000	0.677711000	-0.969102000
C	2.803544000	1.087995000	-0.652778000
C	2.451548000	2.440648000	-0.462745000
C	3.564475000	3.433284000	-0.524603000
C	3.671992000	4.306787000	-1.615385000
C	4.708428000	5.238160000	-1.674511000
C	5.645908000	5.309519000	-0.640885000
C	5.554251000	4.431424000	0.442389000

C	4.524071000	3.493139000	0.496346000
C	3.564475000	-3.433284000	-0.524603000
C	4.524071000	-3.493139000	0.496346000
C	5.554251000	-4.431424000	0.442389000
C	5.645908000	-5.309519000	-0.640885000
C	4.708428000	-5.238160000	-1.674511000
C	3.671992000	-4.306787000	-1.615385000
H	5.001152000	-1.343850000	-1.167534000
H	5.001152000	1.343850000	-1.167534000
H	2.927837000	4.257504000	-2.410641000
H	4.781460000	5.914255000	-2.526554000
H	6.450587000	6.044101000	-0.682284000
H	6.285589000	4.479802000	1.249677000
H	4.441590000	2.809988000	1.341496000
H	4.441590000	-2.809988000	1.341496000
H	6.285589000	-4.479802000	1.249677000
H	6.450587000	-6.044101000	-0.682284000
H	4.781460000	-5.914255000	-2.526554000
H	2.927837000	-4.257504000	-2.410641000
N	0.000000000	2.158674000	-0.418796000
N	-1.980946000	0.000000000	-0.507268000
C	1.144368000	2.908355000	-0.242168000
C	0.691078000	4.216839000	0.156046000
C	-0.691078000	4.216839000	0.156046000
C	-1.144368000	2.908355000	-0.242168000
C	-2.451548000	2.440648000	-0.462745000
C	-2.803544000	1.087995000	-0.652778000
C	-4.169198000	0.677711000	-0.969102000
C	-4.169198000	-0.677711000	-0.969102000
C	-2.803544000	-1.087995000	-0.652778000
C	-2.451548000	-2.440648000	-0.462745000
C	-3.564475000	-3.433284000	-0.524603000
C	-3.671992000	-4.306787000	-1.615385000
C	-4.708428000	-5.238160000	-1.674511000
C	-5.645908000	-5.309519000	-0.640885000
C	-5.554251000	-4.431424000	0.442389000
C	-4.524071000	-3.493139000	0.496346000
C	-3.564475000	3.433284000	-0.524603000
C	-4.524071000	3.493139000	0.496346000
C	-5.554251000	4.431424000	0.442389000
C	-5.645908000	5.309519000	-0.640885000
C	-4.708428000	5.238160000	-1.674511000
C	-3.671992000	4.306787000	-1.615385000
H	-5.001152000	1.343850000	-1.167534000
H	-5.001152000	-1.343850000	-1.167534000
H	-2.927837000	-4.257504000	-2.410641000
H	-4.781460000	-5.914255000	-2.526554000
H	-6.450587000	-6.044101000	-0.682284000
H	-6.285589000	-4.479802000	1.249677000
H	-4.441590000	-2.809988000	1.341496000
H	-4.441590000	2.809988000	1.341496000

H	-6.285589000	4.479802000	1.249677000
H	-6.450587000	6.044101000	-0.682284000
H	-4.781460000	5.914255000	-2.526554000
H	-2.927837000	4.257504000	-2.410641000
H	0.000000000	-1.151873000	-0.611297000
H	0.000000000	1.151873000	-0.611297000
Br	-1.723498000	-5.667441000	0.749268000
Br	1.723498000	-5.667441000	0.749268000
Br	1.723498000	5.667441000	0.749268000
Br	-1.723498000	5.667441000	0.749268000

3. H₂[*opp*-Br₄TPP]; *trans*1; *waved*

N	2.104042000	0.273008000	0.000000000
N	0.003312000	-0.002205000	2.067925000
H	0.003222000	-0.001849000	1.049964000
C	4.264232000	-0.673464000	-3.835618000
C	3.435240000	0.423461000	-3.567322000
C	2.451168000	0.355101000	-2.442640000
C	2.885889000	0.492898000	-1.106688000
C	2.885889000	0.492898000	1.106688000
C	2.451168000	0.355101000	2.442640000
C	1.126788000	0.138856000	2.855096000
C	-1.119926000	-0.144259000	2.855302000
C	-0.676779000	-0.075119000	4.218686000
H	-1.330718000	-0.141208000	5.079099000
C	0.683754000	0.071395000	4.218546000
H	1.337800000	0.138620000	5.078817000
C	3.435240000	0.423461000	3.567322000
C	4.264232000	-0.673464000	3.835618000
C	5.178397000	-0.625108000	4.887925000
H	5.824561000	-1.481128000	5.083343000
C	5.269874000	0.518437000	5.684963000
H	5.989562000	0.558728000	6.502912000
C	4.431332000	1.608099000	5.435355000
C	3.514313000	1.558252000	4.386164000
H	2.865990000	2.409485000	4.178324000
C	4.224370000	0.910856000	0.683739000
C	4.224370000	0.910856000	-0.683739000
C	3.514313000	1.558252000	-4.386164000
H	2.865990000	2.409485000	-4.178324000
C	4.431332000	1.608099000	-5.435355000
C	5.269874000	0.518437000	-5.684963000
H	5.989562000	0.558728000	-6.502912000
C	5.178397000	-0.625108000	-4.887925000
H	5.824561000	-1.481128000	-5.083343000
N	-2.096274000	-0.278960000	0.000000000
N	0.003312000	-0.002205000	-2.067925000
H	0.003222000	-0.001849000	-1.049964000
C	-4.262259000	0.663496000	3.832264000

C	-3.429546000	-0.431139000	3.566060000
C	-2.444218000	-0.361016000	2.442582000
C	-2.878330000	-0.498768000	1.106532000
C	-2.878330000	-0.498768000	-1.106532000
C	-2.444218000	-0.361016000	-2.442582000
C	-1.119926000	-0.144259000	-2.855302000
C	1.126788000	0.138856000	-2.855096000
C	0.683754000	0.071395000	-4.218546000
H	1.337800000	0.138620000	-5.078817000
C	-0.676779000	-0.075119000	-4.218686000
H	-1.330718000	-0.141208000	-5.079099000
C	-3.429546000	-0.431139000	-3.566060000
C	-4.262259000	0.663496000	-3.832264000
C	-5.177277000	0.613559000	-4.883760000
H	-5.825130000	1.468426000	-5.078588000
C	-5.267077000	-0.529906000	-5.681093000
H	-5.987786000	-0.571664000	-6.498068000
C	-4.426446000	-1.618124000	-5.432211000
C	-3.508242000	-1.566527000	-4.384142000
H	-2.857760000	-2.416363000	-4.177347000
C	-4.216369000	-0.917983000	-0.683739000
C	-4.216369000	-0.917983000	0.683739000
C	-3.508242000	-1.566527000	4.384142000
H	-2.857760000	-2.416363000	4.177347000
C	-4.426446000	-1.618124000	5.432211000
C	-5.267077000	-0.529906000	5.681093000
H	-5.987786000	-0.571664000	6.498068000
C	-5.177277000	0.613559000	4.883760000
H	-5.825130000	1.468426000	5.078588000
H	-4.489369000	-2.511813000	-6.053619000
H	-4.197633000	1.547455000	-3.197662000
H	-4.197633000	1.547455000	3.197662000
H	-4.489369000	-2.511813000	6.053619000
H	4.495199000	2.501669000	6.056835000
H	4.199005000	-1.557120000	3.200644000
H	4.199005000	-1.557120000	-3.200644000
H	4.495199000	2.501669000	-6.056835000
Br	-5.685672000	-1.510044000	1.704099000
Br	-5.685672000	-1.510044000	-1.704099000
Br	5.694562000	1.502533000	-1.703073000
Br	5.694562000	1.502533000	1.703073000

4. $\text{H}_2[\text{opp}-(\text{CN})_4\text{TPP}]$; **trans1; saddled**

N	2.077089000	0.000000000	-0.102876000
N	0.000000000	2.095965000	-0.105888000
C	2.868814000	-1.099272000	0.064515000
C	4.224376000	-0.694149000	0.442430000
C	4.224376000	0.694149000	0.442430000
C	2.868814000	1.099272000	0.064515000

C	2.464192000	2.443782000	-0.126611000
C	1.132606000	2.868923000	-0.248306000
C	0.684894000	4.206926000	-0.518077000
C	-0.684894000	4.206926000	-0.518077000
C	-1.132606000	2.868923000	-0.248306000
C	-2.464192000	2.443782000	-0.126611000
C	-3.516444000	3.489443000	-0.249068000
C	-4.403532000	3.456850000	-1.336923000
C	-5.408555000	4.414319000	-1.455292000
C	-5.542997000	5.409742000	-0.485550000
C	-4.658730000	5.455246000	0.594847000
C	-3.643905000	4.507038000	0.708816000
C	3.516444000	3.489443000	-0.249068000
C	3.643905000	4.507038000	0.708816000
C	4.658730000	5.455246000	0.594847000
C	5.542997000	5.409742000	-0.485550000
C	5.408555000	4.414319000	-1.455292000
C	4.403532000	3.456850000	-1.336923000
C	5.315789000	1.493737000	0.855940000
C	5.315789000	-1.493737000	0.855940000
H	0.000000000	1.081780000	-0.008765000
H	1.346266000	5.046290000	-0.696572000
H	-1.346266000	5.046290000	-0.696572000
H	-4.302301000	2.668040000	-2.082732000
H	-6.095446000	4.376867000	-2.300493000
H	-6.341118000	6.147366000	-0.568006000
H	-4.768274000	6.224807000	1.358800000
H	-2.962489000	4.526920000	1.559344000
H	2.962489000	4.526920000	1.559344000
H	4.768274000	6.224807000	1.358800000
H	6.341118000	6.147366000	-0.568006000
H	6.095446000	4.376867000	-2.300493000
H	4.302301000	2.668040000	-2.082732000
N	-2.077089000	0.000000000	-0.102876000
N	0.000000000	-2.095965000	-0.105888000
C	-2.868814000	1.099272000	0.064515000
C	-4.224376000	0.694149000	0.442430000
C	-4.224376000	-0.694149000	0.442430000
C	-2.868814000	-1.099272000	0.064515000
C	-2.464192000	-2.443782000	-0.126611000
C	-1.132606000	-2.868923000	-0.248306000
C	-0.684894000	-4.206926000	-0.518077000
C	0.684894000	-4.206926000	-0.518077000
C	1.132606000	-2.868923000	-0.248306000
C	2.464192000	-2.443782000	-0.126611000
C	3.516444000	-3.489443000	-0.249068000
C	4.403532000	-3.456850000	-1.336923000
C	5.408555000	-4.414319000	-1.455292000
C	5.542997000	-5.409742000	-0.485550000
C	4.658730000	-5.455246000	0.594847000
C	3.643905000	-4.507038000	0.708816000

C	-3.516444000	-3.489443000	-0.249068000
C	-3.643905000	-4.507038000	0.708816000
C	-4.658730000	-5.455246000	0.594847000
C	-5.542997000	-5.409742000	-0.485550000
C	-5.408555000	-4.414319000	-1.455292000
C	-4.403532000	-3.456850000	-1.336923000
C	-5.315789000	-1.493737000	0.855940000
C	-5.315789000	1.493737000	0.855940000
H	0.000000000	-1.081780000	-0.008765000
H	-1.346266000	-5.046290000	-0.696572000
H	1.346266000	-5.046290000	-0.696572000
H	4.302301000	-2.668040000	-2.082732000
H	6.095446000	-4.376867000	-2.300493000
H	6.341118000	-6.147366000	-0.568006000
H	4.768274000	-6.224807000	1.358800000
H	2.962489000	-4.526920000	1.559344000
H	-2.962489000	-4.526920000	1.559344000
H	-4.768274000	-6.224807000	1.358800000
H	-6.341118000	-6.147366000	-0.568006000
H	-6.095446000	-4.376867000	-2.300493000
H	-4.302301000	-2.668040000	-2.082732000
N	6.234073000	2.109569000	1.227139000
N	6.234073000	-2.109569000	1.227139000
N	-6.234073000	-2.109569000	1.227139000
N	-6.234073000	2.109569000	1.227139000

5. H₂[*opp*-(CN)₄TPP]; *trans2*; *saddled*

N	2.149530000	0.000000000	0.102713000
N	0.000000000	-1.998704000	0.152146000
C	2.904257000	1.140913000	-0.036982000
C	4.236297000	0.701938000	-0.357912000
C	4.236297000	-0.701938000	-0.357912000
C	2.904257000	-1.140913000	-0.036982000
C	2.442675000	-2.459441000	0.136301000
C	1.088915000	-2.826728000	0.273598000
C	0.677223000	-4.205304000	0.533440000
C	-0.677223000	-4.205304000	0.533440000
C	-1.088915000	-2.826728000	0.273598000
C	-2.442675000	-2.459441000	0.136301000
C	-3.474111000	-3.533775000	0.199343000
C	-4.345888000	-3.603401000	1.296622000
C	-5.325779000	-4.592807000	1.356295000
C	-5.449643000	-5.516657000	0.316830000
C	-4.579757000	-5.459413000	-0.774676000
C	-3.590804000	-4.478543000	-0.831078000
C	3.474111000	-3.533775000	0.199343000
C	3.590804000	-4.478543000	-0.831078000
C	4.579757000	-5.459413000	-0.774676000
C	5.449643000	-5.516657000	0.316830000

C	5.325779000	-4.592807000	1.356295000
C	4.345888000	-3.603401000	1.296622000
C	5.354037000	-1.492207000	-0.717987000
C	5.354037000	1.492207000	-0.717987000
H	1.346878000	-5.041365000	0.701604000
H	-1.346878000	-5.041365000	0.701604000
H	-4.252809000	-2.871212000	2.099264000
H	-6.001038000	-4.635492000	2.210589000
H	-6.227119000	-6.279685000	0.355025000
H	-4.677956000	-6.175807000	-1.590135000
H	-2.914920000	-4.422336000	-1.684266000
H	2.914920000	-4.422336000	-1.684266000
H	4.677956000	-6.175807000	-1.590135000
H	6.227119000	-6.279685000	0.355025000
H	6.001038000	-4.635492000	2.210589000
H	4.252809000	-2.871212000	2.099264000
N	-2.149530000	0.000000000	0.102713000
N	0.000000000	1.998704000	0.152146000
C	-2.904257000	-1.140913000	-0.036982000
C	-4.236297000	-0.701938000	-0.357912000
C	-4.236297000	0.701938000	-0.357912000
C	-2.904257000	1.140913000	-0.036982000
C	-2.442675000	2.459441000	0.136301000
C	-1.088915000	2.826728000	0.273598000
C	-0.677223000	4.205304000	0.533440000
C	0.677223000	4.205304000	0.533440000
C	1.088915000	2.826728000	0.273598000
C	2.442675000	2.459441000	0.136301000
C	3.474111000	3.533775000	0.199343000
C	4.345888000	3.603401000	1.296622000
C	5.325779000	4.592807000	1.356295000
C	5.449643000	5.516657000	0.316830000
C	4.579757000	5.459413000	-0.774676000
C	3.590804000	4.478543000	-0.831078000
C	-3.474111000	3.533775000	0.199343000
C	-3.590804000	4.478543000	-0.831078000
C	-4.579757000	5.459413000	-0.774676000
C	-5.449643000	5.516657000	0.316830000
C	-5.325779000	4.592807000	1.356295000
C	-4.345888000	3.603401000	1.296622000
C	-5.354037000	1.492207000	-0.717987000
C	-5.354037000	-1.492207000	-0.717987000
H	-1.346878000	5.041365000	0.701604000
H	1.346878000	5.041365000	0.701604000
H	4.252809000	2.871212000	2.099264000
H	6.001038000	4.635492000	2.210589000
H	6.227119000	6.279685000	0.355025000
H	4.677956000	6.175807000	-1.590135000
H	2.914920000	4.422336000	-1.684266000
H	-2.914920000	4.422336000	-1.684266000
H	-4.677956000	6.175807000	-1.590135000

H	-6.227119000	6.279685000	0.355025000
H	-6.001038000	4.635492000	2.210589000
H	-4.252809000	2.871212000	2.099264000
H	1.135890000	0.000000000	0.254623000
H	-1.135890000	0.000000000	0.254623000
N	6.304918000	2.077622000	-1.051556000
N	6.304918000	-2.077622000	-1.051556000
N	-6.304918000	-2.077622000	-1.051556000
N	-6.304918000	2.077622000	-1.051556000

6. H₂[*opp*-(CF₃)₄TPP]; *trans*1; *saddled*

F	-1.256785000	4.820627000	2.983036000
F	-2.897850000	4.323404000	1.664399000
F	-1.604873000	6.037824000	1.195314000
F	1.256785000	4.820627000	2.983036000
F	1.604873000	6.037824000	1.195314000
F	2.897850000	4.323404000	1.664399000
N	0.000000000	2.041626000	-0.385202000
N	-2.097988000	0.000000000	-0.465745000
C	1.096281000	2.745888000	0.015805000
C	0.694631000	3.863503000	0.860330000
C	-0.694631000	3.863503000	0.860330000
C	-1.096281000	2.745888000	0.015805000
C	-2.388469000	2.449098000	-0.532850000
C	-2.759714000	1.136159000	-0.873521000
C	-3.893678000	0.686374000	-1.631703000
C	-3.893678000	-0.686374000	-1.631703000
C	-2.759714000	-1.136159000	-0.873521000
C	-2.388469000	-2.449098000	-0.532850000
C	-3.301496000	-3.552186000	-0.883209000
C	-2.784511000	-4.705697000	-1.503308000
C	-3.622490000	-5.761089000	-1.855638000
C	-4.991192000	-5.689452000	-1.588641000
C	-5.517219000	-4.553896000	-0.963873000
C	-4.683361000	-3.496221000	-0.614902000
C	-3.301496000	3.552186000	-0.883209000
C	-4.683361000	3.496221000	-0.614902000
C	-5.517219000	4.553896000	-0.963873000
C	-4.991192000	5.689452000	-1.588641000
C	-3.622490000	5.761089000	-1.855638000
C	-2.784511000	4.705697000	-1.503308000
C	-1.606382000	4.754480000	1.671177000
C	1.606382000	4.754480000	1.671177000
H	-1.157409000	0.000000000	-0.080298000
H	-4.597388000	1.341106000	-2.131335000
H	-4.597388000	-1.341106000	-2.131335000
H	-1.717819000	-4.758494000	-1.718841000
H	-3.204750000	-6.643534000	-2.340177000
H	-5.645848000	-6.518472000	-1.857593000

H	-6.580688000	-4.502933000	-0.729870000
H	-5.087541000	-2.635867000	-0.082622000
H	-5.087541000	2.635867000	-0.082622000
H	-6.580688000	4.502933000	-0.729870000
H	-5.645848000	6.518472000	-1.857593000
H	-3.204750000	6.643534000	-2.340177000
H	-1.717819000	4.758494000	-1.718841000
F	1.256785000	-4.820627000	2.983036000
F	2.897850000	-4.323404000	1.664399000
F	1.604873000	-6.037824000	1.195314000
F	-1.256785000	-4.820627000	2.983036000
F	-1.604873000	-6.037824000	1.195314000
F	-2.897850000	-4.323404000	1.664399000
N	0.000000000	-2.041626000	-0.385202000
N	2.097988000	0.000000000	-0.465745000
C	-1.096281000	-2.745888000	0.015805000
C	-0.694631000	-3.863503000	0.860330000
C	0.694631000	-3.863503000	0.860330000
C	1.096281000	-2.745888000	0.015805000
C	2.388469000	-2.449098000	-0.532850000
C	2.759714000	-1.136159000	-0.873521000
C	3.893678000	-0.686374000	-1.631703000
C	3.893678000	0.686374000	-1.631703000
C	2.759714000	1.136159000	-0.873521000
C	2.388469000	2.449098000	-0.532850000
C	3.301496000	3.552186000	-0.883209000
C	2.784511000	4.705697000	-1.503308000
C	3.622490000	5.761089000	-1.855638000
C	4.991192000	5.689452000	-1.588641000
C	5.517219000	4.553896000	-0.963873000
C	4.683361000	3.496221000	-0.614902000
C	3.301496000	-3.552186000	-0.883209000
C	4.683361000	-3.496221000	-0.614902000
C	5.517219000	-4.553896000	-0.963873000
C	4.991192000	-5.689452000	-1.588641000
C	3.622490000	-5.761089000	-1.855638000
C	2.784511000	-4.705697000	-1.503308000
C	1.606382000	-4.754480000	1.671177000
C	-1.606382000	-4.754480000	1.671177000
H	1.157409000	0.000000000	-0.080298000
H	4.597388000	-1.341106000	-2.131335000
H	4.597388000	1.341106000	-2.131335000
H	1.717819000	4.758494000	-1.718841000
H	3.204750000	6.643534000	-2.340177000
H	5.645848000	6.518472000	-1.857593000
H	6.580688000	4.502933000	-0.729870000
H	5.087541000	2.635867000	-0.082622000
H	5.087541000	-2.635867000	-0.082622000
H	6.580688000	-4.502933000	-0.729870000
H	5.645848000	-6.518472000	-1.857593000
H	3.204750000	-6.643534000	-2.340177000

H	1.717819000	-4.758494000	-1.718841000
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7. H₂[*opp*-(CF₃)₄TPP]; *trans*2; *saddled*

F	1.251729000	4.997133000	-2.920339000
F	2.900014000	4.449180000	-1.633567000
F	1.584668000	6.117066000	-1.068133000
F	-1.251729000	4.997133000	-2.920339000
F	-1.584668000	6.117066000	-1.068133000
F	-2.900014000	4.449180000	-1.633567000
N	0.000000000	2.107199000	0.243502000
N	1.987441000	0.000000000	0.407288000
C	-1.139923000	2.789511000	-0.089946000
C	-0.702974000	3.917561000	-0.859727000
C	0.702974000	3.917561000	-0.859727000
C	1.139923000	2.789511000	-0.089946000
C	2.402137000	2.424604000	0.472481000
C	2.695827000	1.091242000	0.836024000
C	3.829896000	0.678891000	1.662423000
C	3.829896000	-0.678891000	1.662423000
C	2.695827000	-1.091242000	0.836024000
C	2.402137000	-2.424604000	0.472481000
C	3.361557000	-3.490465000	0.825488000
C	2.911243000	-4.652245000	1.479547000
C	3.804600000	-5.657485000	1.842108000
C	5.164055000	-5.525586000	1.550728000
C	5.624092000	-4.380193000	0.893683000
C	4.734200000	-3.371788000	0.535689000
C	3.361557000	3.490465000	0.825488000
C	4.734200000	3.371788000	0.535689000
C	5.624092000	4.380193000	0.893683000
C	5.164055000	5.525586000	1.550728000
C	3.804600000	5.657485000	1.842108000
C	2.911243000	4.652245000	1.479547000
C	1.607936000	4.865027000	-1.617732000
C	-1.607936000	4.865027000	-1.617732000
H	4.506722000	1.340781000	2.191334000
H	4.506722000	-1.340781000	2.191334000
H	1.851780000	-4.755672000	1.713374000
H	3.438206000	-6.546821000	2.354812000
H	5.862557000	-6.315042000	1.828449000
H	6.681079000	-4.280086000	0.646547000
H	5.087100000	-2.496075000	-0.007580000
H	5.087100000	2.496075000	-0.007580000
H	6.681079000	4.280086000	0.646547000
H	5.862557000	6.315042000	1.828449000
H	3.438206000	6.546821000	2.354812000
H	1.851780000	4.755672000	1.713374000
F	-1.251729000	-4.997133000	-2.920339000
F	-2.900014000	-4.449180000	-1.633567000

F	-1.584668000	-6.117066000	-1.068133000
F	1.251729000	-4.997133000	-2.920339000
F	1.584668000	-6.117066000	-1.068133000
F	2.900014000	-4.449180000	-1.633567000
N	0.000000000	-2.107199000	0.243502000
N	-1.987441000	0.000000000	0.407288000
C	1.139923000	-2.789511000	-0.089946000
C	0.702974000	-3.917561000	-0.859727000
C	-0.702974000	-3.917561000	-0.859727000
C	-1.139923000	-2.789511000	-0.089946000
C	-2.402137000	-2.424604000	0.472481000
C	-2.695827000	-1.091242000	0.836024000
C	-3.829896000	-0.678891000	1.662423000
C	-3.829896000	0.678891000	1.662423000
C	-2.695827000	1.091242000	0.836024000
C	-2.402137000	2.424604000	0.472481000
C	-3.361557000	3.490465000	0.825488000
C	-2.911243000	4.652245000	1.479547000
C	-3.804600000	5.657485000	1.842108000
C	-5.164055000	5.525586000	1.550728000
C	-5.624092000	4.380193000	0.893683000
C	-4.734200000	3.371788000	0.535689000
C	-3.361557000	-3.490465000	0.825488000
C	-4.734200000	-3.371788000	0.535689000
C	-5.624092000	-4.380193000	0.893683000
C	-5.164055000	-5.525586000	1.550728000
C	-3.804600000	-5.657485000	1.842108000
C	-2.911243000	-4.652245000	1.479547000
C	-1.607936000	-4.865027000	-1.617732000
C	1.607936000	-4.865027000	-1.617732000
H	-4.506722000	-1.340781000	2.191334000
H	-4.506722000	1.340781000	2.191334000
H	-1.851780000	4.755672000	1.713374000
H	-3.438206000	6.546821000	2.354812000
H	-5.862557000	6.315042000	1.828449000
H	-6.681079000	4.280086000	0.646547000
H	-5.087100000	2.496075000	-0.007580000
H	-5.087100000	-2.496075000	-0.007580000
H	-6.681079000	-4.280086000	0.646547000
H	-5.862557000	-6.315042000	1.828449000
H	-3.438206000	-6.546821000	2.354812000
H	-1.851780000	-4.755672000	1.713374000
H	0.000000000	1.196140000	0.702922000
H	0.000000000	-1.196140000	0.702922000

8. H₂[*opp*-(CF₃)₄TPP]; *trans*1; *waved*

N	2.138268000	-0.066945000	0.135486000
N	0.025077000	2.018067000	-0.415756000
H	-0.014527000	1.000974000	-0.440675000

C	3.465373000	-4.462143000	1.652324000
C	3.366593000	-3.652381000	0.510660000
C	2.450658000	-2.471479000	0.487582000
C	2.945513000	-1.149363000	0.363907000
C	2.950459000	1.002771000	-0.102863000
C	2.507620000	2.348949000	-0.174075000
C	1.171651000	2.775848000	-0.261377000
C	-1.090680000	2.832964000	-0.432760000
C	-0.614518000	4.180750000	-0.292721000
H	-1.252214000	5.054288000	-0.247157000
C	0.745691000	4.145412000	-0.176805000
H	1.409750000	4.985731000	-0.020265000
C	3.490639000	3.452471000	0.047646000
C	4.093551000	3.578796000	1.307571000
C	4.956645000	4.641507000	1.576161000
H	5.416257000	4.728823000	2.560485000
C	5.235388000	5.582759000	0.584410000
H	5.916910000	6.408332000	0.789756000
C	4.642892000	5.461534000	-0.676208000
C	3.770352000	4.408405000	-0.940168000
H	3.310252000	4.305772000	-1.922554000
C	4.353660000	0.574285000	-0.107825000
C	4.356225000	-0.739986000	0.303028000
C	4.049737000	-4.027034000	-0.652895000
H	3.965539000	-3.405408000	-1.544063000
C	4.827772000	-5.185675000	-0.673080000
C	4.931945000	-5.978703000	0.470241000
H	5.542924000	-6.881424000	0.455809000
C	4.251384000	-5.612114000	1.635404000
H	4.332694000	-6.225577000	2.532868000
N	-2.138268000	0.066945000	-0.135486000
N	-0.025077000	-2.018067000	0.415756000
H	0.014527000	-1.000974000	0.440675000
C	-3.465373000	4.462143000	-1.652324000
C	-3.366593000	3.652381000	-0.510660000
C	-2.450658000	2.471479000	-0.487582000
C	-2.945513000	1.149363000	-0.363907000
C	-2.950459000	-1.002771000	0.102863000
C	-2.507620000	-2.348949000	0.174075000
C	-1.171651000	-2.775848000	0.261377000
C	1.090680000	-2.832964000	0.432760000
C	0.614518000	-4.180750000	0.292721000
H	1.252214000	-5.054288000	0.247157000
C	-0.745691000	-4.145412000	0.176805000
H	-1.409750000	-4.985731000	0.020265000
C	-3.490639000	-3.452471000	-0.047646000
C	-4.093551000	-3.578796000	-1.307571000
C	-4.956645000	-4.641507000	-1.576161000
H	-5.416257000	-4.728823000	-2.560485000
C	-5.235388000	-5.582759000	-0.584410000
H	-5.916910000	-6.408332000	-0.789756000

C	-4.642892000	-5.461534000	0.676208000
C	-3.770352000	-4.408405000	0.940168000
H	-3.310252000	-4.305772000	1.922554000
C	-4.353660000	-0.574285000	0.107825000
C	-4.356225000	0.739986000	-0.303028000
C	-4.049737000	4.027034000	0.652895000
H	-3.965539000	3.405408000	1.544063000
C	-4.827772000	5.185675000	0.673080000
C	-4.931945000	5.978703000	-0.470241000
H	-5.542924000	6.881424000	-0.455809000
C	-4.251384000	5.612114000	-1.635404000
H	-4.332694000	6.225577000	-2.532868000
H	-4.865539000	-6.188222000	1.457636000
H	-3.877602000	-2.837683000	-2.077199000
H	-2.929780000	4.172942000	-2.556451000
H	-5.353909000	5.466628000	1.585341000
H	4.865539000	6.188222000	-1.457636000
H	3.877602000	2.837683000	2.077199000
H	2.929780000	-4.172942000	2.556451000
H	5.353909000	-5.466628000	-1.585341000
C	5.596341000	-1.449963000	0.804680000
F	6.212857000	-2.242382000	-0.112464000
F	6.528243000	-0.549439000	1.235248000
F	5.308983000	-2.222220000	1.890942000
C	5.540144000	1.270287000	-0.746233000
F	6.422452000	0.362505000	-1.255775000
F	5.128160000	2.016654000	-1.815990000
F	6.249212000	2.086295000	0.074244000
C	-5.596341000	1.449963000	-0.804680000
F	-6.528243000	0.549439000	-1.235248000
F	-6.212857000	2.242382000	0.112464000
F	-5.308983000	2.222220000	-1.890942000
C	-5.540144000	-1.270287000	0.746233000
F	-5.128160000	-2.016654000	1.815990000
F	-6.422452000	-0.362505000	1.255775000
F	-6.249212000	-2.086295000	-0.074244000

9. H₂[*opp*-(CH₃)₄TPP]; *trans*1; *saddled*

H	0.997888000	6.061698000	-1.129297000
H	2.452230000	5.053165000	-0.993708000
H	1.900440000	5.987578000	0.392152000
H	-0.997888000	6.061698000	-1.129297000
H	-1.900440000	5.987578000	0.392152000
H	-2.452230000	5.053165000	-0.993708000
N	0.000000000	2.157128000	0.516180000
N	1.984916000	0.000000000	0.595026000
C	-1.133887000	2.919366000	0.353504000
C	-0.693760000	4.241079000	-0.037569000
C	0.693760000	4.241079000	-0.037569000

C	1.133887000	2.919366000	0.353504000
C	2.437411000	2.446387000	0.594374000
C	2.795546000	1.090985000	0.781944000
C	4.142020000	0.678910000	1.167029000
C	4.142020000	-0.678910000	1.167029000
C	2.795546000	-1.090985000	0.781944000
C	2.437411000	-2.446387000	0.594374000
C	3.533689000	-3.449953000	0.727838000
C	3.532500000	-4.354919000	1.799835000
C	4.557031000	-5.291060000	1.942084000
C	5.597809000	-5.338462000	1.010897000
C	5.613382000	-4.436366000	-0.056412000
C	4.592292000	-3.495154000	-0.193003000
C	3.533689000	3.449953000	0.727838000
C	4.592292000	3.495154000	-0.193003000
C	5.613382000	4.436366000	-0.056412000
C	5.597809000	5.338462000	1.010897000
C	4.557031000	5.291060000	1.942084000
C	3.532500000	4.354919000	1.799835000
C	1.555105000	5.390827000	-0.463940000
C	-1.555105000	5.390827000	-0.463940000
H	4.963374000	1.341035000	1.417622000
H	4.963374000	-1.341035000	1.417622000
H	2.716011000	-4.315907000	2.521602000
H	4.545014000	-5.984150000	2.783898000
H	6.396419000	-6.072780000	1.119100000
H	6.424052000	-4.465575000	-0.785200000
H	4.599281000	-2.788661000	-1.023182000
H	4.599281000	2.788661000	-1.023182000
H	6.424052000	4.465575000	-0.785200000
H	6.396419000	6.072780000	1.119100000
H	4.545014000	5.984150000	2.783898000
H	2.716011000	4.315907000	2.521602000
H	-0.997888000	-6.061698000	-1.129297000
H	-2.452230000	-5.053165000	-0.993708000
H	-1.900440000	-5.987578000	0.392152000
H	0.997888000	-6.061698000	-1.129297000
H	1.900440000	-5.987578000	0.392152000
H	2.452230000	-5.053165000	-0.993708000
N	0.000000000	-2.157128000	0.516180000
N	-1.984916000	0.000000000	0.595026000
C	1.133887000	-2.919366000	0.353504000
C	0.693760000	-4.241079000	-0.037569000
C	-0.693760000	-4.241079000	-0.037569000
C	-1.133887000	-2.919366000	0.353504000
C	-2.437411000	-2.446387000	0.594374000
C	-2.795546000	-1.090985000	0.781944000
C	-4.142020000	-0.678910000	1.167029000
C	-4.142020000	0.678910000	1.167029000
C	-2.795546000	1.090985000	0.781944000
C	-2.437411000	2.446387000	0.594374000

C	-3.533689000	3.449953000	0.727838000
C	-3.532500000	4.354919000	1.799835000
C	-4.557031000	5.291060000	1.942084000
C	-5.597809000	5.338462000	1.010897000
C	-5.613382000	4.436366000	-0.056412000
C	-4.592292000	3.495154000	-0.193003000
C	-3.533689000	-3.449953000	0.727838000
C	-4.592292000	-3.495154000	-0.193003000
C	-5.613382000	-4.436366000	-0.056412000
C	-5.597809000	-5.338462000	1.010897000
C	-4.557031000	-5.291060000	1.942084000
C	-3.532500000	-4.354919000	1.799835000
C	-1.555105000	-5.390827000	-0.463940000
C	1.555105000	-5.390827000	-0.463940000
H	-4.963374000	-1.341035000	1.417622000
H	-4.963374000	1.341035000	1.417622000
H	-2.716011000	4.315907000	2.521602000
H	-4.545014000	5.984150000	2.783898000
H	-6.396419000	6.072780000	1.119100000
H	-6.424052000	4.465575000	-0.785200000
H	-4.599281000	2.788661000	-1.023182000
H	-4.599281000	-2.788661000	-1.023182000
H	-6.424052000	-4.465575000	-0.785200000
H	-6.396419000	-6.072780000	1.119100000
H	-4.545014000	-5.984150000	2.783898000
H	-2.716011000	-4.315907000	2.521602000
H	0.000000000	1.150988000	0.702096000
H	0.000000000	-1.150988000	0.702096000

10. H₂[*opp*-(CH₃)₄TPP]; *trans*2; *saddled*

H	-1.002047000	5.956488000	1.382950000
H	-2.441655000	4.933291000	1.207380000
H	-1.929511000	5.962044000	-0.125347000
H	1.002047000	5.956488000	1.382950000
H	1.929511000	5.962044000	-0.125347000
H	2.441655000	4.933291000	1.207380000
N	0.000000000	2.071447000	-0.494790000
N	-2.074787000	0.000000000	-0.561329000
C	1.091659000	2.874027000	-0.292872000
C	0.685597000	4.209904000	0.175591000
C	-0.685597000	4.209904000	0.175591000
C	-1.091659000	2.874027000	-0.292872000
C	-2.418905000	2.465419000	-0.562643000
C	-2.834422000	1.134207000	-0.751103000
C	-4.145045000	0.686503000	-1.122484000
C	-4.145045000	-0.686503000	-1.122484000
C	-2.834422000	-1.134207000	-0.751103000
C	-2.418905000	-2.465419000	-0.562643000
C	-3.480688000	-3.497689000	-0.734516000

C	-3.387757000	-4.425678000	-1.782902000
C	-4.371849000	-5.397934000	-1.961393000
C	-5.463724000	-5.459152000	-1.091817000
C	-5.570728000	-4.535391000	-0.048837000
C	-4.590185000	-3.558087000	0.123674000
C	-3.480688000	3.497689000	-0.734516000
C	-4.590185000	3.558087000	0.123674000
C	-5.570728000	4.535391000	-0.048837000
C	-5.463724000	5.459152000	-1.091817000
C	-4.371849000	5.397934000	-1.961393000
C	-3.387757000	4.425678000	-1.782902000
C	-1.558479000	5.317845000	0.684541000
C	1.558479000	5.317845000	0.684541000
H	-1.066743000	0.000000000	-0.409282000
H	-4.972652000	1.342206000	-1.364459000
H	-4.972652000	-1.342206000	-1.364459000
H	-2.529133000	-4.377920000	-2.453039000
H	-4.286851000	-6.109968000	-2.782864000
H	-6.230130000	-6.222574000	-1.227680000
H	-6.419128000	-4.577774000	0.634822000
H	-4.666182000	-2.839940000	0.940521000
H	-4.666182000	2.839940000	0.940521000
H	-6.419128000	4.577774000	0.634822000
H	-6.230130000	6.222574000	-1.227680000
H	-4.286851000	6.109968000	-2.782864000
H	-2.529133000	4.377920000	-2.453039000
H	1.002047000	-5.956488000	1.382950000
H	2.441655000	-4.933291000	1.207380000
H	1.929511000	-5.962044000	-0.125347000
H	-1.002047000	-5.956488000	1.382950000
H	-1.929511000	-5.962044000	-0.125347000
H	-2.441655000	-4.933291000	1.207380000
N	0.000000000	-2.071447000	-0.494790000
N	2.074787000	0.000000000	-0.561329000
C	-1.091659000	-2.874027000	-0.292872000
C	-0.685597000	-4.209904000	0.175591000
C	0.685597000	-4.209904000	0.175591000
C	1.091659000	-2.874027000	-0.292872000
C	2.418905000	-2.465419000	-0.562643000
C	2.834422000	-1.134207000	-0.751103000
C	4.145045000	-0.686503000	-1.122484000
C	4.145045000	0.686503000	-1.122484000
C	2.834422000	1.134207000	-0.751103000
C	2.418905000	2.465419000	-0.562643000
C	3.480688000	3.497689000	-0.734516000
C	3.387757000	4.425678000	-1.782902000
C	4.371849000	5.397934000	-1.961393000
C	5.463724000	5.459152000	-1.091817000
C	5.570728000	4.535391000	-0.048837000
C	4.590185000	3.558087000	0.123674000
C	3.480688000	-3.497689000	-0.734516000

C	4.590185000	-3.558087000	0.123674000
C	5.570728000	-4.535391000	-0.048837000
C	5.463724000	-5.459152000	-1.091817000
C	4.371849000	-5.397934000	-1.961393000
C	3.387757000	-4.425678000	-1.782902000
C	1.558479000	-5.317845000	0.684541000
C	-1.558479000	-5.317845000	0.684541000
H	1.066743000	0.000000000	-0.409282000
H	4.972652000	-1.342206000	-1.364459000
H	4.972652000	1.342206000	-1.364459000
H	2.529133000	4.377920000	-2.453039000
H	4.286851000	6.109968000	-2.782864000
H	6.230130000	6.222574000	-1.227680000
H	6.419128000	4.577774000	0.634822000
H	4.666182000	2.839940000	0.940521000
H	4.666182000	-2.839940000	0.940521000
H	6.419128000	-4.577774000	0.634822000
H	6.230130000	-6.222574000	-1.227680000
H	4.286851000	-6.109968000	-2.782864000
H	2.529133000	-4.377920000	-2.453039000

11. H₂[*opp*-(CH₃)₄TPP]; *trans1*; *waved*

N	-1.912406000	0.385625000	0.245218000
N	-0.239228000	-1.890821000	1.086572000
H	-0.122983000	-1.001331000	0.589774000
C	-3.458825000	4.643958000	-0.367050000
C	-3.125483000	3.630158000	-1.275093000
C	-2.106242000	2.592367000	-0.917880000
C	-2.607783000	1.485107000	-0.195974000
C	-2.845589000	-0.395755000	0.881980000
C	-2.644915000	-1.647974000	1.506936000
C	-1.432334000	-2.349167000	1.599101000
C	0.777501000	-2.788535000	1.325308000
C	0.190042000	-3.906581000	2.038558000
C	-1.159076000	-3.636772000	2.207945000
C	-3.873193000	-2.252706000	2.116250000
C	-4.220638000	-1.968905000	3.443284000
C	-5.375379000	-2.515111000	4.006447000
H	-5.633654000	-2.288083000	5.041226000
C	-6.199212000	-3.348431000	3.245818000
H	-7.100459000	-3.776568000	3.685590000
C	-5.869955000	-3.620595000	1.915589000
C	-4.715066000	-3.073084000	1.354275000
H	-4.453573000	-3.279399000	0.315931000
C	-4.165432000	0.227222000	0.842731000
C	-4.018257000	1.394956000	0.169761000
C	-3.790294000	3.575865000	-2.506693000
H	-3.541182000	2.778259000	-3.207397000
C	-4.753064000	4.531803000	-2.835221000

C	-5.065612000	5.551255000	-1.932587000
H	-5.816707000	6.298799000	-2.189358000
C	-4.419632000	5.602152000	-0.694685000
H	-4.666200000	6.388687000	0.019270000
N	1.912406000	-0.385625000	-0.245218000
N	0.239228000	1.890821000	-1.086572000
H	0.122983000	1.001331000	-0.589774000
C	3.458825000	-4.643958000	0.367050000
C	3.125483000	-3.630158000	1.275093000
C	2.106242000	-2.592367000	0.917880000
C	2.607783000	-1.485107000	0.195974000
C	2.845589000	0.395755000	-0.881980000
C	2.644915000	1.647974000	-1.506936000
C	1.432334000	2.349167000	-1.599101000
C	-0.777501000	2.788535000	-1.325308000
C	-0.190042000	3.906581000	-2.038558000
C	1.159076000	3.636772000	-2.207945000
C	3.873193000	2.252706000	-2.116250000
C	4.220638000	1.968905000	-3.443284000
C	5.375379000	2.515111000	-4.006447000
H	5.633654000	2.288083000	-5.041226000
C	6.199212000	3.348431000	-3.245818000
H	7.100459000	3.776568000	-3.685590000
C	5.869955000	3.620595000	-1.915589000
C	4.715066000	3.073084000	-1.354275000
H	4.453573000	3.279399000	-0.315931000
C	4.165432000	-0.227222000	-0.842731000
C	4.018257000	-1.394956000	-0.169761000
C	3.790294000	-3.575865000	2.506693000
H	3.541182000	-2.778259000	3.207397000
C	4.753064000	-4.531803000	2.835221000
C	5.065612000	-5.551255000	1.932587000
H	5.816707000	-6.298799000	2.189358000
C	4.419632000	-5.602152000	0.694685000
H	4.666200000	-6.388687000	-0.019270000
H	6.515539000	4.259814000	-1.312238000
H	3.574947000	1.315562000	-4.030786000
H	2.953580000	-4.675774000	-0.598515000
H	5.262322000	-4.479849000	3.798112000
H	-6.515539000	-4.259814000	1.312238000
H	-3.574947000	-1.315562000	4.030786000
H	-2.953580000	4.675774000	0.598515000
H	-5.262322000	4.479849000	-3.798112000
C	0.887892000	-5.148176000	2.504736000
H	1.640915000	-4.930037000	3.273402000
H	0.173305000	-5.860925000	2.929669000
H	1.417303000	-5.651341000	1.686239000
C	-2.138954000	-4.534204000	2.900530000
H	-2.956843000	-4.836893000	2.234777000
H	-1.647284000	-5.442502000	3.263655000
H	-2.607993000	-4.040690000	3.761355000

C	2.138954000	4.534204000	-2.900530000
H	2.956843000	4.836893000	-2.234777000
H	2.607993000	4.040690000	-3.761355000
H	1.647284000	5.442502000	-3.263655000
C	-0.887892000	5.148176000	-2.504736000
H	-1.640915000	4.930037000	-3.273402000
H	-1.417303000	5.651341000	-1.686239000
H	-0.173305000	5.860925000	-2.929669000
H	4.783315000	-2.127527000	0.061789000
H	5.074020000	0.181196000	-1.270702000
H	-4.783315000	2.127527000	-0.061789000
H	-5.074020000	-0.181196000	1.270702000

12. H₂[*opp*-Br₄(CH₃)₄TPP]; *trans*1; *saddled*

H	1.016455000	5.685774000	-1.624748000
H	2.492347000	4.792273000	-1.200614000
H	1.805519000	5.946920000	-0.061831000
H	-1.016455000	5.685774000	-1.624748000
H	-1.805519000	5.946920000	-0.061831000
H	-2.492347000	4.792273000	-1.200614000
N	0.000000000	2.106676000	0.595038000
N	2.040740000	0.000000000	0.727122000
C	-1.134293000	2.842973000	0.346434000
C	-0.693857000	4.097305000	-0.224862000
C	0.693857000	4.097305000	-0.224862000
C	1.134293000	2.842973000	0.346434000
C	2.430362000	2.433917000	0.714079000
C	2.775128000	1.105899000	1.069817000
C	3.987686000	0.684922000	1.770374000
C	3.987686000	-0.684922000	1.770374000
C	2.775128000	-1.105899000	1.069817000
C	2.430362000	-2.433917000	0.714079000
C	3.488904000	-3.477232000	0.761976000
C	3.393699000	-4.543329000	1.668523000
C	4.401477000	-5.502630000	1.739760000
C	5.508738000	-5.418733000	0.890753000
C	5.604431000	-4.368397000	-0.026050000
C	4.604311000	-3.399403000	-0.085152000
C	3.488904000	3.477232000	0.761976000
C	4.604311000	3.399403000	-0.085152000
C	5.604431000	4.368397000	-0.026050000
C	5.508738000	5.418733000	0.890753000
C	4.401477000	5.502630000	1.739760000
C	3.393699000	4.543329000	1.668523000
C	1.548120000	5.181611000	-0.807763000
C	-1.548120000	5.181611000	-0.807763000
H	2.531517000	-4.595900000	2.333545000
H	4.327389000	-6.315207000	2.463115000
H	6.297774000	-6.169134000	0.946640000

H	6.466744000	-4.298977000	-0.689285000
H	4.680792000	-2.565604000	-0.782955000
H	4.680792000	2.565604000	-0.782955000
H	6.466744000	4.298977000	-0.689285000
H	6.297774000	6.169134000	0.946640000
H	4.327389000	6.315207000	2.463115000
H	2.531517000	4.595900000	2.333545000
H	-1.016455000	-5.685774000	-1.624748000
H	-2.492347000	-4.792273000	-1.200614000
H	-1.805519000	-5.946920000	-0.061831000
H	1.016455000	-5.685774000	-1.624748000
H	1.805519000	-5.946920000	-0.061831000
H	2.492347000	-4.792273000	-1.200614000
N	0.000000000	-2.106676000	0.595038000
N	-2.040740000	0.000000000	0.727122000
C	1.134293000	-2.842973000	0.346434000
C	0.693857000	-4.097305000	-0.224862000
C	-0.693857000	-4.097305000	-0.224862000
C	-1.134293000	-2.842973000	0.346434000
C	-2.430362000	-2.433917000	0.714079000
C	-2.775128000	-1.105899000	1.069817000
C	-3.987686000	-0.684922000	1.770374000
C	-3.987686000	0.684922000	1.770374000
C	-2.775128000	1.105899000	1.069817000
C	-2.430362000	2.433917000	0.714079000
C	-3.488904000	3.477232000	0.761976000
C	-3.393699000	4.543329000	1.668523000
C	-4.401477000	5.502630000	1.739760000
C	-5.508738000	5.418733000	0.890753000
C	-5.604431000	4.368397000	-0.026050000
C	-4.604311000	3.399403000	-0.085152000
C	-3.488904000	-3.477232000	0.761976000
C	-4.604311000	-3.399403000	-0.085152000
C	-5.604431000	-4.368397000	-0.026050000
C	-5.508738000	-5.418733000	0.890753000
C	-4.401477000	-5.502630000	1.739760000
C	-3.393699000	-4.543329000	1.668523000
C	-1.548120000	-5.181611000	-0.807763000
C	1.548120000	-5.181611000	-0.807763000
H	-2.531517000	4.595900000	2.333545000
H	-4.327389000	6.315207000	2.463115000
H	-6.297774000	6.169134000	0.946640000
H	-6.466744000	4.298977000	-0.689285000
H	-4.680792000	2.565604000	-0.782955000
H	-4.680792000	-2.565604000	-0.782955000
H	-6.466744000	-4.298977000	-0.689285000
H	-6.297774000	-6.169134000	0.946640000
H	-4.327389000	-6.315207000	2.463115000
H	-2.531517000	-4.595900000	2.333545000
H	0.000000000	1.135511000	0.901444000
H	0.000000000	-1.135511000	0.901444000

Br	-5.248945000	-1.719166000	2.720399000
Br	-5.248945000	1.719166000	2.720399000
Br	5.248945000	-1.719166000	2.720399000
Br	5.248945000	1.719166000	2.720399000

13. H₂[*opp*-Br₄(CH₃)₄TPP]; *trans*2; *saddled*

H	-1.012986000	5.599947000	1.805241000
H	-2.448777000	4.606700000	1.477782000
H	-1.932513000	5.814154000	0.306688000
H	1.012986000	5.599947000	1.805241000
H	1.932513000	5.814154000	0.306688000
H	2.448777000	4.606700000	1.477782000
N	0.000000000	2.005449000	-0.571930000
N	-2.104794000	0.000000000	-0.738833000
C	1.089280000	2.782267000	-0.282153000
C	0.685514000	4.040788000	0.368157000
C	-0.685514000	4.040788000	0.368157000
C	-1.089280000	2.782267000	-0.282153000
C	-2.402153000	2.447043000	-0.688722000
C	-2.801215000	1.146020000	-1.056172000
C	-3.994541000	0.692036000	-1.722477000
C	-3.994541000	-0.692036000	-1.722477000
C	-2.801215000	-1.146020000	-1.056172000
C	-2.402153000	-2.447043000	-0.688722000
C	-3.415456000	-3.532539000	-0.773526000
C	-3.244093000	-4.577669000	-1.692585000
C	-4.199409000	-5.586645000	-1.801885000
C	-5.328256000	-5.573732000	-0.978108000
C	-5.498342000	-4.545051000	-0.047554000
C	-4.551635000	-3.527119000	0.048631000
C	-3.415456000	3.532539000	-0.773526000
C	-4.551635000	3.527119000	0.048631000
C	-5.498342000	4.545051000	-0.047554000
C	-5.328256000	5.573732000	-0.978108000
C	-4.199409000	5.586645000	-1.801885000
C	-3.244093000	4.577669000	-1.692585000
C	-1.563705000	5.064494000	1.021160000
C	1.563705000	5.064494000	1.021160000
H	-1.140776000	0.000000000	-0.401516000
H	-2.361210000	-4.578281000	-2.331828000
H	-4.064821000	-6.384369000	-2.532936000
H	-6.075000000	-6.363704000	-1.062167000
H	-6.376737000	-4.532020000	0.597966000
H	-4.687559000	-2.711368000	0.759061000
H	-4.687559000	2.711368000	0.759061000
H	-6.376737000	4.532020000	0.597966000
H	-6.075000000	6.363704000	-1.062167000
H	-4.064821000	6.384369000	-2.532936000
H	-2.361210000	4.578281000	-2.331828000

H	1.012986000	-5.599947000	1.805241000
H	2.448777000	-4.606700000	1.477782000
H	1.932513000	-5.814154000	0.306688000
H	-1.012986000	-5.599947000	1.805241000
H	-1.932513000	-5.814154000	0.306688000
H	-2.448777000	-4.606700000	1.477782000
N	0.000000000	-2.005449000	-0.571930000
N	2.104794000	0.000000000	-0.738833000
C	-1.089280000	-2.782267000	-0.282153000
C	-0.685514000	-4.040788000	0.368157000
C	0.685514000	-4.040788000	0.368157000
C	1.089280000	-2.782267000	-0.282153000
C	2.402153000	-2.447043000	-0.688722000
C	2.801215000	-1.146020000	-1.056172000
C	3.994541000	-0.692036000	-1.722477000
C	3.994541000	0.692036000	-1.722477000
C	2.801215000	1.146020000	-1.056172000
C	2.402153000	2.447043000	-0.688722000
C	3.415456000	3.532539000	-0.773526000
C	3.244093000	4.577669000	-1.692585000
C	4.199409000	5.586645000	-1.801885000
C	5.328256000	5.573732000	-0.978108000
C	5.498342000	4.545051000	-0.047554000
C	4.551635000	3.527119000	0.048631000
C	3.415456000	-3.532539000	-0.773526000
C	4.551635000	-3.527119000	0.048631000
C	5.498342000	-4.545051000	-0.047554000
C	5.328256000	-5.573732000	-0.978108000
C	4.199409000	-5.586645000	-1.801885000
C	3.244093000	-4.577669000	-1.692585000
C	1.563705000	-5.064494000	1.021160000
C	-1.563705000	-5.064494000	1.021160000
H	1.140776000	0.000000000	-0.401516000
H	2.361210000	4.578281000	-2.331828000
H	4.064821000	6.384369000	-2.532936000
H	6.075000000	6.363704000	-1.062167000
H	6.376737000	4.532020000	0.597966000
H	4.687559000	2.711368000	0.759061000
H	4.687559000	-2.711368000	0.759061000
H	6.376737000	-4.532020000	0.597966000
H	6.075000000	-6.363704000	-1.062167000
H	4.064821000	-6.384369000	-2.532936000
H	2.361210000	-4.578281000	-2.331828000
Br	-5.268684000	1.727826000	-2.634990000
Br	-5.268684000	-1.727826000	-2.634990000
Br	5.268684000	-1.727826000	-2.634990000
Br	5.268684000	1.727826000	-2.634990000

14. H₂[*opp*-(CF₃)₄(CH₃)₄TPP]; *trans*1; *saddled*

H	-4.430792000	1.067449000	-3.492106000
H	-3.926103000	2.534666000	-2.623327000
H	-5.442467000	1.733711000	-2.202623000
H	-4.430792000	-1.067449000	-3.492106000
H	-5.442467000	-1.733711000	-2.202623000
H	-3.926103000	-2.534666000	-2.623327000
N	-2.137072000	0.000000000	-0.024074000
N	0.000000000	2.058051000	0.004433000
C	-2.711948000	-1.137054000	-0.536757000
C	-3.666214000	-0.694961000	-1.528198000
C	-3.666214000	0.694961000	-1.528198000
C	-2.711948000	1.137054000	-0.536757000
C	-2.385181000	2.428845000	-0.072484000
C	-1.096271000	2.687001000	0.508464000
C	-0.695575000	3.682698000	1.496464000
C	0.695575000	3.682698000	1.496464000
C	1.096271000	2.687001000	0.508464000
C	2.385181000	2.428845000	-0.072484000
C	3.334984000	3.531505000	-0.270254000
C	4.710531000	3.363217000	-0.018854000
C	5.598731000	4.416705000	-0.201946000
C	5.132563000	5.661689000	-0.639307000
C	3.769885000	5.845502000	-0.885534000
C	2.877565000	4.792251000	-0.700171000
C	-3.334984000	3.531505000	-0.270254000
C	-2.877565000	4.792251000	-0.700171000
C	-3.769885000	5.845502000	-0.885534000
C	-5.132563000	5.661689000	-0.639307000
C	-5.598731000	4.416705000	-0.201946000
C	-4.710531000	3.363217000	-0.018854000
C	-4.401770000	1.555432000	-2.508424000
C	-4.401770000	-1.555432000	-2.508424000
H	5.065296000	2.401261000	0.350693000
H	6.658505000	4.275809000	0.011916000
H	5.829990000	6.487807000	-0.778612000
H	3.400249000	6.814116000	-1.222150000
H	1.814995000	4.930603000	-0.898248000
H	-1.814995000	4.930603000	-0.898248000
H	-3.400249000	6.814116000	-1.222150000
H	-5.829990000	6.487807000	-0.778612000
H	-6.658505000	4.275809000	0.011916000
H	-5.065296000	2.401261000	0.350693000
H	4.430792000	-1.067449000	-3.492106000
H	3.926103000	-2.534666000	-2.623327000
H	5.442467000	-1.733711000	-2.202623000
H	4.430792000	1.067449000	-3.492106000
H	5.442467000	1.733711000	-2.202623000
H	3.926103000	2.534666000	-2.623327000
N	2.137072000	0.000000000	-0.024074000
N	0.000000000	-2.058051000	0.004433000
C	2.711948000	1.137054000	-0.536757000

C	3.666214000	0.694961000	-1.528198000
C	3.666214000	-0.694961000	-1.528198000
C	2.711948000	-1.137054000	-0.536757000
C	2.385181000	-2.428845000	-0.072484000
C	1.096271000	-2.687001000	0.508464000
C	0.695575000	-3.682698000	1.496464000
C	-0.695575000	-3.682698000	1.496464000
C	-1.096271000	-2.687001000	0.508464000
C	-2.385181000	-2.428845000	-0.072484000
C	-3.334984000	-3.531505000	-0.270254000
C	-4.710531000	-3.363217000	-0.018854000
C	-5.598731000	-4.416705000	-0.201946000
C	-5.132563000	-5.661689000	-0.639307000
C	-3.769885000	-5.845502000	-0.885534000
C	-2.877565000	-4.792251000	-0.700171000
C	3.334984000	-3.531505000	-0.270254000
C	2.877565000	-4.792251000	-0.700171000
C	3.769885000	-5.845502000	-0.885534000
C	5.132563000	-5.661689000	-0.639307000
C	5.598731000	-4.416705000	-0.201946000
C	4.710531000	-3.363217000	-0.018854000
C	4.401770000	-1.555432000	-2.508424000
C	4.401770000	1.555432000	-2.508424000
H	-5.065296000	-2.401261000	0.350693000
H	-6.658505000	-4.275809000	0.011916000
H	-5.829990000	-6.487807000	-0.778612000
H	-3.400249000	-6.814116000	-1.222150000
H	-1.814995000	-4.930603000	-0.898248000
H	1.814995000	-4.930603000	-0.898248000
H	3.400249000	-6.814116000	-1.222150000
H	5.829990000	-6.487807000	-0.778612000
H	6.658505000	-4.275809000	0.011916000
H	5.065296000	-2.401261000	0.350693000
H	-1.349214000	0.000000000	0.614539000
H	1.349214000	0.000000000	0.614539000
C	1.609592000	-4.460691000	2.412620000
F	1.259014000	-4.372878000	3.723272000
F	1.620769000	-5.793403000	2.095963000
F	2.898651000	-4.024283000	2.353576000
C	-1.609592000	-4.460691000	2.412620000
F	-1.620769000	-5.793403000	2.095963000
F	-1.259014000	-4.372878000	3.723272000
F	-2.898651000	-4.024283000	2.353576000
C	1.609592000	4.460691000	2.412620000
F	1.259014000	4.372878000	3.723272000
F	2.898651000	4.024283000	2.353576000
F	1.620769000	5.793403000	2.095963000
C	-1.609592000	4.460691000	2.412620000
F	-2.898651000	4.024283000	2.353576000
F	-1.259014000	4.372878000	3.723272000
F	-1.620769000	5.793403000	2.095963000

15. H₂[*opp*-(CF₃)₄(CH₃)₄TPP]; trans2; saddled

H	4.407113000	1.065757000	3.461746000
H	3.856648000	2.526393000	2.608630000
H	5.388496000	1.772920000	2.170790000
H	4.407113000	-1.065757000	3.461746000
H	5.388496000	-1.772920000	2.170790000
H	3.856648000	-2.526393000	2.608630000
N	2.024650000	0.000000000	-0.056911000
N	0.000000000	2.105503000	-0.174274000
C	2.658927000	-1.090019000	0.470620000
C	3.637154000	-0.686329000	1.496923000
C	3.637154000	0.686329000	1.496923000
C	2.658927000	1.090019000	0.470620000
C	2.403320000	2.400357000	-0.004920000
C	1.142730000	2.732686000	-0.592428000
C	0.704174000	3.769511000	-1.479244000
C	-0.704174000	3.769511000	-1.479244000
C	-1.142730000	2.732686000	-0.592428000
C	-2.403320000	2.400357000	-0.004920000
C	-3.408946000	3.455888000	0.200790000
C	-4.762292000	3.216603000	-0.101740000
C	-5.722003000	4.199531000	0.116268000
C	-5.350396000	5.438789000	0.648182000
C	-4.009286000	5.691841000	0.946140000
C	-3.044628000	4.713108000	0.715936000
C	3.408946000	3.455888000	0.200790000
C	3.044628000	4.713108000	0.715936000
C	4.009286000	5.691841000	0.946140000
C	5.350396000	5.438789000	0.648182000
C	5.722003000	4.199531000	0.116268000
C	4.762292000	3.216603000	-0.101740000
C	4.355650000	1.559258000	2.480950000
C	4.355650000	-1.559258000	2.480950000
H	0.000000000	1.254488000	0.382722000
H	-5.043177000	2.253541000	-0.527248000
H	-6.764401000	4.003789000	-0.136075000
H	-6.103297000	6.207608000	0.822068000
H	-3.713518000	6.656881000	1.357828000
H	-1.998948000	4.911345000	0.950912000
H	1.998948000	4.911345000	0.950912000
H	3.713518000	6.656881000	1.357828000
H	6.103297000	6.207608000	0.822068000
H	6.764401000	4.003789000	-0.136075000
H	5.043177000	2.253541000	-0.527248000
H	-4.407113000	-1.065757000	3.461746000
H	-3.856648000	-2.526393000	2.608630000
H	-5.388496000	-1.772920000	2.170790000
H	-4.407113000	1.065757000	3.461746000

H	-5.388496000	1.772920000	2.170790000
H	-3.856648000	2.526393000	2.608630000
N	-2.024650000	0.000000000	-0.056911000
N	0.000000000	-2.105503000	-0.174274000
C	-2.658927000	1.090019000	0.470620000
C	-3.637154000	0.686329000	1.496923000
C	-3.637154000	-0.686329000	1.496923000
C	-2.658927000	-1.090019000	0.470620000
C	-2.403320000	-2.400357000	-0.004920000
C	-1.142730000	-2.732686000	-0.592428000
C	-0.704174000	-3.769511000	-1.479244000
C	0.704174000	-3.769511000	-1.479244000
C	1.142730000	-2.732686000	-0.592428000
C	2.403320000	-2.400357000	-0.004920000
C	3.408946000	-3.455888000	0.200790000
C	4.762292000	-3.216603000	-0.101740000
C	5.722003000	-4.199531000	0.116268000
C	5.350396000	-5.438789000	0.648182000
C	4.009286000	-5.691841000	0.946140000
C	3.044628000	-4.713108000	0.715936000
C	-3.408946000	-3.455888000	0.200790000
C	-3.044628000	-4.713108000	0.715936000
C	-4.009286000	-5.691841000	0.946140000
C	-5.350396000	-5.438789000	0.648182000
C	-5.722003000	-4.199531000	0.116268000
C	-4.762292000	-3.216603000	-0.101740000
C	-4.355650000	-1.559258000	2.480950000
C	-4.355650000	1.559258000	2.480950000
H	0.000000000	-1.254488000	0.382722000
H	5.043177000	-2.253541000	-0.527248000
H	6.764401000	-4.003789000	-0.136075000
H	6.103297000	-6.207608000	0.822068000
H	3.713518000	-6.656881000	1.357828000
H	1.998948000	-4.911345000	0.950912000
H	-1.998948000	-4.911345000	0.950912000
H	-3.713518000	-6.656881000	1.357828000
H	-6.103297000	-6.207608000	0.822068000
H	-6.764401000	-4.003789000	-0.136075000
H	-5.043177000	-2.253541000	-0.527248000
C	-1.615696000	4.638484000	-2.317277000
F	-1.240778000	4.701409000	-3.618866000
F	-2.896379000	4.188165000	-2.327480000
F	-1.635185000	5.925119000	-1.847912000
C	1.615696000	4.638484000	-2.317277000
F	1.635185000	5.925119000	-1.847912000
F	2.896379000	4.188165000	-2.327480000
F	1.240778000	4.701409000	-3.618866000
C	-1.615696000	-4.638484000	-2.317277000
F	-1.240778000	-4.701409000	-3.618866000
F	-1.635185000	-5.925119000	-1.847912000
F	-2.896379000	-4.188165000	-2.327480000

C	1.615696000	-4.638484000	-2.317277000
F	1.635185000	-5.925119000	-1.847912000
F	1.240778000	-4.701409000	-3.618866000
F	2.896379000	-4.188165000	-2.327480000

16. H₂[adj-Br₄TPP]; trans; saddled

N	2.053628000	-0.007714000	-0.666148000
N	-0.004399000	2.111135000	-0.785814000
C	2.809162000	-1.102301000	-0.348883000
C	4.051106000	-0.675476000	0.292257000
C	4.042002000	0.693564000	0.295720000
C	2.800876000	1.103541000	-0.361476000
C	2.448820000	2.422570000	-0.728666000
C	1.143874000	2.816138000	-1.082870000
C	0.691773000	4.039133000	-1.695814000
C	-0.691233000	4.053815000	-1.667723000
C	-1.144193000	2.833875000	-1.055921000
C	-2.455244000	2.417781000	-0.742747000
C	-3.508432000	3.465838000	-0.652801000
C	-4.616676000	3.462294000	-1.513847000
C	-5.568949000	4.477978000	-1.443541000
C	-5.435665000	5.501606000	-0.501388000
C	-4.347710000	5.500968000	0.375311000
C	-3.388236000	4.493315000	0.296333000
C	3.506893000	3.467826000	-0.729700000
C	3.436711000	4.550934000	0.159469000
C	4.443728000	5.512503000	0.177619000
C	5.519242000	5.415904000	-0.709875000
C	5.587617000	4.348299000	-1.609036000
C	4.592443000	3.373467000	-1.611873000
H	-0.021223000	1.153841000	-0.432510000
Br	1.723596000	5.323842000	-2.595785000
Br	-1.742788000	5.365725000	-2.502470000
H	-4.703677000	2.673933000	-2.261125000
H	-6.413439000	4.476538000	-2.133085000
H	-6.178041000	6.298530000	-0.450702000
H	-4.241049000	6.294097000	1.115691000
H	-2.526165000	4.500320000	0.963726000
H	2.590265000	4.623687000	0.842098000
H	4.388809000	6.343237000	0.881459000
H	6.304811000	6.172225000	-0.699206000
H	6.423954000	4.272039000	-2.304041000
H	4.643732000	2.531245000	-2.301397000
N	-2.011797000	-0.015609000	-0.659122000
N	-0.010619000	-2.109207000	-0.706614000
C	-2.821772000	1.080340000	-0.491488000
C	-4.173358000	0.676585000	-0.115008000
C	-4.182926000	-0.681398000	-0.128061000
C	-2.832766000	-1.099093000	-0.492598000

C	-2.459183000	-2.449171000	-0.681707000
C	-1.135657000	-2.888115000	-0.851673000
C	-0.681611000	-4.212786000	-1.162279000
C	0.690394000	-4.200281000	-1.174312000
C	1.128410000	-2.869186000	-0.860270000
C	2.446104000	-2.441722000	-0.639882000
C	3.517548000	-3.467525000	-0.737463000
C	4.548158000	-3.301975000	-1.676640000
C	5.590689000	-4.222987000	-1.753857000
C	5.621475000	-5.320260000	-0.889467000
C	4.593671000	-5.501054000	0.040041000
C	3.545028000	-4.585731000	0.110943000
C	-3.529641000	-3.481742000	-0.713774000
C	-3.529742000	-4.553087000	0.194998000
C	-4.539597000	-5.514995000	0.160369000
C	-5.564058000	-5.423860000	-0.785431000
C	-5.573628000	-4.363633000	-1.695618000
C	-4.566076000	-3.400053000	-1.659589000
H	-0.035038000	-1.093629000	-0.601979000
H	-1.335405000	-5.054465000	-1.357358000
H	1.355154000	-5.030485000	-1.380105000
H	4.531321000	-2.431032000	-2.331919000
H	6.387576000	-4.078782000	-2.483623000
H	6.445482000	-6.032420000	-0.938344000
H	4.617006000	-6.350822000	0.722701000
H	2.759529000	-4.705507000	0.856903000
H	-2.736230000	-4.615789000	0.940050000
H	-4.530229000	-6.334434000	0.879593000
H	-6.352854000	-6.175940000	-0.812271000
H	-6.365977000	-4.289099000	-2.440903000
H	-4.566882000	-2.574940000	-2.371887000
H	-4.990894000	1.345895000	0.128493000
H	-5.010415000	-1.343473000	0.102572000
Br	5.317192000	1.737799000	1.211145000
Br	5.340086000	-1.718932000	1.188382000

17. H₂[adj-Br₄TPP]; cis1; saddled

N	2.041926000	-0.138726000	-0.749738000
N	-0.143622000	2.062925000	-0.698040000
C	2.844455000	-1.208688000	-0.480086000
C	4.000786000	-0.783792000	0.296179000
C	3.873445000	0.570250000	0.469736000
C	2.670511000	0.977202000	-0.260338000
C	2.305380000	2.307950000	-0.571841000
C	1.018575000	2.720636000	-0.994409000
C	0.702260000	3.968553000	-1.696296000
C	-0.664699000	4.058142000	-1.744091000
C	-1.179521000	2.868019000	-1.080652000
C	-2.538560000	2.542637000	-0.836610000

C	-3.561702000	3.615337000	-0.819772000
C	-4.664919000	3.590259000	-1.687956000
C	-5.580424000	4.641712000	-1.696711000
C	-5.415268000	5.723578000	-0.827833000
C	-4.332378000	5.746564000	0.055300000
C	-3.411183000	4.701900000	0.057947000
C	3.362800000	3.344884000	-0.473490000
C	3.187916000	4.467354000	0.350787000
C	4.184651000	5.434813000	0.443660000
C	5.357660000	5.305686000	-0.305626000
C	5.534957000	4.197462000	-1.138604000
C	4.549645000	3.216845000	-1.212746000
Br	1.855938000	5.145861000	-2.611619000
Br	-1.619966000	5.356078000	-2.721692000
H	-4.772104000	2.760904000	-2.386928000
H	-6.418155000	4.623784000	-2.394263000
H	-6.127187000	6.549183000	-0.841713000
H	-4.199816000	6.586908000	0.736912000
H	-2.551717000	4.725243000	0.727955000
H	2.264948000	4.566404000	0.921570000
H	4.045662000	6.297047000	1.096002000
H	6.133432000	6.069468000	-0.241437000
H	6.446374000	4.097245000	-1.728509000
H	4.681789000	2.347391000	-1.856066000
N	-2.120419000	0.122303000	-0.700316000
N	0.100475000	-2.110757000	-0.778031000
C	-2.949176000	1.224923000	-0.594803000
C	-4.253355000	0.734832000	-0.274590000
C	-4.186564000	-0.634928000	-0.218738000
C	-2.835970000	-1.040567000	-0.502602000
C	-2.391091000	-2.369937000	-0.617303000
C	-1.077541000	-2.822639000	-0.842179000
C	-0.712112000	-4.169447000	-1.189680000
C	0.653007000	-4.233171000	-1.319485000
C	1.183466000	-2.938663000	-1.020275000
C	2.516405000	-2.541821000	-0.850840000
C	3.598873000	-3.534610000	-1.031340000
C	4.655854000	-3.240142000	-1.910380000
C	5.712436000	-4.132508000	-2.073132000
C	5.734908000	-5.330731000	-1.354358000
C	4.687951000	-5.635351000	-0.480394000
C	3.625411000	-4.747440000	-0.322863000
C	-3.433261000	-3.434949000	-0.498623000
C	-3.411130000	-4.319953000	0.590378000
C	-4.379237000	-5.316777000	0.714350000
C	-5.379957000	-5.444910000	-0.252066000
C	-5.407548000	-4.571871000	-1.342512000
C	-4.441496000	-3.572038000	-1.464271000
H	0.283427000	-1.114017000	-0.609420000
H	-1.424984000	-4.972577000	-1.334068000
H	1.251017000	-5.094523000	-1.592891000

H	4.642327000	-2.296145000	-2.455278000
H	6.526056000	-3.889199000	-2.756666000
H	6.568914000	-6.023069000	-1.470861000
H	4.708277000	-6.561541000	0.094445000
H	2.830886000	-4.963923000	0.390790000
H	-2.628636000	-4.214185000	1.342298000
H	-4.354035000	-5.992139000	1.569805000
H	-6.136387000	-6.223932000	-0.155854000
H	-6.181423000	-4.671682000	-2.103907000
H	-4.456784000	-2.890117000	-2.314796000
H	-5.119878000	1.363648000	-0.106390000
H	-4.994225000	-1.323035000	-0.000594000
Br	4.910477000	1.570653000	1.687337000
Br	5.296951000	-1.857367000	1.142652000
H	-1.112975000	0.288465000	-0.814297000

18. H₂[*adj*-(CN)₄TPP]; *trans*; *saddled*

N	2.068954000	-0.000146000	-0.613643000
N	0.006657000	2.135399000	-0.717414000
C	2.854457000	-1.098216000	-0.426390000
C	4.201060000	-0.695719000	-0.013859000
C	4.202447000	0.691774000	-0.003075000
C	2.858182000	1.100426000	-0.420569000
C	2.475590000	2.443294000	-0.640476000
C	1.157309000	2.878717000	-0.869237000
C	0.726331000	4.198016000	-1.253681000
C	-0.677003000	4.204309000	-1.271675000
C	-1.128019000	2.889001000	-0.906220000
C	-2.454637000	2.440238000	-0.746748000
C	-3.529044000	3.474016000	-0.748385000
C	-4.443591000	3.552710000	-1.809349000
C	-5.435240000	4.532464000	-1.810361000
C	-5.532672000	5.431938000	-0.746030000
C	-4.637468000	5.347826000	0.322191000
C	-3.637646000	4.376441000	0.320141000
C	3.533149000	3.489304000	-0.636390000
C	3.613743000	4.406764000	0.421763000
C	4.612776000	5.375549000	0.430095000
C	5.522690000	5.448867000	-0.626367000
C	5.439998000	4.546081000	-1.688277000
C	4.455527000	3.562085000	-1.690738000
H	-0.015116000	1.130741000	-0.527553000
H	-4.356784000	2.852263000	-2.639896000
H	-6.129170000	4.599109000	-2.648170000
H	-6.304594000	6.201641000	-0.751443000
H	-4.711713000	6.046513000	1.155191000
H	-2.929365000	4.313030000	1.146695000
H	2.897076000	4.342889000	1.240778000
H	4.680757000	6.076937000	1.260951000

H	6.300148000	6.212637000	-0.621716000
H	6.147967000	4.606247000	-2.514202000
H	4.386080000	2.848034000	-2.511406000
N	-2.008027000	-0.000723000	-0.654223000
N	-0.006673000	-2.107715000	-0.609901000
C	-2.833501000	1.095477000	-0.578243000
C	-4.219401000	0.694225000	-0.343906000
C	-4.224930000	-0.660625000	-0.321045000
C	-2.842074000	-1.082564000	-0.535044000
C	-2.460483000	-2.439732000	-0.625616000
C	-1.133013000	-2.890390000	-0.713306000
C	-0.684703000	-4.237159000	-0.929761000
C	0.685044000	-4.230382000	-0.947292000
C	1.128807000	-2.880483000	-0.728192000
C	2.455757000	-2.448167000	-0.610115000
C	3.511922000	-3.492263000	-0.710866000
C	4.406240000	-3.470814000	-1.792995000
C	5.409093000	-4.432357000	-1.897027000
C	5.535157000	-5.419740000	-0.917921000
C	4.645143000	-5.452732000	0.158201000
C	3.632309000	-4.500880000	0.257579000
C	-3.528382000	-3.479680000	-0.650515000
C	-3.612269000	-4.447818000	0.363484000
C	-4.613822000	-5.419351000	0.335760000
C	-5.541056000	-5.441638000	-0.709042000
C	-5.464395000	-4.485068000	-1.724640000
C	-4.467486000	-3.509409000	-1.694789000
H	-0.028376000	-1.088758000	-0.547454000
H	-1.343682000	-5.085760000	-1.070231000
H	1.348398000	-5.072670000	-1.102934000
H	4.310819000	-2.689170000	-2.547060000
H	6.100602000	-4.404520000	-2.738814000
H	6.331327000	-6.160630000	-0.989585000
H	4.748325000	-6.215499000	0.929855000
H	2.946651000	-4.510661000	1.104870000
H	-2.892435000	-4.424518000	1.182032000
H	-4.672565000	-6.158095000	1.135406000
H	-6.322117000	-6.201989000	-0.731290000
H	-6.181376000	-4.500107000	-2.545801000
H	-4.403199000	-2.763951000	-2.487577000
H	-5.056090000	1.370021000	-0.206151000
H	-5.068371000	-1.322400000	-0.157559000
C	-1.457779000	5.313646000	-1.676292000
N	-2.036758000	6.257580000	-2.039328000
C	1.516661000	5.304533000	-1.647643000
N	2.086022000	6.253559000	-2.012946000
C	5.293784000	1.476749000	0.438225000
N	6.220981000	2.062950000	0.834492000
C	5.284472000	-1.498588000	0.414501000
N	6.195061000	-2.118946000	0.796830000

19. H₂[*adj*-(CN)₄TPP]; *cis1*; *saddled*

N	2.065359000	-0.131408000	-0.696301000
N	-0.135563000	2.066009000	-0.674774000
C	2.888848000	-1.180774000	-0.436401000
C	4.144425000	-0.717652000	0.144242000
C	4.055370000	0.669666000	0.180283000
C	2.749700000	1.010866000	-0.395654000
C	2.331772000	2.336381000	-0.675023000
C	1.007930000	2.753926000	-0.962477000
C	0.669047000	4.064725000	-1.527694000
C	-0.718749000	4.151300000	-1.501613000
C	-1.184120000	2.890190000	-0.935349000
C	-2.546589000	2.540353000	-0.704918000
C	-3.564646000	3.611997000	-0.617992000
C	-4.680095000	3.636680000	-1.471649000
C	-5.607389000	4.673142000	-1.388245000
C	-5.441909000	5.689032000	-0.443652000
C	-4.343505000	5.666099000	0.418662000
C	-3.408133000	4.638721000	0.329612000
C	3.377965000	3.386260000	-0.662099000
C	3.296949000	4.455643000	0.246204000
C	4.287688000	5.431240000	0.267455000
C	5.349965000	5.367849000	-0.637216000
C	5.429995000	4.317219000	-1.554179000
C	4.459286000	3.321468000	-1.557451000
H	-4.790800000	2.858841000	-2.227126000
H	-6.454001000	4.697338000	-2.074206000
H	-6.164220000	6.503186000	-0.386159000
H	-4.209457000	6.456997000	1.156277000
H	-2.543807000	4.622229000	0.993762000
H	2.462354000	4.497563000	0.945771000
H	4.230801000	6.246570000	0.987912000
H	6.118765000	6.140369000	-0.627555000
H	6.254182000	4.273690000	-2.265382000
H	4.513872000	2.496122000	-2.267073000
N	-2.115758000	0.116134000	-0.694960000
N	0.117701000	-2.114288000	-0.701708000
C	-2.952261000	1.210978000	-0.551635000
C	-4.263606000	0.698750000	-0.288068000
C	-4.194277000	-0.669186000	-0.314227000
C	-2.832124000	-1.055828000	-0.578491000
C	-2.380464000	-2.382375000	-0.707309000
C	-1.052277000	-2.831673000	-0.830463000
C	-0.662226000	-4.191161000	-1.101973000
C	0.706099000	-4.258843000	-1.117634000
C	1.214558000	-2.948509000	-0.843066000
C	2.542217000	-2.542076000	-0.676600000
C	3.615662000	-3.558927000	-0.757900000
C	4.649556000	-3.399330000	-1.696837000
C	5.678473000	-4.333681000	-1.779609000

C	5.695895000	-5.433434000	-0.918967000
C	4.673142000	-5.601419000	0.017712000
C	3.635279000	-4.675218000	0.094812000
C	-3.437740000	-3.441114000	-0.714410000
C	-3.528062000	-4.364858000	0.338299000
C	-4.514494000	-5.352189000	0.331827000
C	-5.421994000	-5.429527000	-0.727650000
C	-5.339892000	-4.514389000	-1.780108000
C	-4.355062000	-3.525390000	-1.773101000
H	0.288381000	-1.108493000	-0.580373000
H	-1.362381000	-4.999951000	-1.273124000
H	1.324379000	-5.128342000	-1.307657000
H	4.637305000	-2.533714000	-2.359442000
H	6.474674000	-4.197910000	-2.511174000
H	6.511288000	-6.154711000	-0.971436000
H	4.692944000	-6.449114000	0.702460000
H	2.851906000	-4.787584000	0.844268000
H	-2.819503000	-4.300070000	1.164412000
H	-4.576099000	-6.060396000	1.158279000
H	-6.192226000	-6.201123000	-0.732812000
H	-6.042187000	-4.572162000	-2.611868000
H	-4.286278000	-2.811177000	-2.594030000
H	-5.134603000	1.315009000	-0.098240000
H	-5.002797000	-1.371980000	-0.152661000
H	-1.109163000	0.288675000	-0.805912000
C	5.194490000	-1.489185000	0.693573000
N	6.057297000	-2.112956000	1.169630000
C	5.009011000	1.508906000	0.804274000
N	5.807900000	2.149194000	1.362840000
C	1.511368000	5.026427000	-2.134923000
N	2.155125000	5.831465000	-2.680586000
C	-1.487436000	5.205044000	-2.047999000
N	-2.108149000	6.071359000	-2.521715000

20. H₂[*adj*-(CF₃)₄TPP]; trans; saddled

N	2.144449000	0.041913000	-0.690341000
N	0.047817000	2.200682000	-0.663393000
C	2.853185000	-1.046322000	-0.318798000
C	3.895124000	-0.677622000	0.640732000
C	3.775546000	0.688401000	0.830054000
C	2.740381000	1.130193000	-0.102541000
C	2.476083000	2.439446000	-0.579947000
C	1.205401000	2.758415000	-1.148986000
C	0.787810000	3.768569000	-2.070741000
C	-0.613487000	3.860104000	-1.999834000
C	-1.071647000	2.855315000	-1.091865000
C	-2.381983000	2.493181000	-0.635219000
C	-3.378136000	3.566384000	-0.409503000
C	-4.656939000	3.530085000	-0.991083000

C	-5.586402000	4.531242000	-0.718646000
C	-5.256536000	5.581095000	0.142908000
C	-3.986525000	5.631504000	0.721495000
C	-3.051865000	4.637237000	0.440120000
C	3.494718000	3.488901000	-0.487890000
C	3.140794000	4.811936000	-0.156098000
C	4.113922000	5.798994000	-0.051893000
C	5.456998000	5.488305000	-0.286772000
C	5.820227000	4.182796000	-0.627468000
C	4.850543000	3.191129000	-0.728216000
H	0.012925000	1.391826000	-0.047147000
H	-4.902011000	2.723257000	-1.680555000
H	-6.569582000	4.498070000	-1.188221000
H	-5.985667000	6.363112000	0.355558000
H	-3.721381000	6.449566000	1.391097000
H	-2.058183000	4.678482000	0.886691000
H	2.098189000	5.050427000	0.050943000
H	3.827413000	6.814465000	0.221144000
H	6.218754000	6.263851000	-0.205544000
H	6.864137000	3.938748000	-0.822935000
H	5.129745000	2.179498000	-1.019201000
N	-1.933138000	0.065293000	-0.611422000
N	0.080068000	-2.016051000	-0.765825000
C	-2.724944000	1.164349000	-0.343619000
C	-4.028889000	0.742946000	0.172528000
C	-4.038190000	-0.612594000	0.123063000
C	-2.727049000	-1.016686000	-0.386729000
C	-2.364508000	-2.364483000	-0.645843000
C	-1.050995000	-2.784548000	-0.906685000
C	-0.612657000	-4.087540000	-1.333569000
C	0.752009000	-4.067695000	-1.432357000
C	1.214824000	-2.762603000	-1.030000000
C	2.533204000	-2.362402000	-0.803082000
C	3.623327000	-3.315306000	-1.121650000
C	4.587872000	-2.934982000	-2.070172000
C	5.610656000	-3.809886000	-2.429984000
C	5.694309000	-5.071333000	-1.835880000
C	4.747714000	-5.454394000	-0.882081000
C	3.716778000	-4.585233000	-0.529937000
C	-3.434888000	-3.396501000	-0.652333000
C	-3.368955000	-4.513658000	0.198126000
C	-4.380266000	-5.474637000	0.190353000
C	-5.472211000	-5.337814000	-0.670587000
C	-5.548761000	-4.232172000	-1.521601000
C	-4.540595000	-3.268444000	-1.511080000
H	0.057406000	-1.002132000	-0.640477000
H	-1.277570000	-4.916069000	-1.547600000
H	1.400689000	-4.878419000	-1.741412000
H	4.520860000	-1.947161000	-2.526215000
H	6.347356000	-3.504474000	-3.173277000
H	6.500387000	-5.752226000	-2.109789000

H	4.819771000	-6.430218000	-0.401604000
H	2.995653000	-4.868377000	0.236083000
H	-2.523425000	-4.612592000	0.879180000
H	-4.318836000	-6.329410000	0.864320000
H	-6.262006000	-6.089406000	-0.677014000
H	-6.394663000	-4.121796000	-2.200457000
H	-4.594564000	-2.408915000	-2.179316000
H	-4.814469000	1.400831000	0.526873000
H	-4.834876000	-1.285494000	0.422533000
C	4.822898000	-1.637816000	1.338942000
F	5.513522000	-1.089182000	2.366060000
F	4.137106000	-2.707600000	1.848868000
F	5.763436000	-2.136056000	0.480233000
C	4.341117000	1.486477000	1.984236000
F	3.780552000	2.723287000	2.087841000
F	4.074772000	0.874685000	3.176832000
F	5.690436000	1.662311000	1.906820000
C	1.668467000	4.403996000	-3.125296000
F	1.708740000	5.762132000	-3.018040000
F	2.949254000	3.957398000	-3.084352000
F	1.218847000	4.099140000	-4.376612000
C	-1.525335000	4.798286000	-2.752525000
F	-0.942628000	5.373798000	-3.828664000
F	-2.640329000	4.154564000	-3.202913000
F	-1.944634000	5.825975000	-1.952278000

21. H₂[*adj*-(CF₃)₄TPP]; *cis1*; *saddled*

N	2.143499000	-0.024207000	-0.687009000
N	-0.034077000	2.142844000	-0.589812000
C	2.870042000	-1.090020000	-0.280539000
C	3.850740000	-0.693560000	0.720646000
C	3.685880000	0.673906000	0.892402000
C	2.668667000	1.078880000	-0.071769000
C	2.374992000	2.379916000	-0.570155000
C	1.097256000	2.682785000	-1.130266000
C	0.746545000	3.717619000	-2.094473000
C	-0.630578000	3.872740000	-2.003409000
C	-1.080174000	2.874842000	-1.043330000
C	-2.420960000	2.584887000	-0.602258000
C	-3.381736000	3.674880000	-0.346216000
C	-4.690340000	3.660059000	-0.860998000
C	-5.577393000	4.692792000	-0.567003000
C	-5.174653000	5.753313000	0.249621000
C	-3.875532000	5.781303000	0.762195000
C	-2.982999000	4.755899000	0.460172000
C	3.395909000	3.429228000	-0.511865000
C	3.037975000	4.763107000	-0.227992000
C	4.007075000	5.758484000	-0.171816000
C	5.349083000	5.444953000	-0.405591000

C	5.718099000	4.127142000	-0.690831000
C	4.753743000	3.127262000	-0.741381000
H	-4.990268000	2.851371000	-1.526582000
H	-6.582701000	4.678667000	-0.988422000
H	-5.869609000	6.561696000	0.477333000
H	-3.554619000	6.608322000	1.395480000
H	-1.966615000	4.776488000	0.852791000
H	1.995992000	5.000979000	-0.019585000
H	3.717502000	6.782854000	0.061393000
H	6.107442000	6.227188000	-0.364320000
H	6.762301000	3.881435000	-0.883077000
H	5.036737000	2.105994000	-0.991747000
N	-2.045558000	0.150172000	-0.668366000
N	0.151348000	-2.039248000	-0.711951000
C	-2.811618000	1.266508000	-0.355921000
C	-4.053522000	0.764353000	0.156800000
C	-4.023493000	-0.605068000	0.089617000
C	-2.748588000	-1.009295000	-0.439765000
C	-2.329770000	-2.331707000	-0.693892000
C	-1.005761000	-2.743424000	-0.948297000
C	-0.598029000	-4.008929000	-1.498759000
C	0.770699000	-4.031575000	-1.573264000
C	1.269686000	-2.796481000	-1.040124000
C	2.585786000	-2.410826000	-0.783625000
C	3.683123000	-3.351339000	-1.082610000
C	4.742468000	-2.916025000	-1.898835000
C	5.778756000	-3.782812000	-2.236169000
C	5.782479000	-5.092763000	-1.750599000
C	4.742856000	-5.531986000	-0.926104000
C	3.698932000	-4.670362000	-0.596674000
C	-3.379361000	-3.387897000	-0.696550000
C	-3.274211000	-4.503178000	0.152285000
C	-4.256888000	-5.492967000	0.150834000
C	-5.359430000	-5.385760000	-0.700969000
C	-5.474721000	-4.282067000	-1.550167000
C	-4.493848000	-3.290288000	-1.547144000
H	0.261869000	-1.095217000	-0.342492000
H	-1.288793000	-4.780291000	-1.818723000
H	1.395525000	-4.823040000	-1.969880000
H	4.737745000	-1.890922000	-2.269228000
H	6.589024000	-3.433707000	-2.876168000
H	6.599799000	-5.767655000	-2.005256000
H	4.753955000	-6.545958000	-0.525888000
H	2.907076000	-4.998156000	0.076065000
H	-2.418039000	-4.580034000	0.822776000
H	-4.164923000	-6.347034000	0.822039000
H	-6.126851000	-6.160169000	-0.702918000
H	-6.327886000	-4.196604000	-2.223393000
H	-4.576818000	-2.433478000	-2.216098000
H	-4.853614000	1.387190000	0.538902000
H	-4.796983000	-1.297841000	0.400062000

H	-1.093751000	0.260107000	-1.016128000
C	4.765279000	-1.636002000	1.453417000
F	5.337188000	-1.106556000	2.559614000
F	4.096803000	-2.763669000	1.853875000
F	5.798934000	-2.052329000	0.655833000
C	4.214287000	1.495632000	2.045278000
F	3.687661000	2.748705000	2.087599000
F	3.884547000	0.926822000	3.244258000
F	5.572225000	1.632145000	2.019044000
C	1.635160000	4.275600000	-3.182006000
F	1.738697000	5.635846000	-3.130196000
F	2.900152000	3.777626000	-3.142540000
F	1.160016000	3.948688000	-4.421587000
C	-1.526844000	4.807004000	-2.769965000
F	-0.953103000	5.349124000	-3.869301000
F	-2.663956000	4.170240000	-3.193049000
F	-1.930034000	5.862727000	-1.993721000

22. H₂[*adj*-(CH₃)₄TPP]; *trans*; *saddled*

N	2.047656000	0.008605000	-0.586209000
N	0.013930000	2.130624000	-0.735829000
C	2.830077000	-1.075942000	-0.293506000
C	4.099809000	-0.662770000	0.324175000
C	4.086326000	0.708456000	0.336200000
C	2.815510000	1.107061000	-0.298587000
C	2.455746000	2.430473000	-0.658224000
C	1.153546000	2.858315000	-0.994802000
C	0.714373000	4.124876000	-1.541591000
C	-0.673590000	4.144095000	-1.502987000
C	-1.116881000	2.879010000	-0.965333000
C	-2.427336000	2.438912000	-0.686110000
C	-3.494661000	3.472411000	-0.569484000
C	-4.600291000	3.486710000	-1.435317000
C	-5.586870000	4.465510000	-1.312905000
C	-5.490107000	5.439331000	-0.315187000
C	-4.401346000	5.426513000	0.560631000
C	-3.411531000	4.452390000	0.432256000
C	3.531909000	3.459741000	-0.683580000
C	3.506211000	4.552734000	0.195798000
C	4.522559000	5.506940000	0.173809000
C	5.573768000	5.390193000	-0.739997000
C	5.605807000	4.308894000	-1.625052000
C	4.596374000	3.346982000	-1.591028000
H	0.007153000	1.150965000	-0.450929000
H	-4.669367000	2.728298000	-2.215254000
H	-6.433228000	4.469379000	-2.000380000
H	-6.262141000	6.203066000	-0.218365000
H	-4.324435000	6.176632000	1.348489000
H	-2.558062000	4.440670000	1.110837000

H	2.680811000	4.640042000	0.903003000
H	4.495582000	6.344828000	0.871189000
H	6.366106000	6.138925000	-0.761349000
H	6.421633000	4.213830000	-2.342278000
H	4.618607000	2.495599000	-2.271529000
N	-1.999681000	-0.003103000	-0.651546000
N	0.004129000	-2.094764000	-0.675934000
C	-2.804360000	1.093210000	-0.473048000
C	-4.160933000	0.687117000	-0.116001000
C	-4.175112000	-0.671611000	-0.146327000
C	-2.823830000	-1.088362000	-0.500539000
C	-2.446312000	-2.437427000	-0.687846000
C	-1.119336000	-2.874332000	-0.841222000
C	-0.658752000	-4.195053000	-1.152344000
C	0.714898000	-4.178776000	-1.149633000
C	1.146295000	-2.850027000	-0.819868000
C	2.462604000	-2.412190000	-0.588233000
C	3.529486000	-3.444127000	-0.710539000
C	4.532327000	-3.288663000	-1.680946000
C	5.545258000	-4.237353000	-1.817205000
C	5.575632000	-5.356237000	-0.980753000
C	4.580738000	-5.524276000	-0.013958000
C	3.563342000	-4.578904000	0.116141000
C	-3.514092000	-3.473567000	-0.730593000
C	-3.515964000	-4.549844000	0.173363000
C	-4.521915000	-5.515748000	0.130861000
C	-5.543780000	-5.424549000	-0.817868000
C	-5.553198000	-4.359686000	-1.722581000
C	-4.548344000	-3.393031000	-1.679032000
H	-0.016617000	-1.079392000	-0.562022000
H	-1.307254000	-5.037511000	-1.361868000
H	1.380694000	-5.007825000	-1.356845000
H	4.508005000	-2.409163000	-2.324741000
H	6.313813000	-4.103252000	-2.579073000
H	6.370434000	-6.095498000	-1.082790000
H	4.600308000	-6.392445000	0.645517000
H	2.793463000	-4.701411000	0.878340000
H	-2.725210000	-4.613394000	0.921184000
H	-4.511819000	-6.338528000	0.846516000
H	-6.329858000	-6.179466000	-0.851226000
H	-6.344048000	-4.283643000	-2.469556000
H	-4.550490000	-2.564381000	-2.387160000
H	-4.980095000	1.352313000	0.133838000
H	-5.006215000	-1.333769000	0.071848000
C	-1.534401000	5.251176000	-2.030798000
H	-0.986686000	5.845255000	-2.772590000
H	-2.445592000	4.869130000	-2.503453000
H	-1.856652000	5.936172000	-1.233549000
C	1.561220000	5.199771000	-2.155679000
H	1.845114000	5.973584000	-1.428266000
H	2.489898000	4.800758000	-2.574461000

H	1.010936000	5.697683000	-2.964404000
C	5.104661000	1.579613000	1.009904000
H	4.639600000	2.443679000	1.498522000
H	5.648187000	1.011276000	1.775701000
H	5.850032000	1.979891000	0.308411000
C	5.140803000	-1.537636000	0.954857000
H	4.693682000	-2.410669000	1.445175000
H	5.860036000	-1.926350000	0.219838000
H	5.711344000	-0.980482000	1.708962000

23. H₂[adj-(CH₃)₄TPP]; cis1; saddled

symmetry c1

N	2.144444000	-0.097741000	-0.594894000
N	-0.099929000	2.147321000	-0.684375000
C	2.941590000	-1.195929000	-0.337218000
C	4.155875000	-0.706633000	0.255921000
C	4.067984000	0.677704000	0.313900000
C	2.807396000	1.074128000	-0.288402000
C	2.381352000	2.384145000	-0.613409000
C	1.077551000	2.814888000	-0.957020000
C	0.692839000	4.084903000	-1.547137000
C	-0.692467000	4.171519000	-1.516525000
C	-1.193097000	2.948102000	-0.952073000
C	-2.517726000	2.543286000	-0.693743000
C	-3.584128000	3.572811000	-0.609074000
C	-4.716412000	3.520474000	-1.439704000
C	-5.711909000	4.493346000	-1.346758000
C	-5.597027000	5.530166000	-0.416858000
C	-4.481030000	5.585829000	0.422645000
C	-3.483136000	4.617103000	0.325144000
C	3.434282000	3.440241000	-0.590100000
C	3.340962000	4.521780000	0.299286000
C	4.327950000	5.506294000	0.327592000
C	5.417326000	5.431643000	-0.545027000
C	5.516390000	4.362668000	-1.440257000
C	4.535737000	3.371648000	-1.457058000
H	-0.269396000	1.173981000	-0.394098000
H	-4.798866000	2.714833000	-2.169151000
H	-6.579202000	4.444091000	-2.005821000
H	-6.376262000	6.289246000	-0.343668000
H	-4.390118000	6.385073000	1.158965000
H	-2.611045000	4.655651000	0.978567000
H	2.485268000	4.576192000	0.972788000
H	4.247952000	6.334765000	1.032003000
H	6.186733000	6.203981000	-0.527384000
H	6.360814000	4.302107000	-2.127424000
H	4.608837000	2.531926000	-2.148632000
N	-2.006398000	0.148667000	-0.660347000

N	0.147161000	-2.004098000	-0.686894000
C	-2.871584000	1.190915000	-0.477735000
C	-4.196227000	0.716030000	-0.096954000
C	-4.122426000	-0.642098000	-0.107909000
C	-2.749626000	-0.983832000	-0.485110000
C	-2.314441000	-2.312634000	-0.696582000
C	-0.982213000	-2.744172000	-0.893319000
C	-0.634138000	-4.109728000	-1.290431000
C	0.723981000	-4.183154000	-1.281605000
C	1.192448000	-2.865758000	-0.869118000
C	2.541298000	-2.515507000	-0.627163000
C	3.573310000	-3.578879000	-0.719736000
C	4.630929000	-3.455185000	-1.636010000
C	5.602068000	-4.449649000	-1.743092000
C	5.535961000	-5.584793000	-0.930522000
C	4.486419000	-5.721946000	-0.018145000
C	3.511029000	-4.729884000	0.084142000
C	-3.369868000	-3.367884000	-0.716058000
C	-3.345914000	-4.425742000	0.208542000
C	-4.334327000	-5.410551000	0.192227000
C	-5.361117000	-5.359521000	-0.754365000
C	-5.394293000	-4.314780000	-1.681847000
C	-4.409554000	-3.326426000	-1.660479000
H	-1.336771000	-4.891712000	-1.558178000
H	1.347595000	-5.031384000	-1.543760000
H	4.677425000	-2.568212000	-2.268566000
H	6.411401000	-4.341003000	-2.465814000
H	6.296861000	-6.361506000	-1.011060000
H	4.429236000	-6.604164000	0.620180000
H	2.695794000	-4.829741000	0.800602000
H	-2.544829000	-4.462001000	0.946928000
H	-4.304382000	-6.219132000	0.923466000
H	-6.132060000	-6.130677000	-0.769227000
H	-6.188670000	-4.270769000	-2.427801000
H	-4.431580000	-2.511560000	-2.384176000
H	-5.049561000	1.335365000	0.158737000
H	-4.908885000	-1.348948000	0.134355000
H	1.175766000	-0.261635000	-0.903037000
C	5.270869000	-1.533127000	0.820231000
H	5.768454000	-1.003865000	1.642563000
H	4.911550000	-2.495931000	1.198740000
H	6.036458000	-1.755856000	0.062886000
C	5.069166000	1.550122000	1.012185000
H	5.547119000	0.990749000	1.826764000
H	5.867300000	1.896708000	0.340930000
H	4.605346000	2.442104000	1.443673000
C	1.580266000	5.095580000	-2.211864000
H	1.919401000	5.879422000	-1.520161000
H	2.477395000	4.635574000	-2.636787000
H	1.036870000	5.591122000	-3.026617000
C	-1.509068000	5.293429000	-2.081486000

H	-0.960698000	5.809183000	-2.879511000
H	-2.459565000	4.936840000	-2.492611000
H	-1.756604000	6.043046000	-1.315977000

24. H₂[*adj*-Br₄(CH₃)₄TPP]; *trans*; saddled

N	2.010951000	0.016915000	-0.562607000
N	0.010121000	2.124251000	-0.723423000
C	2.782524000	-1.077456000	-0.267417000
C	4.021798000	-0.680800000	0.420812000
C	4.015576000	0.689977000	0.446295000
C	2.774131000	1.103395000	-0.233548000
C	2.440010000	2.428749000	-0.612766000
C	1.147062000	2.850068000	-0.984996000
C	0.711786000	4.094036000	-1.584077000
C	-0.676050000	4.098623000	-1.587797000
C	-1.122715000	2.855309000	-0.997748000
C	-2.422985000	2.448526000	-0.647928000
C	-3.494771000	3.478133000	-0.633312000
C	-4.602607000	3.360349000	-1.486548000
C	-5.624826000	4.306958000	-1.451537000
C	-5.558798000	5.375529000	-0.553435000
C	-4.458415000	5.500729000	0.299613000
C	-3.428641000	4.563460000	0.252688000
C	3.527479000	3.443268000	-0.635207000
C	3.493249000	4.559157000	0.214343000
C	4.524071000	5.497593000	0.194640000
C	5.597062000	5.341698000	-0.687484000
C	5.637200000	4.237313000	-1.543068000
C	4.613798000	3.290612000	-1.510529000
H	0.016830000	1.149387000	-0.426548000
H	-4.656710000	2.511440000	-2.168080000
H	-6.481788000	4.204655000	-2.117484000
H	-6.365994000	6.107447000	-0.514573000
H	-4.408207000	6.327346000	1.008917000
H	-2.573055000	4.646195000	0.923060000
H	2.651672000	4.675777000	0.897874000
H	4.491576000	6.353337000	0.869537000
H	6.400617000	6.078261000	-0.707021000
H	6.469798000	4.112203000	-2.235862000
H	4.641137000	2.421269000	-2.167837000
N	-2.033484000	0.019140000	-0.641540000
N	0.011899000	-2.083683000	-0.774092000
C	-2.769095000	1.119063000	-0.293605000
C	-3.988212000	0.692477000	0.392996000
C	-3.992194000	-0.677402000	0.374117000
C	-2.775277000	-1.089335000	-0.320922000
C	-2.434083000	-2.405017000	-0.709494000
C	-1.131859000	-2.787578000	-1.084620000
C	-0.674588000	-3.984255000	-1.740985000

C	0.709490000	-3.979309000	-1.740805000
C	1.158342000	-2.783059000	-1.077014000
C	2.454349000	-2.387183000	-0.684875000
C	3.528158000	-3.415039000	-0.738797000
C	4.594875000	-3.268016000	-1.636743000
C	5.583874000	-4.246348000	-1.725336000
C	5.528837000	-5.374192000	-0.901767000
C	4.479193000	-5.519481000	0.009319000
C	3.481552000	-4.549497000	0.084926000
C	-3.488989000	-3.451739000	-0.711777000
C	-3.397275000	-4.551624000	0.153642000
C	-4.395081000	-5.522918000	0.166497000
C	-5.486632000	-5.415201000	-0.699776000
C	-5.579065000	-4.327966000	-1.573006000
C	-4.590441000	-3.346487000	-1.572776000
H	0.020692000	-1.127957000	-0.416893000
H	4.626126000	-2.387400000	-2.278271000
H	6.398052000	-4.131477000	-2.441440000
H	6.302018000	-6.139830000	-0.971307000
H	4.433306000	-6.396768000	0.654891000
H	2.649905000	-4.665849000	0.780268000
H	-2.540913000	-4.629801000	0.823289000
H	-4.322088000	-6.367492000	0.851990000
H	-6.265717000	-6.178280000	-0.693416000
H	-6.428419000	-4.242530000	-2.251003000
H	-4.659312000	-2.489627000	-2.242435000
C	-1.528920000	5.170376000	-2.195097000
H	-0.995526000	5.659689000	-3.020099000
H	-2.470756000	4.771205000	-2.584000000
H	-1.791439000	5.949576000	-1.465418000
C	1.569689000	5.160563000	-2.194037000
H	1.836999000	5.941276000	-1.467784000
H	2.507916000	4.756534000	-2.586769000
H	1.035746000	5.650566000	-3.018202000
C	5.014559000	1.554485000	1.154438000
H	4.541716000	2.433656000	1.606645000
H	5.513132000	0.989096000	1.952505000
H	5.797038000	1.929621000	0.479747000
C	5.029310000	-1.568395000	1.086170000
H	4.558695000	-2.453470000	1.529747000
H	5.788196000	-1.938274000	0.382076000
H	5.555411000	-1.026191000	1.882380000
Br	-1.712241000	-5.263000000	-2.643275000
Br	1.752236000	-5.251015000	-2.649413000
Br	-5.250033000	1.720445000	1.348666000
Br	-5.260041000	-1.730930000	1.290253000

25. H₂[*adj*-Br₄(CH₃)₄TPP]; *cis1*; *saddled*

N	2.149694000	-0.022794000	-0.611525000
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N	-0.021349000	2.146900000	-0.637892000
C	2.867190000	-1.132072000	-0.191299000
C	4.014813000	-0.628927000	0.518825000
C	3.999430000	0.756588000	0.426895000
C	2.828007000	1.142947000	-0.328014000
C	2.431127000	2.437005000	-0.740406000
C	1.105538000	2.820238000	-1.055127000
C	0.636171000	3.996429000	-1.752562000
C	-0.749610000	4.035571000	-1.642953000
C	-1.166800000	2.870264000	-0.913547000
C	-2.447165000	2.468459000	-0.489394000
C	-3.511734000	3.482539000	-0.346994000
C	-4.768139000	3.282828000	-0.946058000
C	-5.781978000	4.225576000	-0.796148000
C	-5.562066000	5.376704000	-0.034036000
C	-4.317614000	5.584429000	0.568284000
C	-3.298627000	4.648392000	0.407687000
C	3.488560000	3.475049000	-0.829556000
C	3.381099000	4.679909000	-0.115294000
C	4.376931000	5.650643000	-0.205444000
C	5.494323000	5.436690000	-1.018084000
C	5.612277000	4.241722000	-1.733745000
C	4.620026000	3.267569000	-1.636086000
H	-0.050975000	1.274358000	-0.115797000
H	-4.937780000	2.375470000	-1.525702000
H	-6.750838000	4.058587000	-1.267130000
H	-6.360097000	6.108390000	0.094363000
H	-4.146048000	6.474865000	1.173938000
H	-2.331116000	4.796723000	0.887727000
H	2.507544000	4.840790000	0.517248000
H	4.283893000	6.577096000	0.361937000
H	6.270690000	6.198305000	-1.092716000
H	6.478179000	4.071180000	-2.374033000
H	4.704292000	2.334444000	-2.193954000
N	-2.035630000	0.084552000	-0.769403000
N	0.114030000	-2.048242000	-0.696621000
C	-2.733822000	1.108750000	-0.196500000
C	-3.797626000	0.576162000	0.645512000
C	-3.758507000	-0.787723000	0.498609000
C	-2.654704000	-1.074177000	-0.413670000
C	-2.297125000	-2.346754000	-0.931575000
C	-0.965907000	-2.672811000	-1.264211000
C	-0.506048000	-3.789687000	-2.084734000
C	0.853804000	-3.864594000	-1.918277000
C	1.217552000	-2.767209000	-1.026637000
C	2.514414000	-2.446469000	-0.531362000
C	3.509570000	-3.534838000	-0.423195000
C	4.753407000	-3.449919000	-1.069152000
C	5.651140000	-4.513081000	-1.016780000
C	5.324005000	-5.673642000	-0.308874000
C	4.093430000	-5.764200000	0.347267000

C	3.190477000	-4.705552000	0.285797000
C	-3.362534000	-3.359958000	-1.066564000
C	-3.212660000	-4.642835000	-0.512404000
C	-4.244656000	-5.572041000	-0.596475000
C	-5.434887000	-5.241001000	-1.251543000
C	-5.589285000	-3.972933000	-1.818555000
C	-4.564925000	-3.035506000	-1.717380000
H	4.991653000	-2.551687000	-1.639215000
H	6.604422000	-4.444396000	-1.541497000
H	6.024474000	-6.508312000	-0.274623000
H	3.832435000	-6.667888000	0.898440000
H	2.220595000	-4.776324000	0.778125000
H	-2.284413000	-4.891438000	0.001253000
H	-4.124214000	-6.558640000	-0.148693000
H	-6.242332000	-5.970845000	-1.318545000
H	-6.514845000	-3.712950000	-2.332799000
H	-4.681445000	-2.040411000	-2.146116000
H	1.291212000	-0.121167000	-1.152314000
C	4.984785000	-1.434528000	1.328108000
H	5.286437000	-0.879499000	2.226204000
H	4.550751000	-2.388818000	1.643127000
H	5.898646000	-1.667789000	0.763454000
C	4.970441000	1.671812000	1.106970000
H	5.399748000	1.183872000	1.991014000
H	5.804209000	1.950186000	0.446915000
H	4.494036000	2.604959000	1.426194000
C	1.454493000	4.953626000	-2.565045000
H	1.736121000	5.848396000	-1.991589000
H	2.382596000	4.496029000	-2.921563000
H	0.881678000	5.291938000	-3.438652000
C	-1.646028000	5.044993000	-2.290950000
H	-1.199652000	5.416158000	-3.222463000
H	-2.629144000	4.621471000	-2.522658000
H	-1.818264000	5.913813000	-1.639611000
Br	1.991660000	-5.040234000	-2.858804000
Br	-1.486819000	-4.777952000	-3.357346000
Br	-4.764231000	-2.015622000	1.517849000
Br	-4.851633000	1.497003000	1.911067000

26. H₂[*adj*-(CF₃)₄(CH₃)₄TPP]; *trans*; *saddled*

N	2.005283000	-0.036664000	-0.669521000
N	-0.023569000	2.023895000	-0.871585000
C	2.693601000	-1.140211000	-0.209095000
C	3.760384000	-0.735713000	0.725959000
C	3.764828000	0.635110000	0.718020000
C	2.682301000	1.040346000	-0.202178000
C	2.383773000	2.370505000	-0.623969000
C	1.116604000	2.747980000	-1.108548000
C	0.707574000	3.935867000	-1.834964000

C	-0.671429000	3.907268000	-1.953679000
C	-1.150725000	2.713550000	-1.274955000
C	-2.447170000	2.332552000	-0.920565000
C	-3.578183000	3.264484000	-1.129983000
C	-4.650128000	2.870816000	-1.948337000
C	-5.716814000	3.737197000	-2.180354000
C	-5.737753000	4.997861000	-1.578838000
C	-4.685766000	5.389285000	-0.745649000
C	-3.612492000	4.530314000	-0.525692000
C	3.445786000	3.399131000	-0.526495000
C	3.235340000	4.588950000	0.191855000
C	4.245810000	5.542221000	0.301628000
C	5.483652000	5.325794000	-0.311042000
C	5.704517000	4.147672000	-1.030442000
C	4.696218000	3.190551000	-1.133245000
H	-0.016679000	1.052846000	-0.562096000
H	-4.628526000	1.883151000	-2.409275000
H	-6.537379000	3.424844000	-2.826417000
H	-6.577146000	5.671718000	-1.751288000
H	-4.708392000	6.364688000	-0.259183000
H	-2.795708000	4.822004000	0.133683000
H	2.270909000	4.749532000	0.674809000
H	4.070404000	6.455332000	0.871361000
H	6.274090000	6.071827000	-0.226224000
H	6.666561000	3.975184000	-1.513695000
H	4.863183000	2.268615000	-1.690895000
N	-2.077181000	-0.069718000	-0.788017000
N	0.003221000	-2.217049000	-0.718948000
C	-2.720068000	1.034659000	-0.353500000
C	-3.664781000	0.692260000	0.709216000
C	-3.576867000	-0.681424000	0.873657000
C	-2.637706000	-1.144214000	-0.143063000
C	-2.411391000	-2.458921000	-0.633810000
C	-1.146427000	-2.765139000	-1.227833000
C	-0.720128000	-3.651889000	-2.257680000
C	0.689881000	-3.638312000	-2.283968000
C	1.138677000	-2.742099000	-1.267918000
C	2.423309000	-2.431468000	-0.694223000
C	3.410806000	-3.514688000	-0.550979000
C	4.759201000	-3.309025000	-0.893063000
C	5.691933000	-4.330232000	-0.741363000
C	5.296484000	-5.575889000	-0.243885000
C	3.957136000	-5.797822000	0.087573000
C	3.020283000	-4.779672000	-0.073266000
C	-3.453112000	-3.480592000	-0.554635000
C	-3.131891000	-4.825398000	-0.284795000
C	-4.133114000	-5.783400000	-0.177270000
C	-5.473297000	-5.420801000	-0.344576000
C	-5.806063000	-4.091888000	-0.622810000
C	-4.808168000	-3.129768000	-0.727922000
H	0.017656000	-1.519153000	0.019149000

H	5.057085000	-2.341838000	-1.296944000
H	6.731754000	-4.159713000	-1.021341000
H	6.028769000	-6.374336000	-0.123631000
H	3.642285000	-6.767889000	0.472589000
H	1.975564000	-4.950977000	0.187796000
H	-2.090103000	-5.104487000	-0.132789000
H	-3.870823000	-6.817470000	0.045209000
H	-6.256832000	-6.174022000	-0.260087000
H	-6.848432000	-3.807675000	-0.765827000
H	-5.063364000	-2.098769000	-0.968626000
C	-1.485063000	4.884054000	-2.744997000
H	-0.902674000	5.252369000	-3.599892000
H	-2.406775000	4.431095000	-3.123804000
H	-1.778598000	5.759535000	-2.148980000
C	1.607214000	4.955043000	-2.463387000
H	1.765275000	5.824306000	-1.809266000
H	2.595026000	4.540082000	-2.688892000
H	1.166811000	5.325372000	-3.398208000
C	4.599117000	1.517179000	1.595248000
H	4.063565000	2.431130000	1.878057000
H	4.887734000	0.987957000	2.513299000
H	5.525214000	1.837622000	1.096530000
C	4.555115000	-1.607963000	1.651913000
H	4.070758000	-2.577630000	1.812025000
H	5.565523000	-1.814601000	1.271719000
H	4.669679000	-1.117211000	2.628691000
C	-1.633376000	-4.379950000	-3.214582000
F	-2.864552000	-3.806749000	-3.279205000
F	-1.150106000	-4.393102000	-4.482961000
F	-1.811560000	-5.687097000	-2.849155000
C	1.539445000	-4.273779000	-3.356372000
F	2.866763000	-4.244084000	-3.083396000
F	1.200813000	-5.580859000	-3.553128000
F	1.389020000	-3.627363000	-4.549793000
C	-4.080431000	-1.481675000	2.052243000
F	-3.636663000	-0.951926000	3.233124000
F	-5.441394000	-1.536902000	2.112765000
F	-3.628873000	-2.766128000	2.050060000
C	-4.443514000	1.686782000	1.528828000
F	-5.483422000	2.227337000	0.823501000
F	-4.987418000	1.169026000	2.655649000
F	-3.643415000	2.729231000	1.920007000

27. H₂[*adj*-(CF₃)₄(CH₃)₄TPP]; *cis1*; *saddled*

N	2.110773000	-0.037914000	-0.605824000
N	-0.037974000	2.114725000	-0.653047000
C	2.736902000	-1.160953000	-0.077096000
C	3.756894000	-0.660267000	0.817845000
C	3.778539000	0.723580000	0.711098000

C	2.745537000	1.115840000	-0.218312000
C	2.403952000	2.406524000	-0.693004000
C	1.092954000	2.743828000	-1.110751000
C	0.646712000	3.783843000	-2.007687000
C	-0.742337000	3.782570000	-2.009213000
C	-1.187252000	2.750306000	-1.102162000
C	-2.460787000	2.392552000	-0.645330000
C	-3.591559000	3.320155000	-0.770404000
C	-4.852349000	2.838079000	-1.172610000
C	-5.937367000	3.703168000	-1.287755000
C	-5.787940000	5.060471000	-0.989831000
C	-4.544922000	5.548350000	-0.572715000
C	-3.458265000	4.687587000	-0.462881000
C	3.458212000	3.441319000	-0.740118000
C	3.235321000	4.726273000	-0.211798000
C	4.232355000	5.698102000	-0.258938000
C	5.472788000	5.405678000	-0.834327000
C	5.708077000	4.132575000	-1.362151000
C	4.711651000	3.159923000	-1.314299000
H	-0.058201000	1.362413000	0.030212000
H	-4.963618000	1.779737000	-1.407430000
H	-6.905050000	3.317257000	-1.608615000
H	-6.640165000	5.735290000	-1.070856000
H	-4.430534000	6.601719000	-0.315827000
H	-2.497224000	5.056308000	-0.104885000
H	2.271271000	4.948106000	0.246924000
H	4.045696000	6.686152000	0.162588000
H	6.252363000	6.166785000	-0.871755000
H	6.669936000	3.900315000	-1.820057000
H	4.888306000	2.169757000	-1.735474000
N	-2.107845000	0.008515000	-0.738010000
N	0.013930000	-2.132148000	-0.594824000
C	-2.679798000	1.064485000	-0.112224000
C	-3.547929000	0.612750000	0.964356000
C	-3.534901000	-0.777288000	0.902621000
C	-2.645642000	-1.119723000	-0.191767000
C	-2.373478000	-2.388251000	-0.792312000
C	-1.058660000	-2.642057000	-1.276444000
C	-0.602578000	-3.501840000	-2.353923000
C	0.783236000	-3.548886000	-2.248155000
C	1.122341000	-2.699690000	-1.114662000
C	2.405256000	-2.456549000	-0.480551000
C	3.305516000	-3.588012000	-0.227337000
C	4.690672000	-3.500371000	-0.459822000
C	5.518494000	-4.593901000	-0.230505000
C	4.978513000	-5.798641000	0.232589000
C	3.602894000	-5.903275000	0.455987000
C	2.770977000	-4.811865000	0.220558000
C	-3.427369000	-3.392191000	-0.897406000
C	-3.139562000	-4.763693000	-0.744329000
C	-4.152835000	-5.710689000	-0.834173000

C	-5.468151000	-5.309408000	-1.088199000
C	-5.767024000	-3.953155000	-1.248577000
C	-4.758456000	-3.002173000	-1.149139000
H	5.100835000	-2.572383000	-0.857158000
H	6.587355000	-4.516432000	-0.430633000
H	5.627613000	-6.656882000	0.407080000
H	3.176822000	-6.841370000	0.811826000
H	1.697959000	-4.887508000	0.396196000
H	-2.117610000	-5.070188000	-0.526962000
H	-3.920010000	-6.766986000	-0.701247000
H	-6.260941000	-6.054414000	-1.160823000
H	-6.790097000	-3.638852000	-1.453858000
H	-4.982636000	-1.945828000	-1.289646000
H	1.367896000	-0.097934000	-1.297317000
C	4.531880000	-1.454440000	1.824175000
H	4.591906000	-0.901831000	2.771742000
H	4.062871000	-2.423523000	2.020221000
H	5.562265000	-1.649725000	1.495766000
C	4.628526000	1.650175000	1.523034000
H	4.859663000	1.206910000	2.500151000
H	5.584517000	1.864610000	1.023746000
H	4.132228000	2.613099000	1.687152000
C	1.519217000	4.622772000	-2.889023000
H	1.751894000	5.593455000	-2.427760000
H	2.475491000	4.130104000	-3.096105000
H	1.019199000	4.825175000	-3.845233000
C	-1.601561000	4.590073000	-2.932848000
H	-1.116999000	4.683822000	-3.914143000
H	-2.583730000	4.128471000	-3.075627000
H	-1.771439000	5.608084000	-2.554947000
C	1.719063000	-4.145048000	-3.264353000
F	2.990694000	-4.301140000	-2.805722000
F	1.304030000	-5.373337000	-3.685987000
F	1.826066000	-3.347998000	-4.376129000
C	-1.437420000	-4.058804000	-3.478083000
F	-2.632095000	-3.413633000	-3.597051000
F	-0.824424000	-3.939278000	-4.688751000
F	-1.715990000	-5.389697000	-3.312242000
C	-4.187537000	-1.734430000	1.865613000
F	-4.182433000	-1.281072000	3.148537000
F	-5.499567000	-1.971625000	1.545687000
F	-3.560024000	-2.944716000	1.889057000
C	-4.119649000	1.435726000	2.086038000
F	-4.101286000	2.774475000	1.836811000
F	-5.413872000	1.104338000	2.362564000
F	-3.403367000	1.272690000	3.243249000

28. H₂[*adj*-(CF₃)₄Ph₄TPP]; *trans*; *saddled*

N	2.004448000	-0.003440000	-0.621791000
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N	-0.020141000	2.042911000	-0.865699000
C	2.718073000	-1.117918000	-0.241755000
C	3.866618000	-0.728260000	0.605429000
C	3.889069000	0.645595000	0.595112000
C	2.718366000	1.071782000	-0.198555000
C	2.388412000	2.409754000	-0.551639000
C	1.117444000	2.797617000	-1.011411000
C	0.710398000	4.029885000	-1.660782000
C	-0.659071000	3.972997000	-1.870013000
C	-1.147421000	2.735125000	-1.270924000
C	-2.449147000	2.347025000	-0.940107000
C	-3.603280000	3.233527000	-1.201057000
C	-4.675723000	2.735721000	-1.959525000
C	-5.752292000	3.557149000	-2.286347000
C	-5.779840000	4.880913000	-1.842933000
C	-4.731984000	5.375846000	-1.061049000
C	-3.653439000	4.558065000	-0.740608000
C	3.437187000	3.465651000	-0.426909000
C	3.488588000	4.278437000	0.712790000
C	4.479909000	5.249218000	0.843263000
C	5.408499000	5.441159000	-0.181584000
C	5.353076000	4.646495000	-1.328000000
C	4.382644000	3.651572000	-1.442698000
H	-0.006465000	1.059655000	-0.593494000
H	-4.642050000	1.704017000	-2.310507000
H	-6.570951000	3.163942000	-2.889123000
H	-6.620720000	5.525606000	-2.099083000
H	-4.755958000	6.404365000	-0.701603000
H	-2.838093000	4.936319000	-0.126467000
H	2.760310000	4.124665000	1.508439000
H	4.526728000	5.856625000	1.746933000
H	6.176517000	6.208823000	-0.085888000
H	6.068352000	4.799924000	-2.135928000
H	4.335503000	3.025840000	-2.333496000
N	-2.070169000	-0.053500000	-0.759628000
N	0.001814000	-2.177482000	-0.704746000
C	-2.710970000	1.057283000	-0.346545000
C	-3.645890000	0.742506000	0.732101000
C	-3.550728000	-0.625641000	0.934291000
C	-2.623751000	-1.113758000	-0.081266000
C	-2.406230000	-2.435587000	-0.552652000
C	-1.155998000	-2.737308000	-1.181311000
C	-0.753003000	-3.608814000	-2.232666000
C	0.654357000	-3.568450000	-2.311240000
C	1.123517000	-2.682677000	-1.296777000
C	2.425515000	-2.397961000	-0.749383000
C	3.381914000	-3.512733000	-0.649752000
C	4.745544000	-3.338104000	-0.943995000
C	5.643527000	-4.387546000	-0.785213000
C	5.196130000	-5.635775000	-0.342317000
C	3.839402000	-5.831694000	-0.073175000

C	2.939356000	-4.781759000	-0.231417000
C	-3.434717000	-3.465008000	-0.427448000
C	-3.089366000	-4.803019000	-0.153224000
C	-4.075621000	-5.770298000	0.000319000
C	-5.424666000	-5.423785000	-0.124916000
C	-5.781509000	-4.102376000	-0.409177000
C	-4.798662000	-3.131162000	-0.560801000
H	0.032157000	-1.487631000	0.040419000
H	5.088890000	-2.369541000	-1.303847000
H	6.698797000	-4.233506000	-1.009389000
H	5.903049000	-6.455421000	-0.213777000
H	3.483279000	-6.803715000	0.268448000
H	1.884271000	-4.930302000	-0.000547000
H	-2.039887000	-5.069145000	-0.034219000
H	-3.794391000	-6.798605000	0.226293000
H	-6.196691000	-6.183764000	-0.003274000
H	-6.831174000	-3.831009000	-0.519729000
H	-5.073664000	-2.106129000	-0.805218000
C	-1.686236000	-4.365250000	-3.146228000
F	-2.930884000	-3.818362000	-3.171191000
F	-1.250893000	-4.389848000	-4.430758000
F	-1.822560000	-5.669751000	-2.753240000
C	1.481618000	-4.166340000	-3.423516000
F	2.817017000	-4.065615000	-3.219167000
F	1.198964000	-5.488729000	-3.601643000
F	1.238172000	-3.530926000	-4.608173000
C	-4.032055000	-1.392894000	2.143381000
F	-3.562106000	-0.833772000	3.299741000
F	-5.391312000	-1.441628000	2.234225000
F	-3.583472000	-2.678571000	2.164353000
C	-4.442652000	1.755241000	1.513663000
F	-5.537121000	2.186038000	0.816805000
F	-4.911454000	1.290527000	2.697258000
F	-3.686712000	2.860635000	1.798084000
C	-1.430625000	4.931620000	-2.679845000
C	-2.270125000	4.464028000	-3.705097000
C	-1.326909000	6.315374000	-2.469629000
C	-3.006423000	5.355860000	-4.479888000
C	-2.061539000	7.207391000	-3.248856000
C	-2.908009000	6.731235000	-4.252272000
H	-2.353903000	3.391151000	-3.875848000
H	-0.680849000	6.688863000	-1.677213000
H	-3.663165000	4.975410000	-5.262076000
H	-1.977705000	8.279005000	-3.066206000
H	-3.489169000	7.428695000	-4.855732000
C	1.598835000	5.074220000	-2.225232000
C	2.022407000	6.176846000	-1.473069000
C	1.992317000	4.972445000	-3.567180000
C	2.845431000	7.146553000	-2.043040000
C	2.811726000	5.946053000	-4.139252000
C	3.243884000	7.033131000	-3.377326000

H	1.721118000	6.257470000	-0.429637000
H	1.651350000	4.121605000	-4.157087000
H	3.181576000	7.990459000	-1.440648000
H	3.112498000	5.854509000	-5.183277000
H	3.888549000	7.791618000	-3.821893000
C	4.784622000	1.482508000	1.427337000
C	4.440448000	1.730032000	2.764258000
C	5.986253000	2.004653000	0.929913000
C	5.271320000	2.498161000	3.580468000
C	6.814688000	2.774703000	1.743701000
C	6.459357000	3.026003000	3.071394000
H	3.513473000	1.313114000	3.158369000
H	6.254589000	1.822212000	-0.109800000
H	4.990709000	2.681890000	4.618014000
H	7.738791000	3.185806000	1.337242000
H	7.107803000	3.629452000	3.707041000
C	4.709256000	-1.595803000	1.447518000
C	4.122325000	-2.602176000	2.233714000
C	6.102961000	-1.432070000	1.501170000
C	4.906145000	-3.434505000	3.028841000
C	6.886941000	-2.261921000	2.300453000
C	6.293490000	-3.269629000	3.063678000
H	3.041419000	-2.738413000	2.202267000
H	6.572481000	-0.660373000	0.893947000
H	4.432756000	-4.216100000	3.623399000
H	7.968454000	-2.125060000	2.321886000
H	6.907877000	-3.923905000	3.682656000

29. H₂[*adj*-(CF₃)₄Ph₄TPP]; *cis1*; *saddled*

N	2.123181000	-0.035318000	-0.606651000
N	-0.032472000	2.120084000	-0.634072000
C	2.776669000	-1.160838000	-0.116053000
C	3.868124000	-0.655289000	0.696829000
C	3.909825000	0.725943000	0.543942000
C	2.796242000	1.120873000	-0.287345000
C	2.419416000	2.416422000	-0.700722000
C	1.099552000	2.779706000	-1.048900000
C	0.648631000	3.896650000	-1.845463000
C	-0.742881000	3.885129000	-1.858938000
C	-1.186050000	2.785268000	-1.026682000
C	-2.457018000	2.415401000	-0.565849000
C	-3.597305000	3.333221000	-0.674630000
C	-4.848836000	2.836916000	-1.086530000
C	-5.932059000	3.695883000	-1.248621000
C	-5.788272000	5.061782000	-0.991895000
C	-4.556661000	5.562407000	-0.557627000
C	-3.474325000	4.706256000	-0.393714000
C	3.471826000	3.472457000	-0.752935000
C	3.526937000	4.470193000	0.229722000

C	4.521284000	5.446073000	0.188277000
C	5.447409000	5.456318000	-0.857301000
C	5.387412000	4.476432000	-1.850731000
C	4.415717000	3.478728000	-1.788632000
H	-0.054248000	1.321509000	-0.004995000
H	-4.952384000	1.774375000	-1.305252000
H	-6.891510000	3.299867000	-1.581633000
H	-6.635968000	5.734713000	-1.121619000
H	-4.443782000	6.624457000	-0.340924000
H	-2.520747000	5.090929000	-0.035417000
H	2.800495000	4.455577000	1.041921000
H	4.572684000	6.200812000	0.973050000
H	6.215992000	6.228466000	-0.898100000
H	6.099158000	4.488775000	-2.676167000
H	4.362222000	2.710806000	-2.560087000
N	-2.083498000	0.035492000	-0.715897000
N	0.048345000	-2.110832000	-0.633010000
C	-2.666625000	1.073080000	-0.067569000
C	-3.538577000	0.589416000	0.991289000
C	-3.513972000	-0.798477000	0.896954000
C	-2.617133000	-1.108910000	-0.201167000
C	-2.340840000	-2.361844000	-0.833757000
C	-1.026987000	-2.610161000	-1.320196000
C	-0.572201000	-3.476247000	-2.394031000
C	0.810870000	-3.548088000	-2.272240000
C	1.152485000	-2.695834000	-1.141490000
C	2.437747000	-2.458546000	-0.508964000
C	3.314661000	-3.602251000	-0.223545000
C	4.706292000	-3.549554000	-0.417132000
C	5.508766000	-4.632527000	-0.078343000
C	4.935119000	-5.795205000	0.446632000
C	3.550383000	-5.871858000	0.615208000
C	2.744704000	-4.788379000	0.275248000
C	-3.395327000	-3.362439000	-0.966672000
C	-3.109213000	-4.737363000	-0.844117000
C	-4.120820000	-5.682113000	-0.968332000
C	-5.433323000	-5.274813000	-1.226068000
C	-5.731464000	-3.914681000	-1.352428000
C	-4.724754000	-2.965987000	-1.217473000
H	5.148858000	-2.652325000	-0.846615000
H	6.586552000	-4.574419000	-0.228760000
H	5.566329000	-6.642465000	0.715058000
H	3.096998000	-6.778227000	1.016614000
H	1.665772000	-4.836504000	0.422685000
H	-2.089703000	-5.049551000	-0.623505000
H	-3.888705000	-6.741300000	-0.859873000
H	-6.224647000	-6.017963000	-1.327212000
H	-6.752717000	-3.595505000	-1.559300000
H	-4.948764000	-1.906401000	-1.331386000
H	1.332819000	-0.102676000	-1.243473000
C	1.745410000	-4.179533000	-3.269724000

F	2.992286000	-4.406829000	-2.777928000
F	1.279407000	-5.379445000	-3.717906000
F	1.921837000	-3.376181000	-4.368122000
C	-1.397664000	-4.002016000	-3.541178000
F	-2.587555000	-3.347169000	-3.657807000
F	-0.766790000	-3.848110000	-4.739519000
F	-1.684181000	-5.334361000	-3.418666000
C	-4.161409000	-1.778801000	1.840354000
F	-4.125186000	-1.364416000	3.136373000
F	-5.481043000	-1.990172000	1.537630000
F	-3.548031000	-2.996148000	1.816111000
C	-4.125070000	1.379766000	2.129817000
F	-4.151850000	2.720551000	1.901604000
F	-5.404793000	1.002749000	2.413884000
F	-3.390942000	1.218744000	3.276819000
C	-1.591761000	4.725029000	-2.721743000
C	-1.425236000	6.117677000	-2.765921000
C	-2.583161000	4.134385000	-3.523220000
C	-2.246493000	6.903264000	-3.572911000
C	-3.404049000	4.920895000	-4.326991000
C	-3.241675000	6.308941000	-4.351558000
H	-0.662402000	6.585058000	-2.145685000
H	-2.714123000	3.052959000	-3.496785000
H	-2.112753000	7.985126000	-3.588279000
H	-4.175255000	4.449008000	-4.935738000
H	-3.888599000	6.924539000	-4.977078000
C	1.510597000	4.740057000	-2.708640000
C	2.025295000	5.967236000	-2.272633000
C	1.812535000	4.295804000	-4.003674000
C	2.844345000	6.726199000	-3.106781000
C	2.626741000	5.058748000	-4.841418000
C	3.148769000	6.273386000	-4.392709000
H	1.804469000	6.309150000	-1.262416000
H	1.403550000	3.345775000	-4.348217000
H	3.252370000	7.671121000	-2.748075000
H	2.852903000	4.702829000	-5.846832000
H	3.790421000	6.867295000	-5.043981000
C	4.793625000	1.645757000	1.298383000
C	4.427787000	2.044457000	2.591069000
C	5.995915000	2.115446000	0.754221000
C	5.242953000	2.911683000	3.319550000
C	6.807397000	2.985434000	1.479697000
C	6.432460000	3.386862000	2.764302000
H	3.498378000	1.670125000	3.020422000
H	6.277227000	1.814777000	-0.254221000
H	4.948178000	3.214977000	4.324551000
H	7.732148000	3.355556000	1.037314000
H	7.067404000	4.067813000	3.331395000
C	4.667979000	-1.426641000	1.663314000
C	4.031955000	-2.329033000	2.532995000
C	6.059938000	-1.270048000	1.748236000

C	4.773393000	-3.074307000	3.445584000
C	6.800445000	-2.016914000	2.663122000
C	6.161701000	-2.925483000	3.509808000
H	2.950835000	-2.452365000	2.474117000
H	6.562855000	-0.574774000	1.078359000
H	4.266264000	-3.777220000	4.106340000
H	7.882669000	-1.893448000	2.709629000
H	6.742884000	-3.514586000	4.219469000