

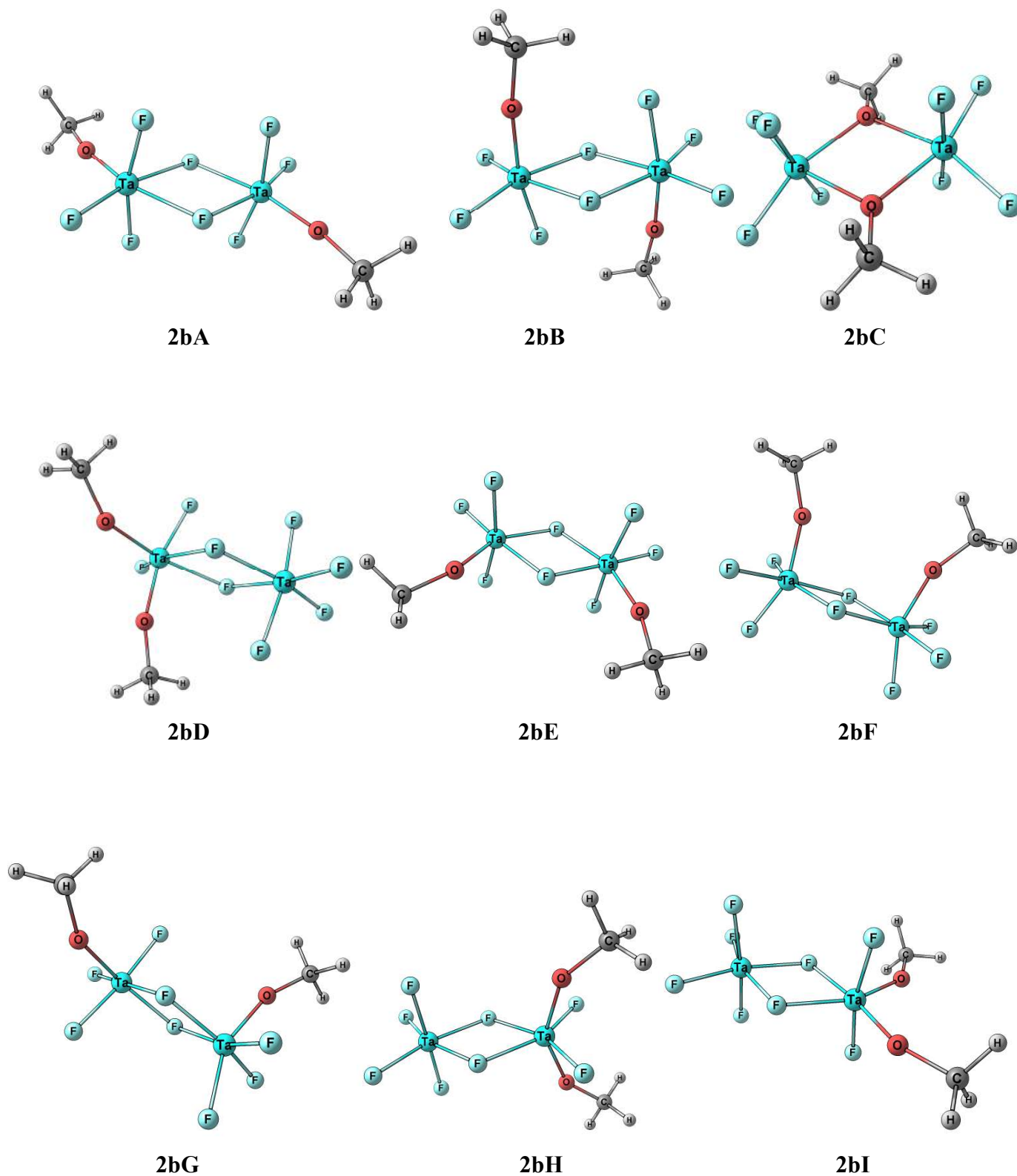
Convenient Synthesis of Fluoride-Alkoxides of Nb(V) and Ta(V): a Spectroscopic, Crystallographic and Computational Study

Marco Bortoluzzi, Nicola Guazzelli, Fabio Marchetti, Guido Pampaloni, Stefano Zacchini

Supplementary Material

Figure S1	<i>p. 2</i>
Figure S2	<i>p. 4</i>
Figure S3	<i>p. 5</i>
Figure S4	<i>p. 6</i>
Figure S5	<i>p. 7</i>
Figure S6	<i>p. 8</i>
Figure S7	<i>p. 9</i>
Figure S8	<i>p. 10</i>
Figure S9	<i>p. 11</i>
Figure S10	<i>p. 12</i>
Figure S11	<i>p. 13</i>
Table S1	<i>p. 14</i>
Figure S12	<i>p. 15</i>
Figure S13	<i>p. 16</i>
Figure S14	<i>p. 17</i>
Figure S15	<i>p. 18</i>
Figure S16	<i>p. 19</i>
Figure S17	<i>p. 20</i>
Figure S18	<i>p. 21</i>
Figure S19	<i>p. 22</i>
Figure S20	<i>p. 23</i>
Table S2	<i>p. 24</i>
Cartesian coordinates (Å) and energies (a.u.) of the gas-phase optimized structures.....	<i>p. 25</i>

Figure S1. DFT-calculated dinuclear structures of TaF₄OMe (**2b**) and relative energy values e (Kcal·mol⁻¹), *in vacuo* and with implicit solvation (CH₂Cl₂)



	2bA	2bB	2bC	2bD	2bE
M06/triple- ζ	-7.1	-7.3	-7.8	-3.5	-6.2
M06/triple- ζ /C-PCM	-9.9	-5.8	-8.6	-3.9	-8.5
	2bF	2bG	2bH	2bI	
M06/triple- ζ	-0.7	-4.8	0	-3.7	
M06/triple- ζ /C-PCM	-4.1	-7.3	0	-4.3	

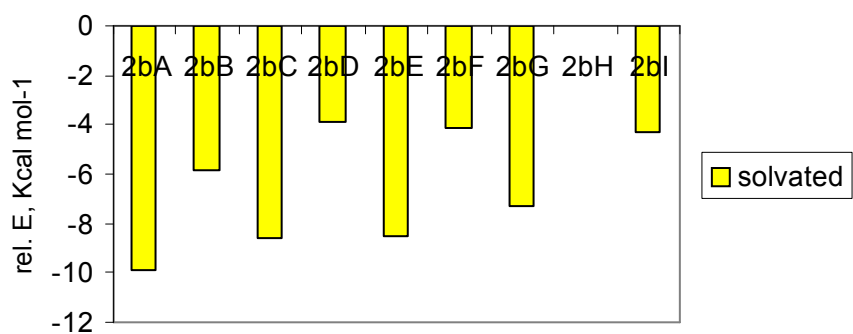
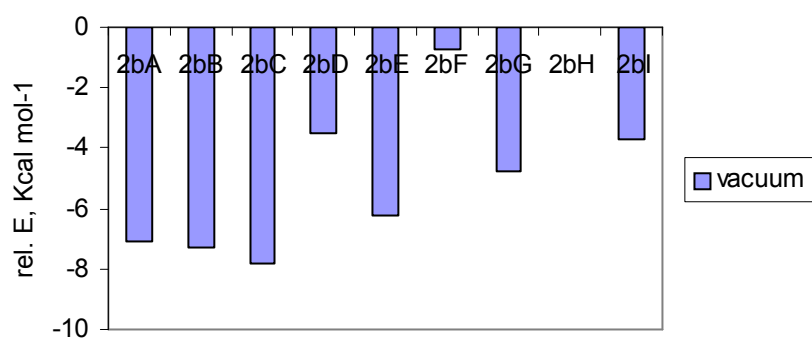
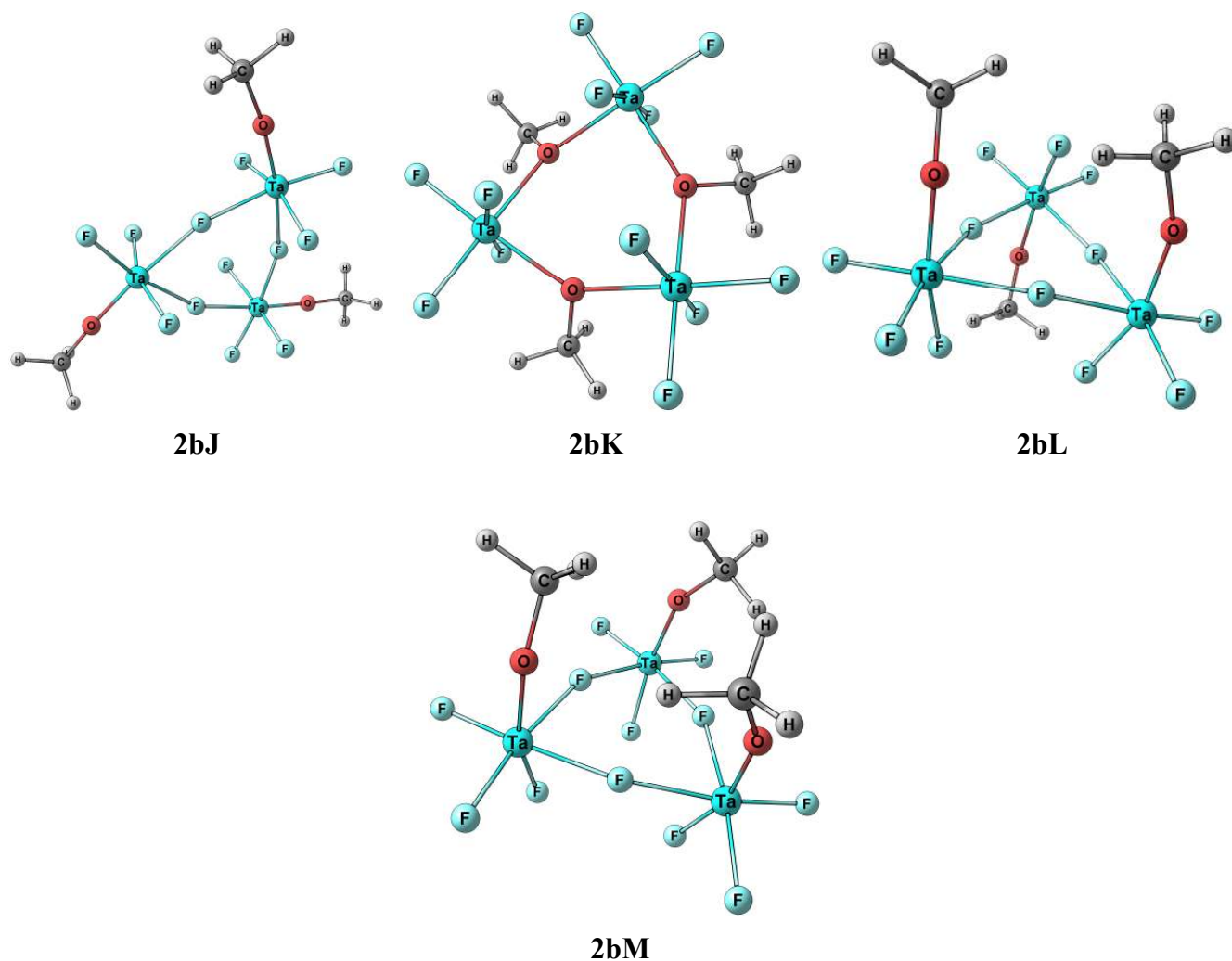


Figure S2. DFT-calculated trinuclear structures of TaF₄OMe (**2b**) and relative energy values (Kcal·mol⁻¹), *in vacuo* and with implicit solvation (CH₂Cl₂)



	2bJ	2bK	2bL	2bM
M06/triple- ζ	-26.2	0	-26.2	-17.4
M06/triple- ζ /C-PCM	-32.4	0	-26.3	-22.3

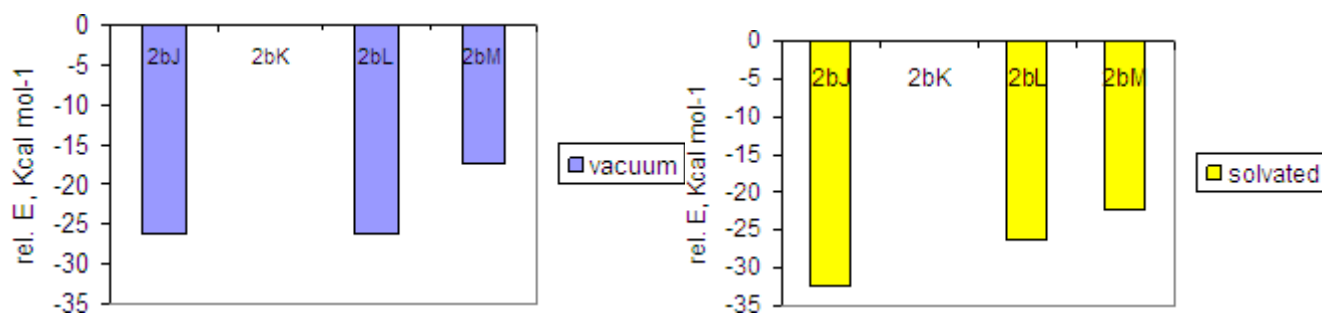
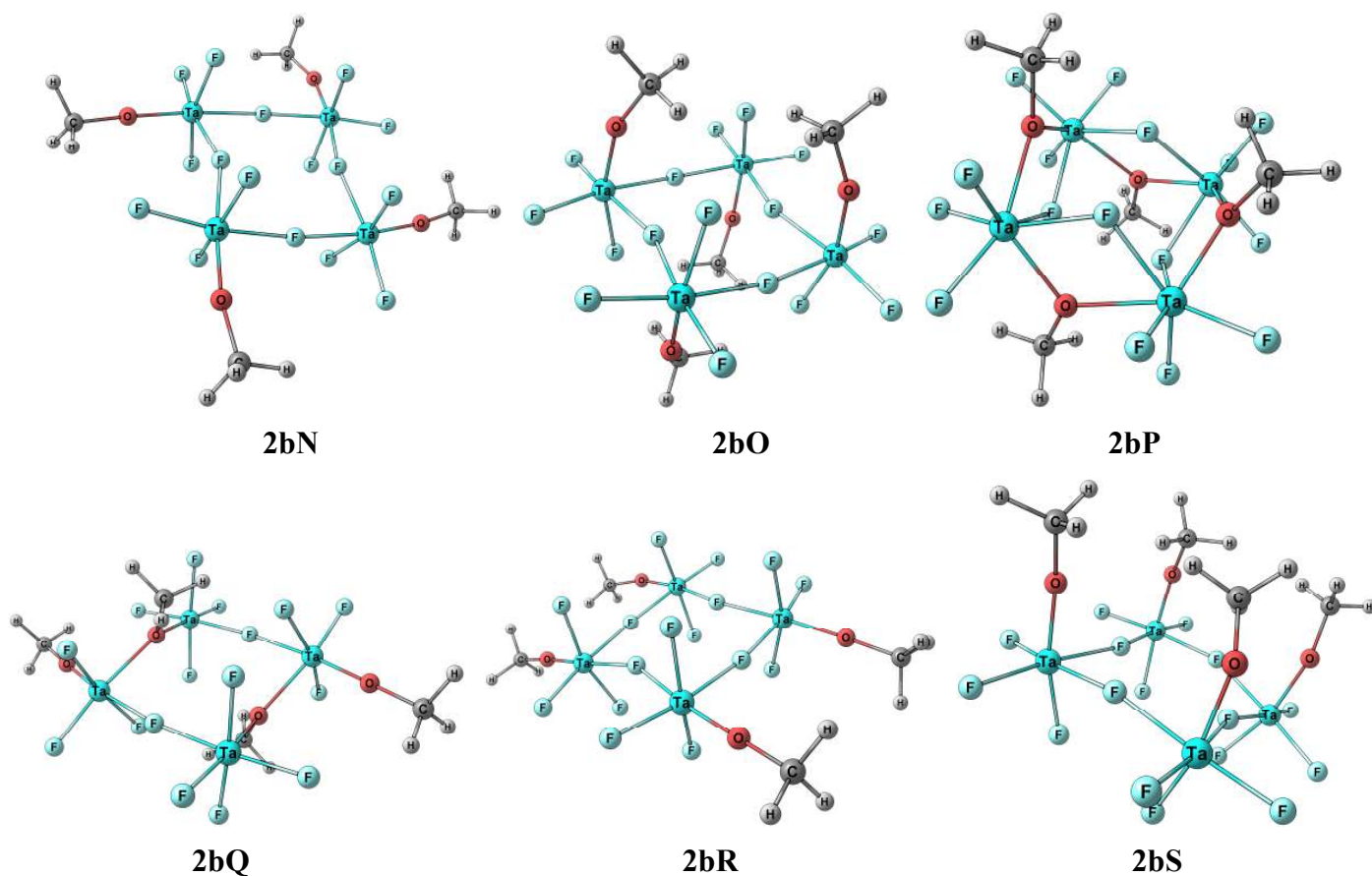


Figure S3. DFT-calculated tetranuclear structures of TaF₄OMe (**2b**) and relative energy values (Kcal·mol⁻¹), *in vacuo* and with implicit solvation (CH₂Cl₂)



	2bN	2bO	2bP	2bQ	2bR	2bS
M06/triple- ζ	-27.2	-28.4	0	-13.1	-19.1	-11.7
M06/triple- ζ /C-PCM	-30.7	-25.4	0	-10.5	-26.6	-16.6

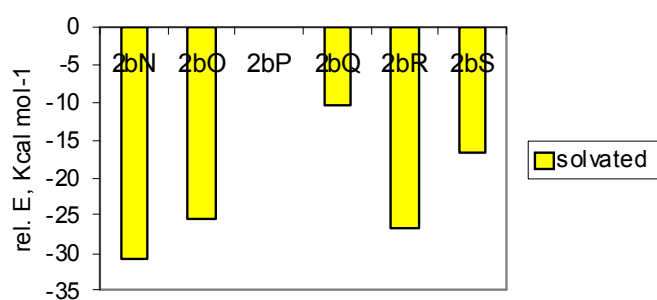
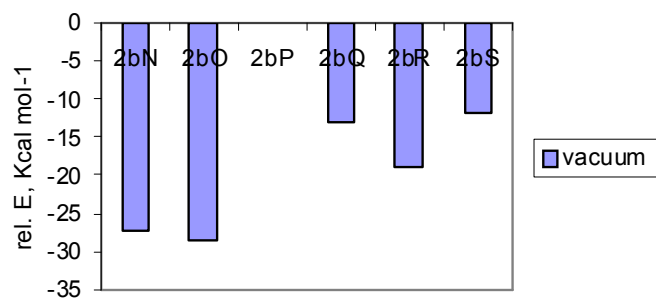


Figure S4. Relative energies (Kcal·mol⁻¹), referred to the TaF₄(OMe) fragment, of the dinuclear, trinuclear and tetranuclear forms of TaF₄(OMe) (**2b**), *in vacuo* and with implicit solvation (CH₂Cl₂)

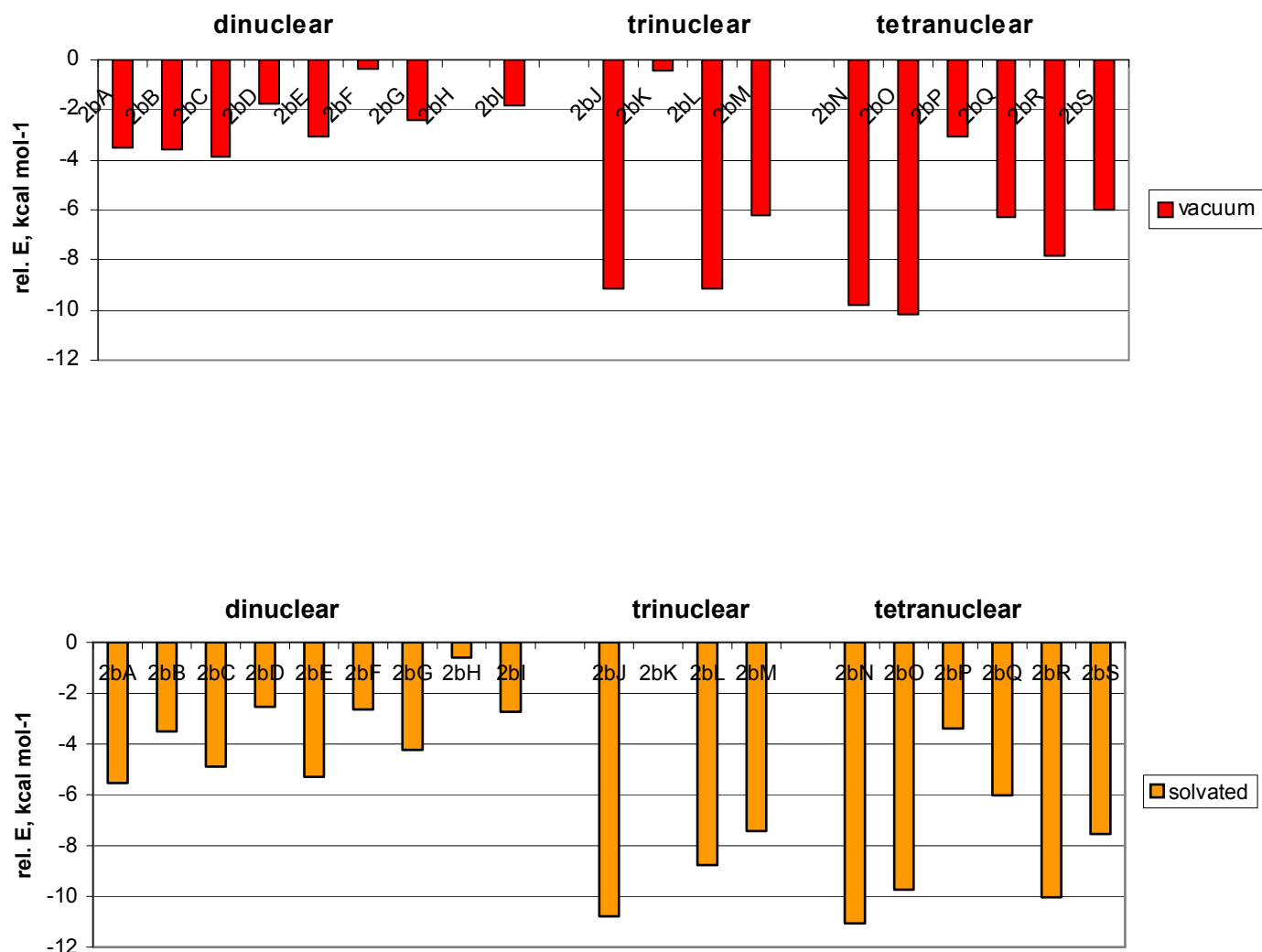
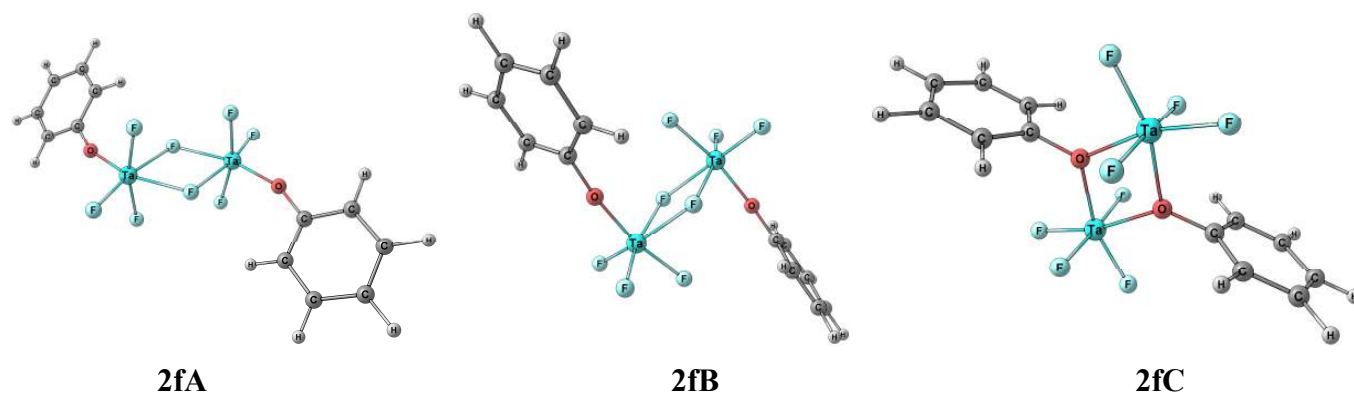


Figure S5. DFT-calculated dinuclear structures of TaF₄OPh (**2f**) and relative energy values (Kcal·mol⁻¹), *in vacuo* and with implicit solvation (CH₂Cl₂)



	2fA	2fB	2fC
M06/triple- ζ	-1.8	0	-1.5
M06/triple- ζ /C-PCM	-2.9	0	-1.9

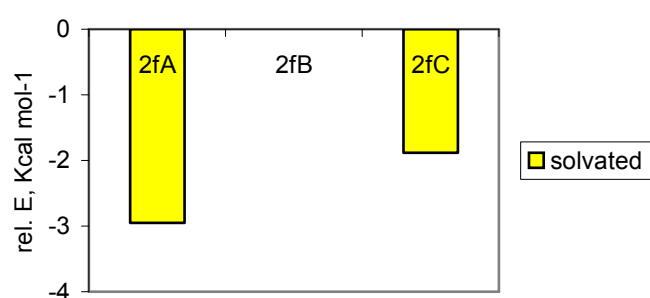
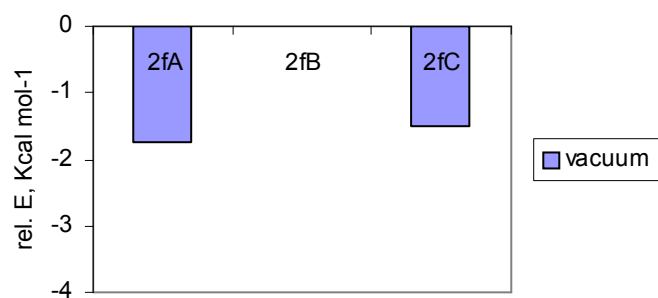
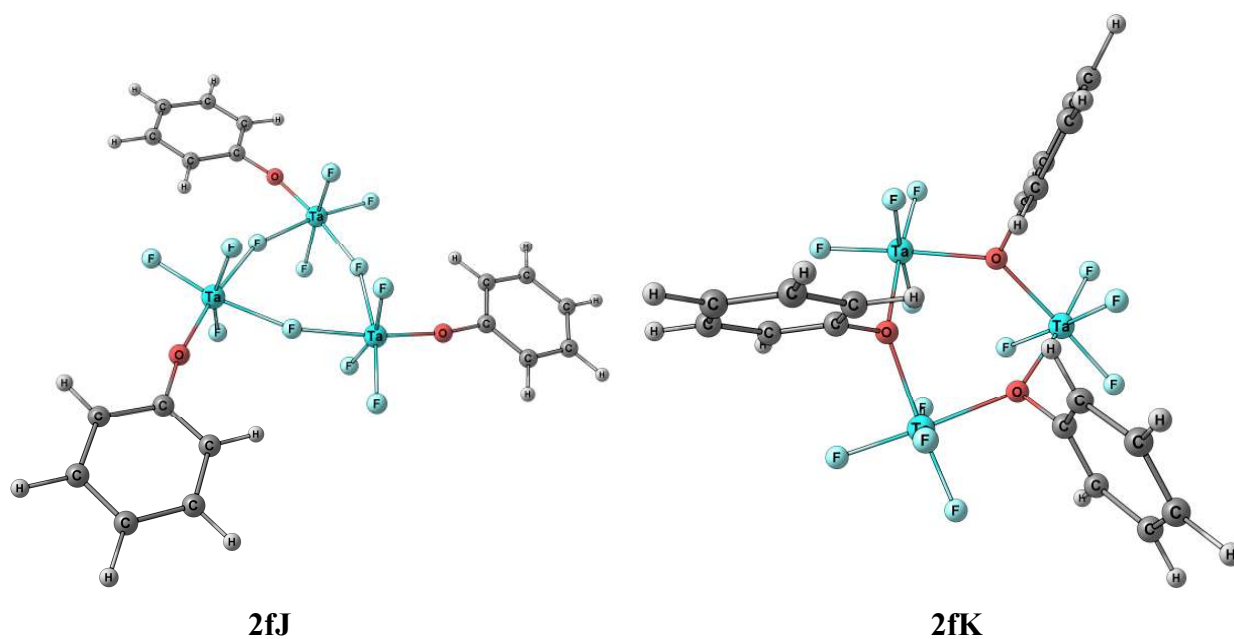


Figure S6. DFT-calculated trinuclear structures of TaF₄OPh (**2f**) and relative energy values (Kcal·mol⁻¹), *in vacuo* and with implicit solvation (CH₂Cl₂)



	2fJ	2fK
M06/triple- ζ	-31.5	0
M06/triple- ζ /C-PCM	-33.9	0

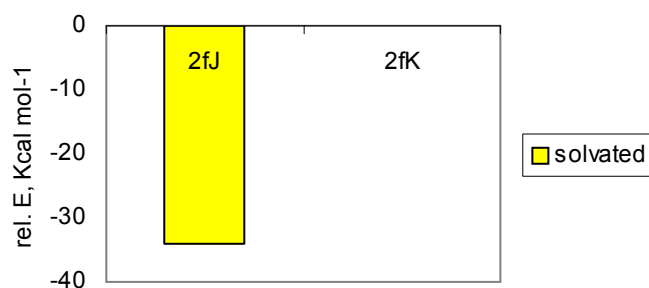
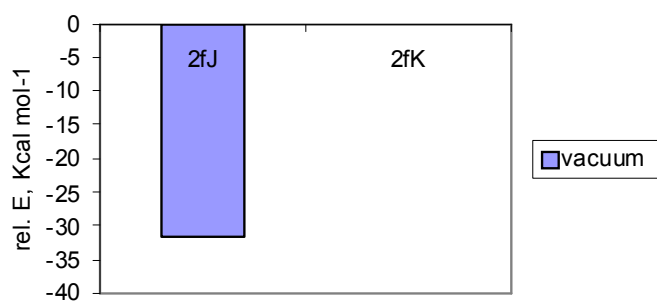
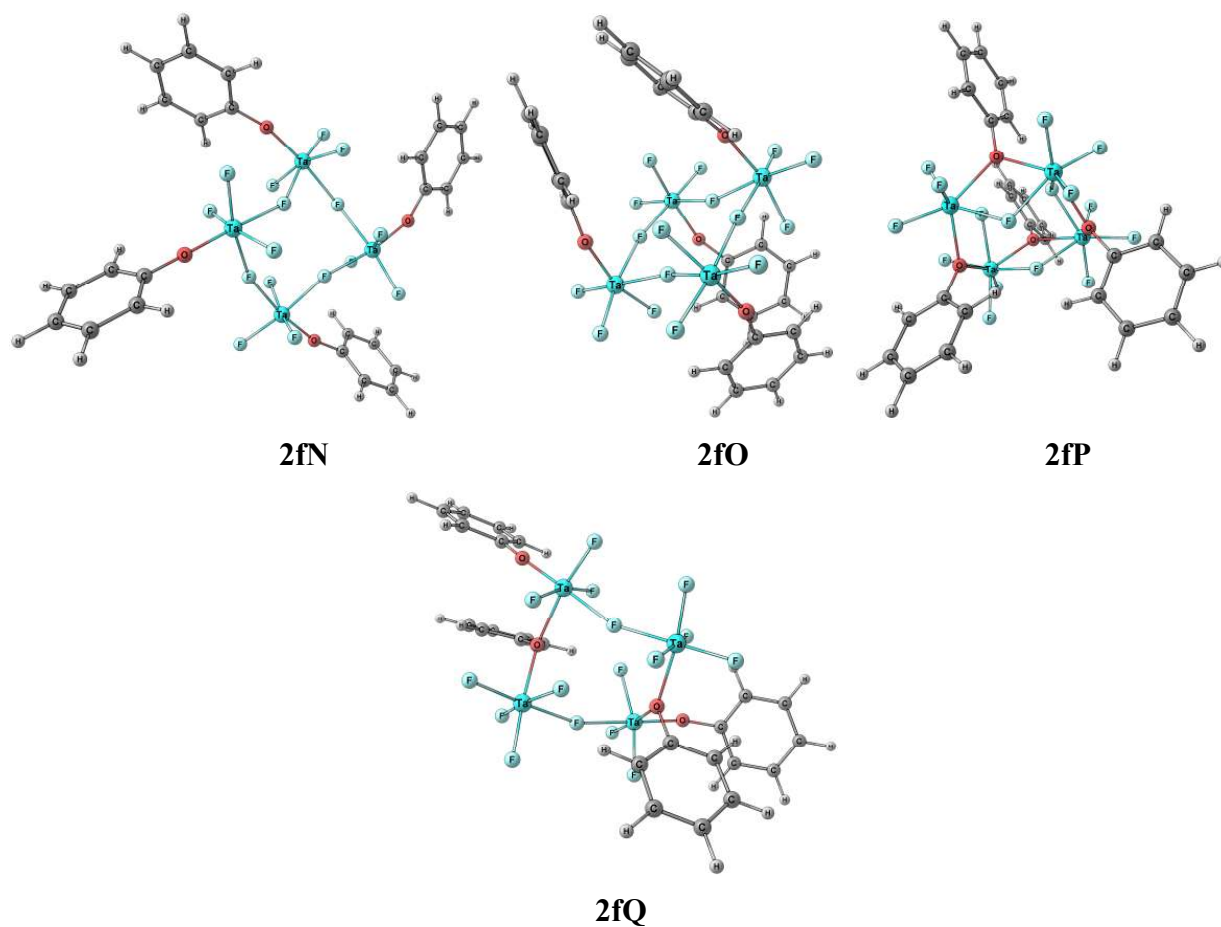


Figure S7. DFT-calculated tetranuclear structures of TaF₄OPh (**2f**) and relative energy values (Kcal·mol⁻¹), *in vacuo* and with implicit solvation (CH₂Cl₂)



	2fN	2fO	2fP	2fQ
M06/triple- ζ	-28.5	-27.0	0	-17.9
M06/triple- ζ /C-PCM	-28.0	23.2	0	-14.9

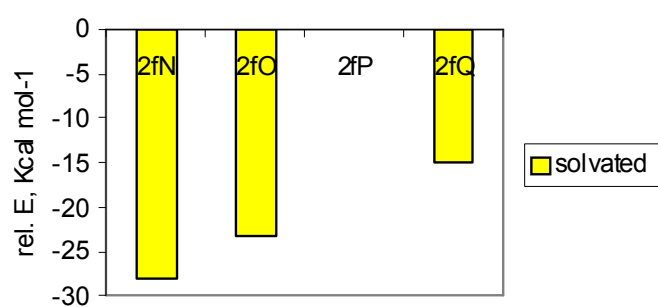
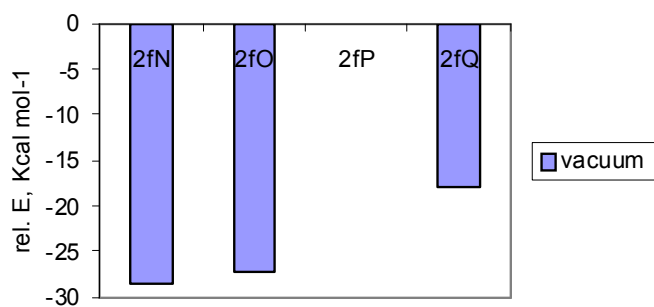


Figure S8. Relative energies ($\text{Kcal}\cdot\text{mol}^{-1}$), referred to the $\text{TaF}_4(\text{OPh})$ fragment, of the dinuclear, trinuclear and tetranuclear forms of $\text{TaF}_4(\text{OPh})$ (**2f**), *in vacuo* and with implicit solvation (CH_2Cl_2)

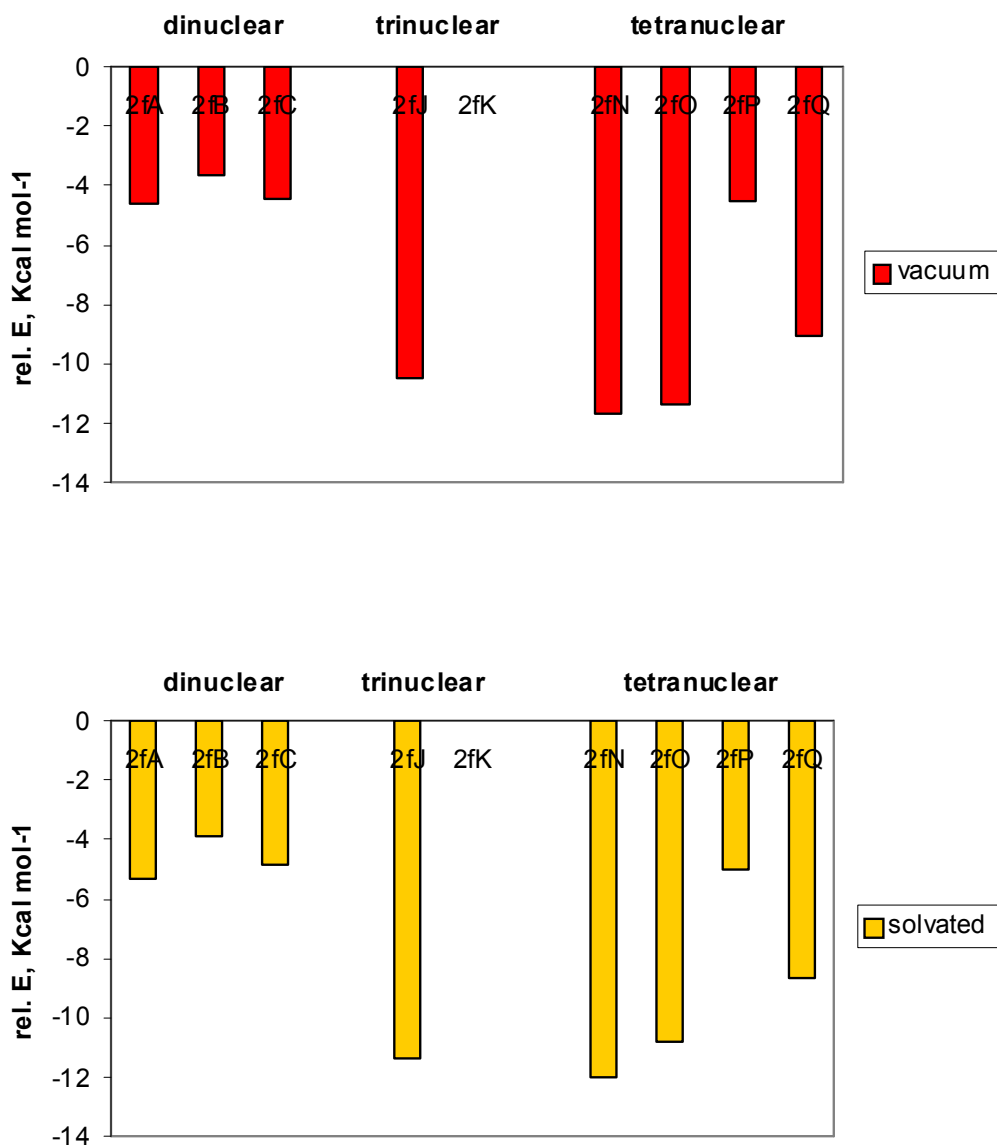


Figure S9. DFT-calculated structures of TaF₄OEt (**2d**) and relative energy values (Kcal·mol⁻¹), *in vacuo* and with implicit solvation (CH₂Cl₂)

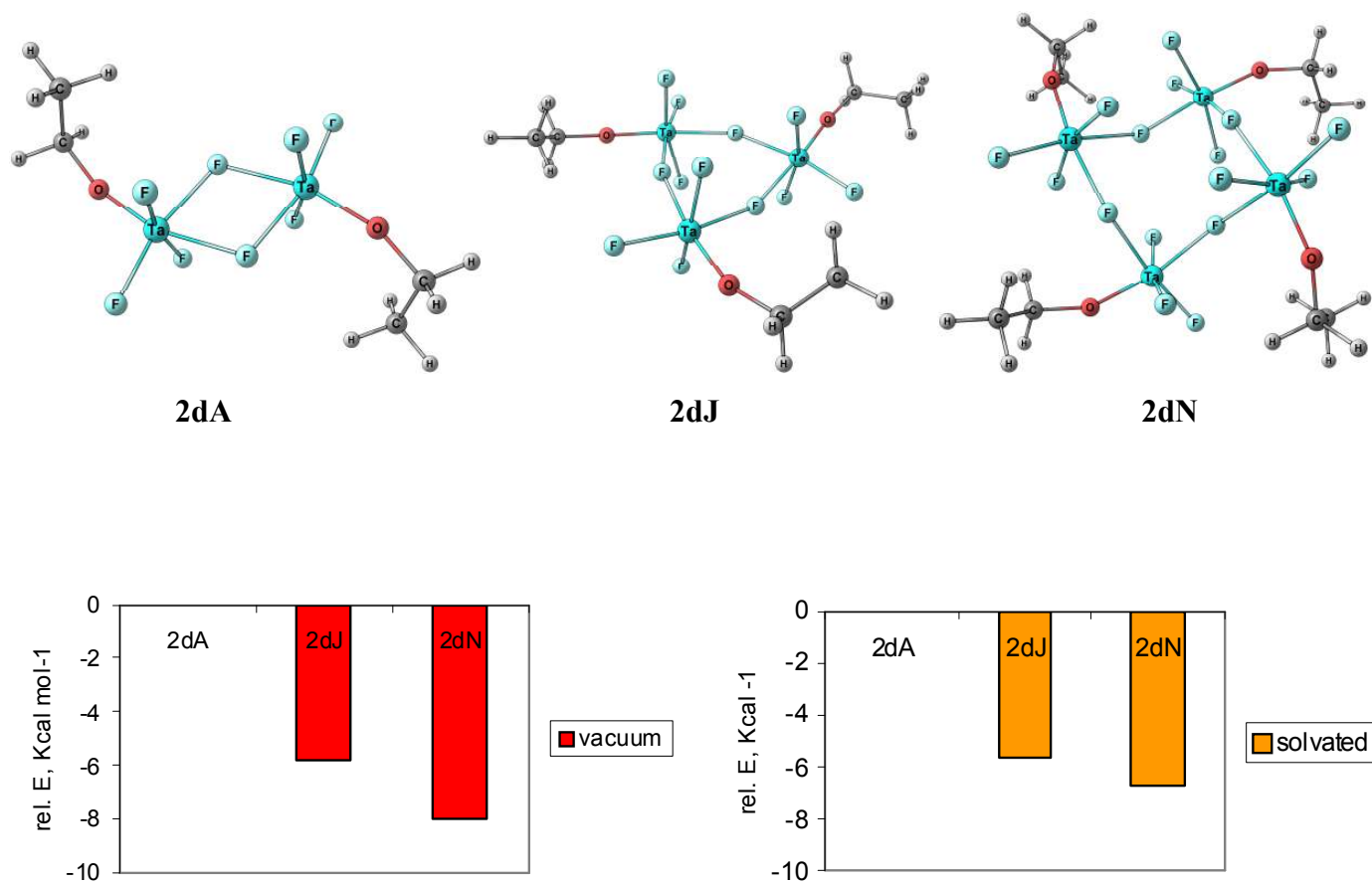
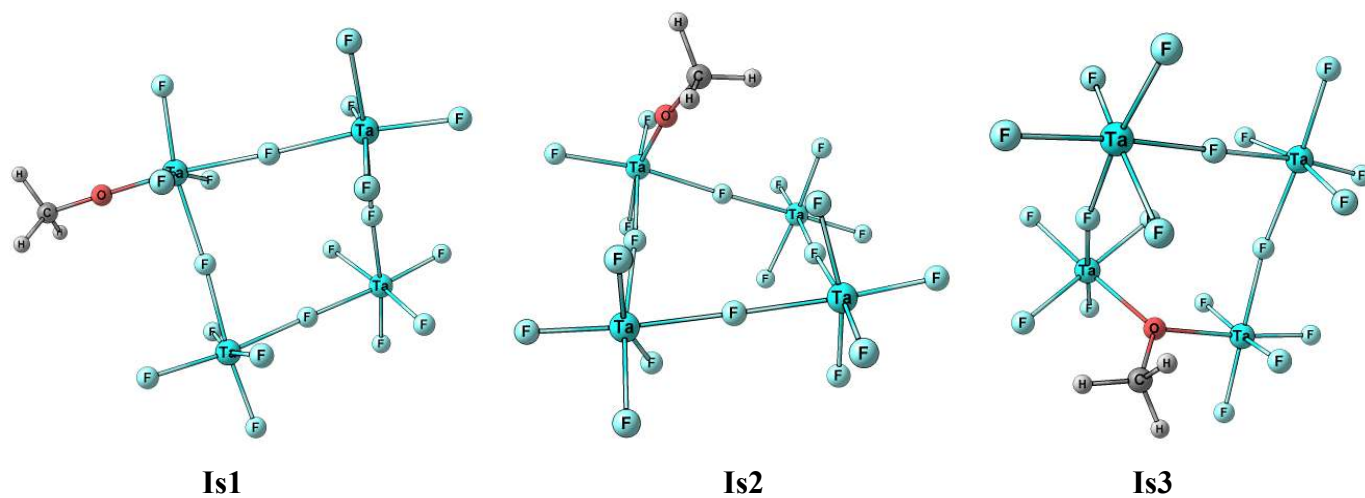


Figure S10. DFT-calculated structures of $\text{Ta}_4\text{F}_{19}(\text{OMe})$ and relative energy values ($\text{Kcal}\cdot\text{mol}^{-1}$), *in vacuo* and with implicit solvation (CH_2Cl_2)



	Is1	Is2	Is3
M06/triple- ζ	-14.2	-12.5	0
M06/triple- ζ /C-PCM	-16.1	-12.9	0

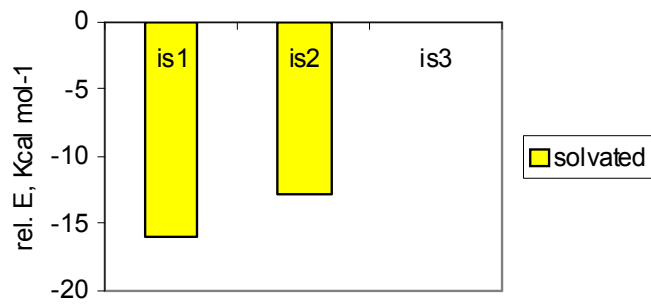
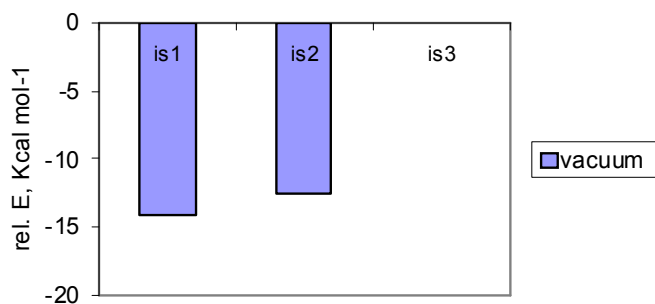


Figure S11. DFT-calculated structures of NbF₃(OPh)₂ (**3e**) and relative energy values (Kcal·mol⁻¹), *in vacuo* and with implicit solvation (CH₂Cl₂)

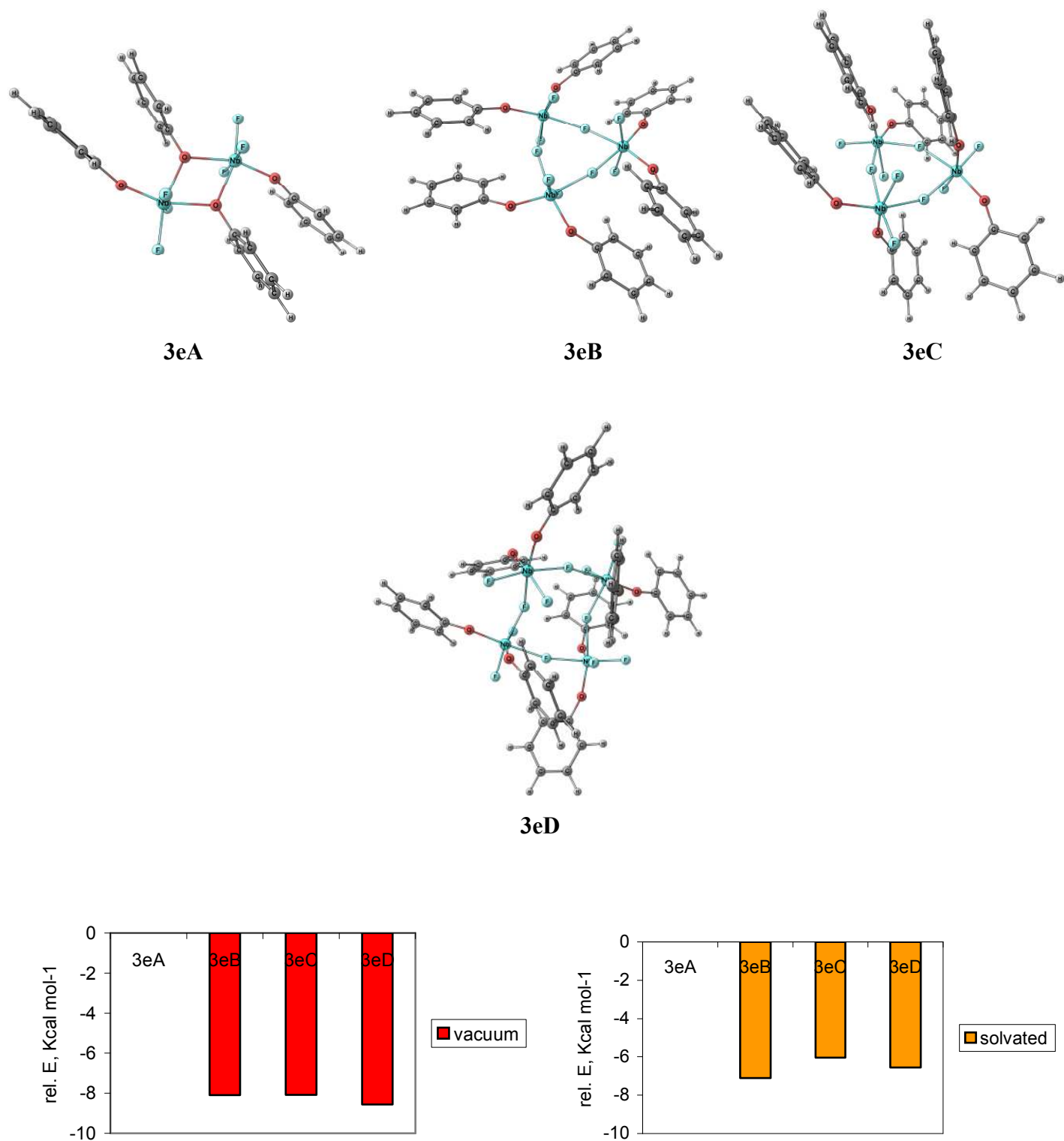
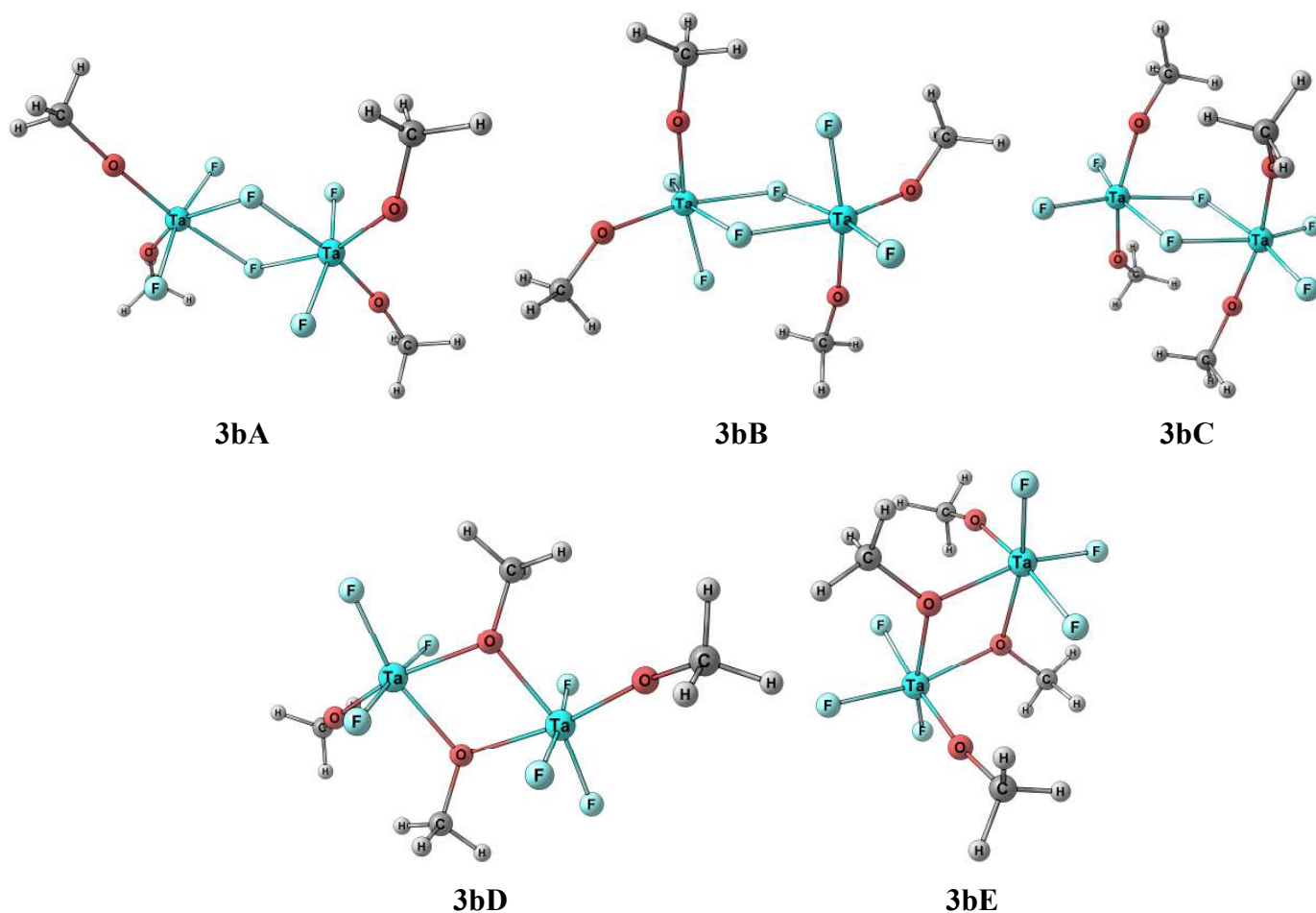


Table S1. Selected calculated average bond distances (Å) and angles (deg) for [NbF₂(μ-F)(OPh)₂]₃ (**3eB**).

	Gas phase	Solvation included
Nb–O	1.862	1.857
Nb–F _{bridging}	2.103	2.107
Nb–F _{terminal}	1.901	1.912
F _{bridging} –Nb–F _{bridging}	81.1	80.6
Nb–F _{bridging} –Nb	152.6	153.5
F _{terminal} –Nb–F _{terminal}	161.8	160.0
O–Nb–O	102.7	103.8

Figure S12. DFT-calculated dinuclear structures of $\text{TaF}_3(\text{OMe})_2$ (**3b**) and relative energy values ($\text{Kcal}\cdot\text{mol}^{-1}$), *in vacuo* and with implicit solvation (CH_2Cl_2)



	3bA	3bB	3bC	3bD	3bE
M06/triple- ζ	-4.1	-7.5	0	-9.6	-8.0
M06/triple- ζ /C-PCM	-9.3	-8.2	0	-13.3	-9.5

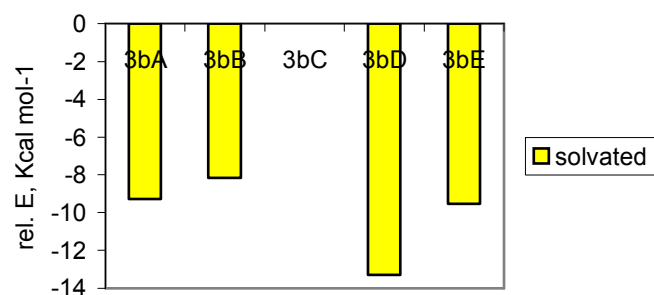
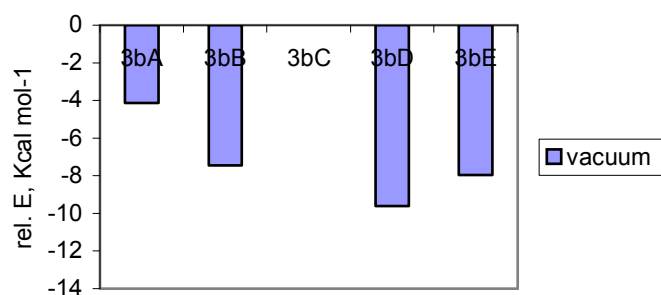
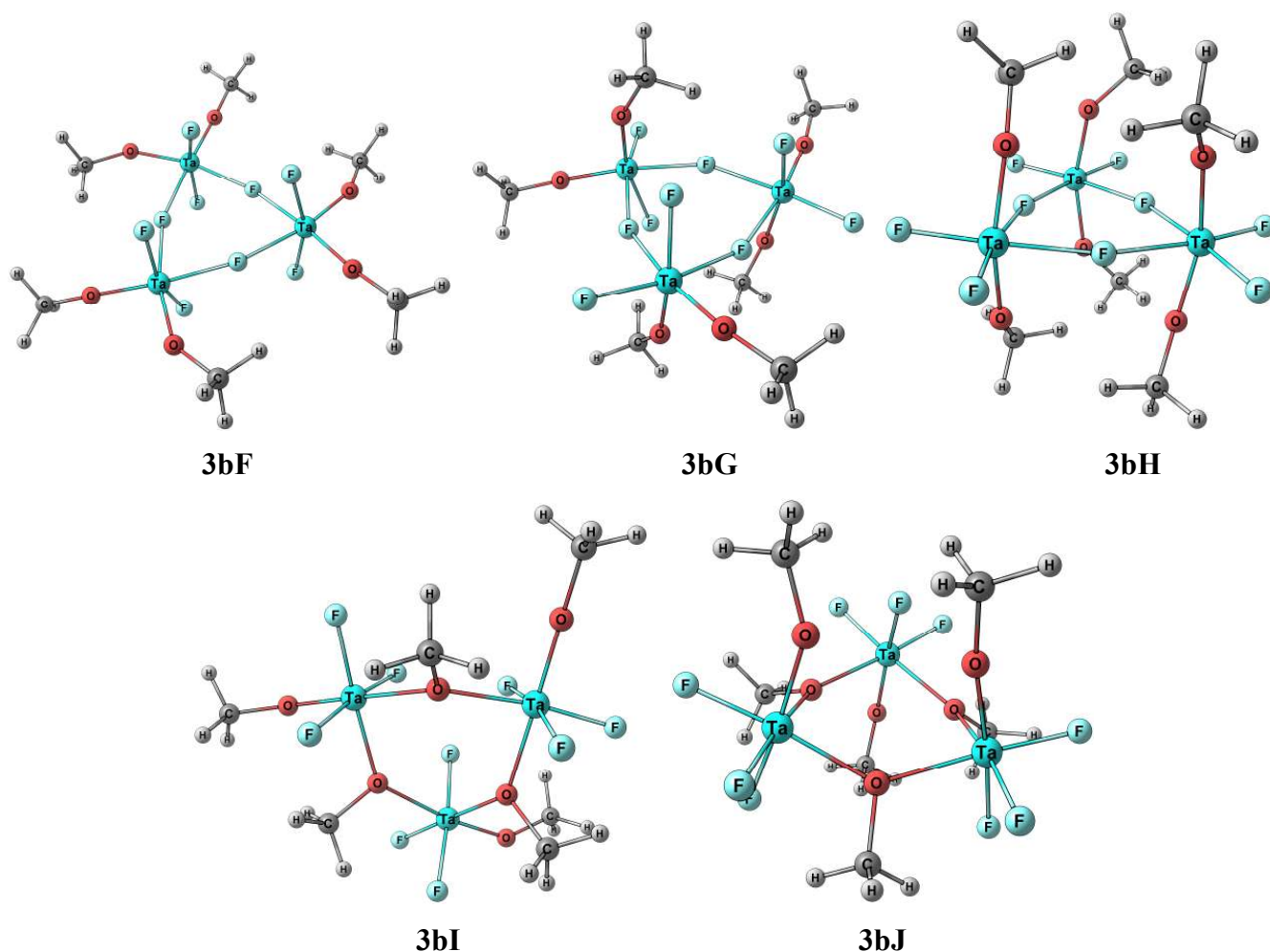


Figure S13. DFT-calculated trinuclear structures of $\text{TaF}_3(\text{OMe})_2$ (**3b**) and relative energy values ($\text{Kcal}\cdot\text{mol}^{-1}$), *in vacuo* and with implicit solvation (CH_2Cl_2)



	3bF	3bG	3bH	3bI	3bJ
M06/triple- ζ	-17.2	-24.9	-14.6	0	-1.6
M06/triple- ζ /C-PCM	-24.0	-23.8	-11.6	-0.5	0

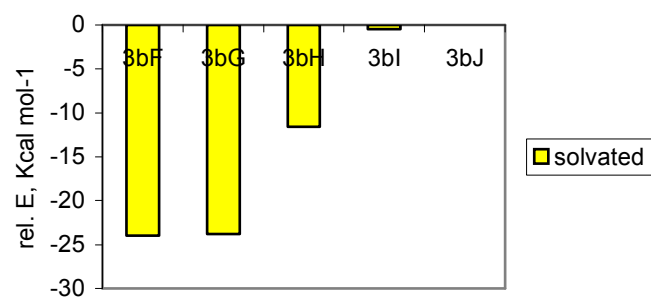
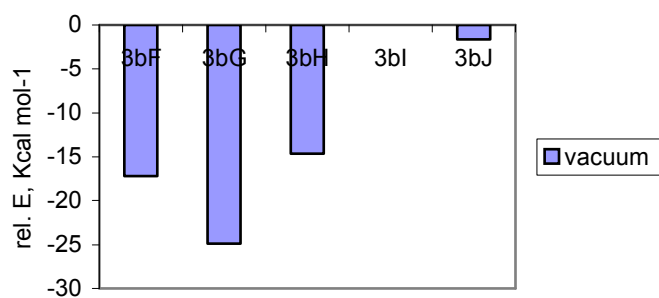
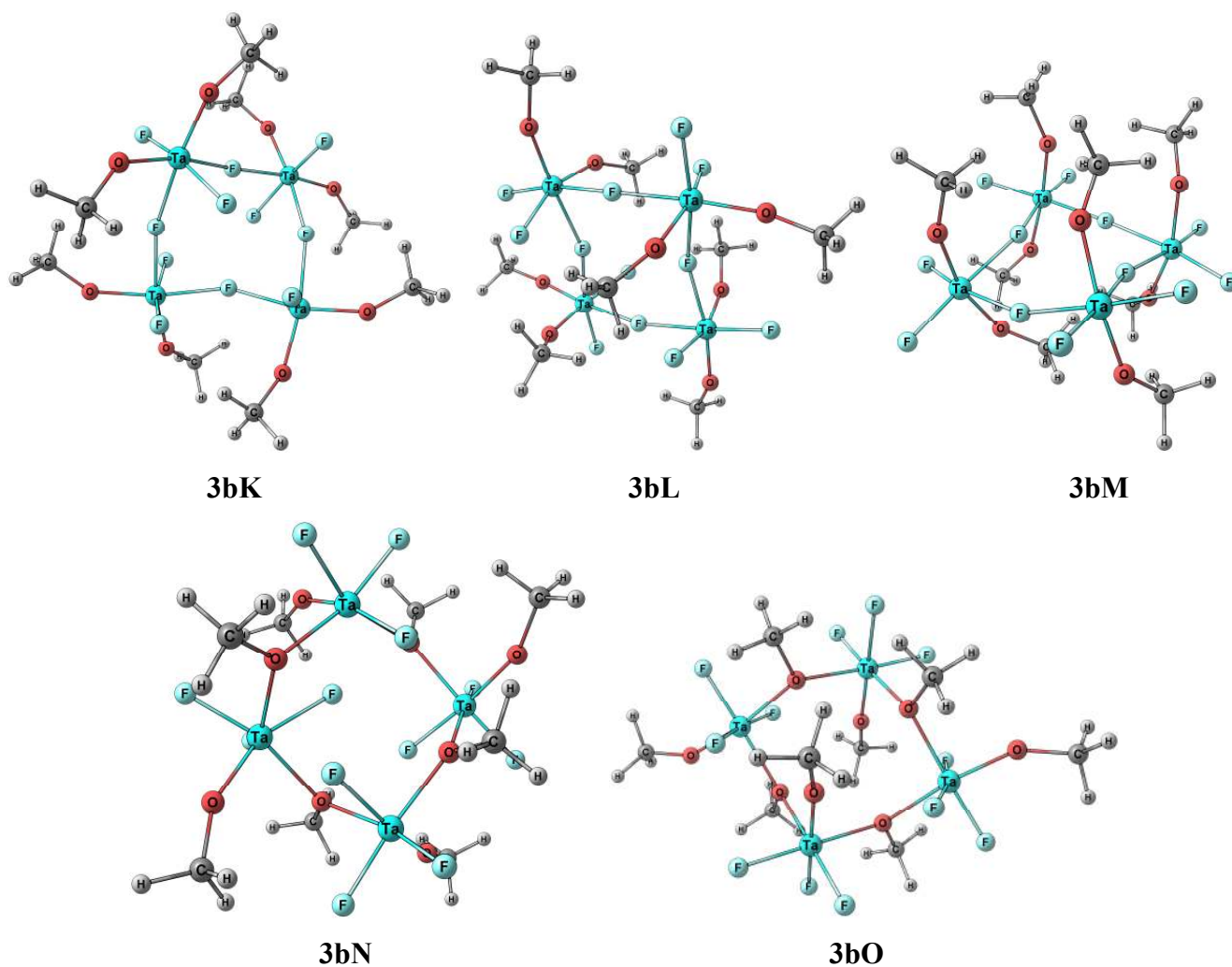


Figure S14. DFT-calculated tetranuclear structures of $\text{TaF}_3(\text{OMe})_2$ (**3b**) and relative energy values ($\text{Kcal}\cdot\text{mol}^{-1}$), *in vacuo* and with implicit solvation (CH_2Cl_2)



	3bK	3bL	3bM	3bN	3bO
M06/triple- ζ	-22.6	-33.6	-15.1	-3.1	0
M06/triple- ζ /C-PCM	-25.4	-29.2	-12.0	-0.6	0

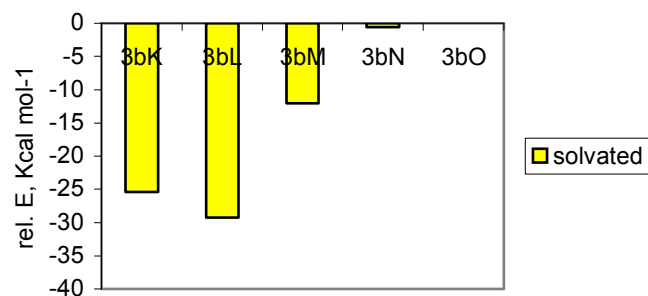
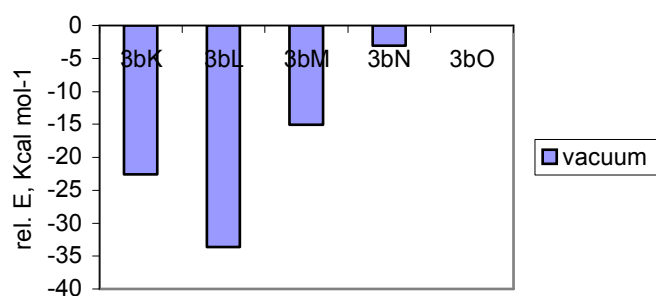


Figure S15. Relative energies ($\text{Kcal}\cdot\text{mol}^{-1}$), referred to the $\text{TaF}_3(\text{OMe})_2$ fragment, of the dinuclear, trinuclear and tetranuclear forms of $\text{TaF}_3(\text{OMe})_2$ (**3b**), *in vacuo* and with implicit solvation (CH_2Cl_2)

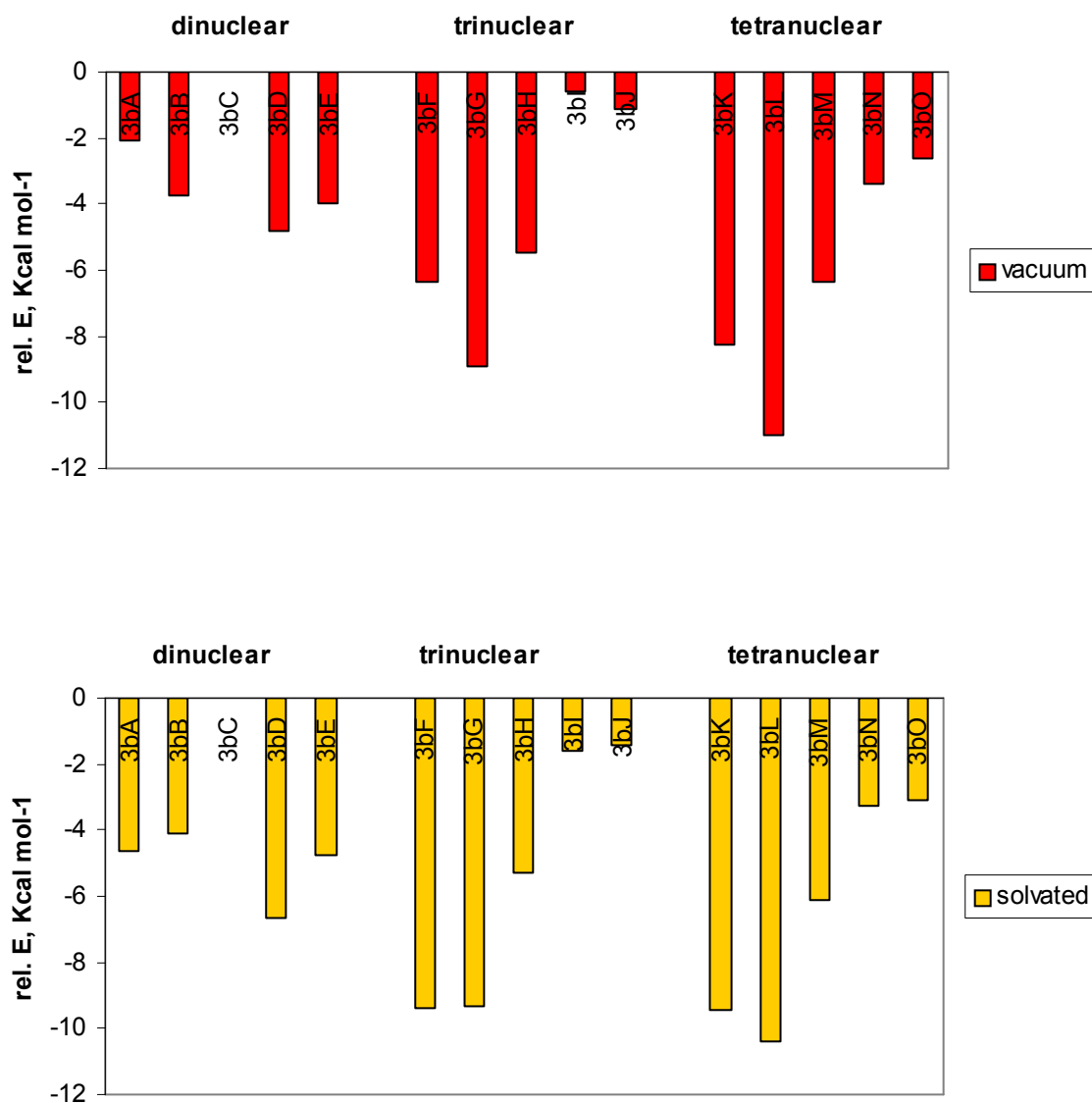
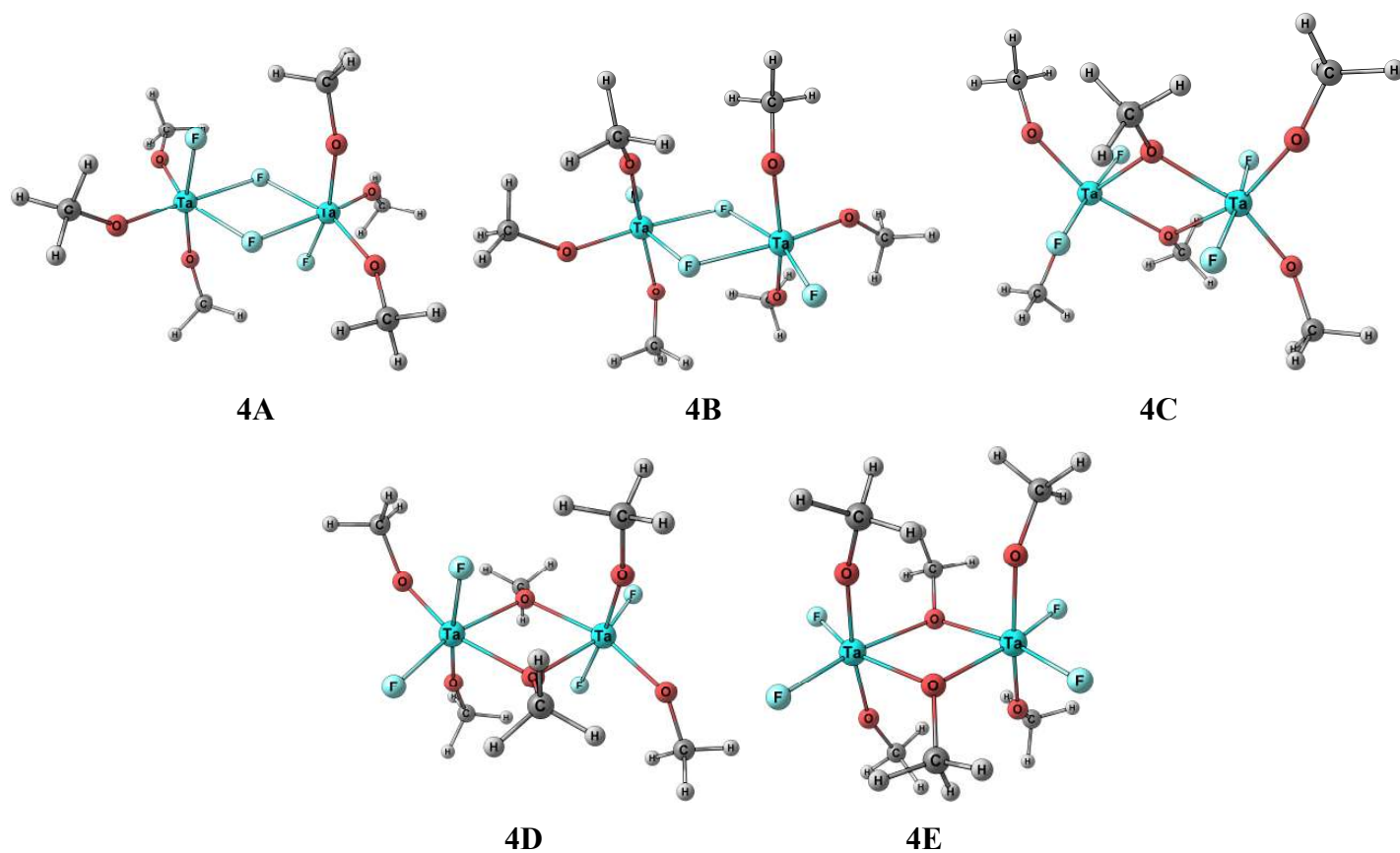


Figure S16. DFT-calculated dinuclear structures of $\text{TaF}_2(\text{OMe})_3$ (**4**) and relative energy values ($\text{Kcal}\cdot\text{mol}^{-1}$), *in vacuo* and with implicit solvation (CH_2Cl_2)



	4A	4B	4C	4D	4E
M06/triple- ζ	-5.5	0	-10.7	-12.9	-3.0
M06/triple- ζ /C-PCM	-4.9	0	-13.6	-13.2	-3.1

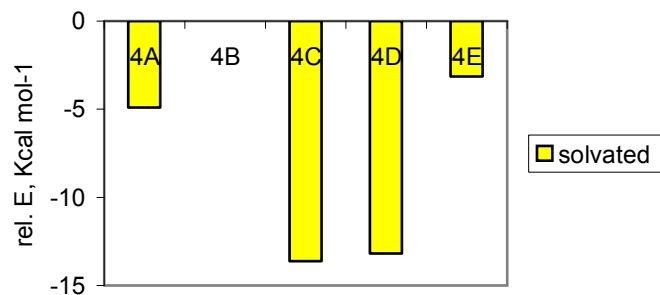
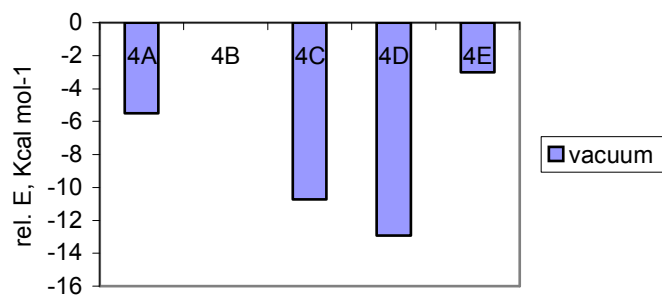
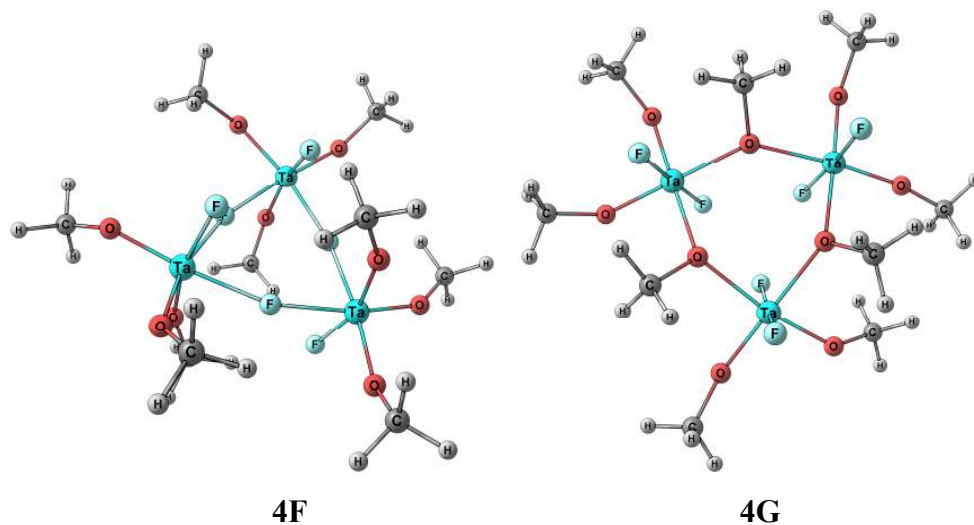


Figure S17. DFT-calculated trinuclear structures of TaF₂(OMe)₃ (**4**) and relative energy values (Kcal·mol⁻¹), *in vacuo* and with implicit solvation (CH₂Cl₂)



	4F	4G
M06/triple- ζ	-24.2	0
M06/triple- ζ /C-PCM	-20.0	0

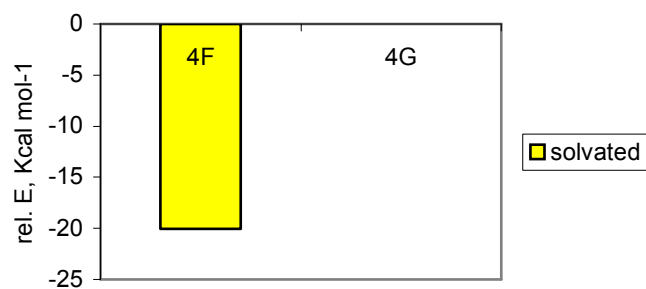
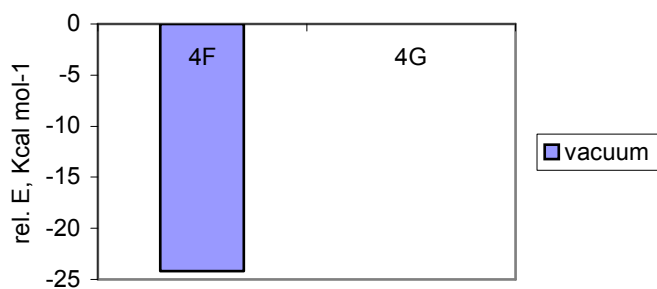
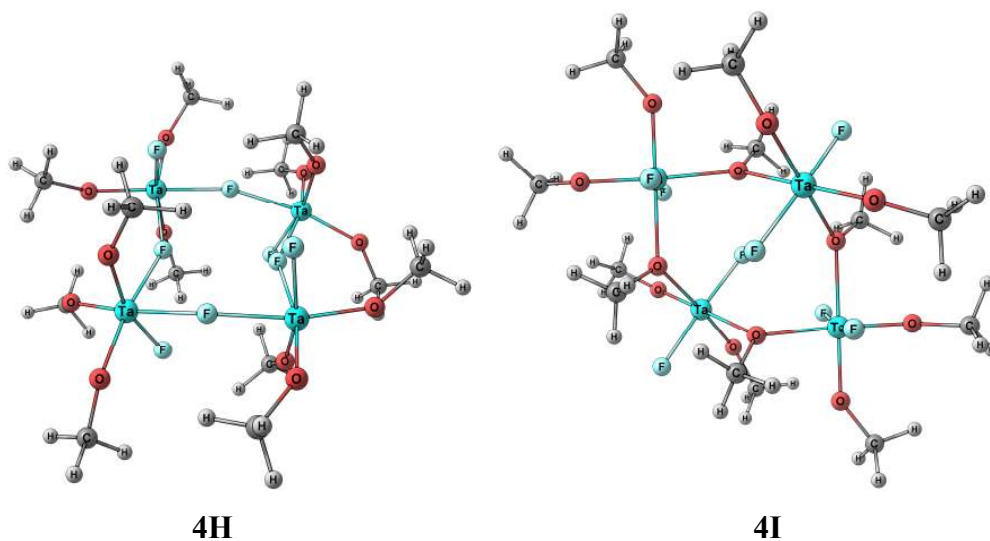


Figure S18. DFT-calculated tetranuclear structures of $\text{TaF}_2(\text{OMe})_3$ (**4**) and relative energy values ($\text{Kcal}\cdot\text{mol}^{-1}$), *in vacuo* and with implicit solvation (CH_2Cl_2)



	4H	4I
M06/triple- ζ	-28.1	0
M06/triple- ζ /C-PCM	-25.5	0

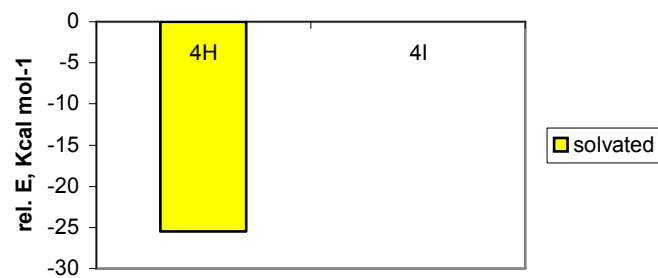
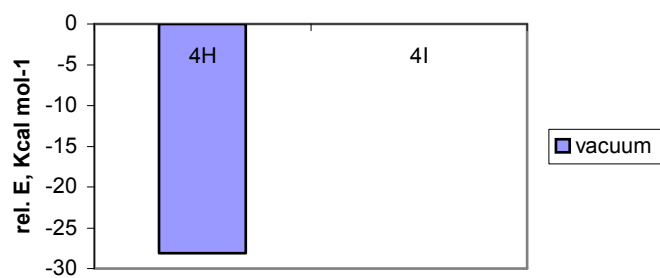


Figure S19. Relative energies ($\text{Kcal}\cdot\text{mol}^{-1}$), referred to the $\text{TaF}_2(\text{OMe})_3$ fragment, of the dinuclear, trinuclear and tetranuclear forms of $\text{TaF}_2(\text{OMe})_3$ (**4**), *in vacuo* and with implicit solvation (CH_2Cl_2)

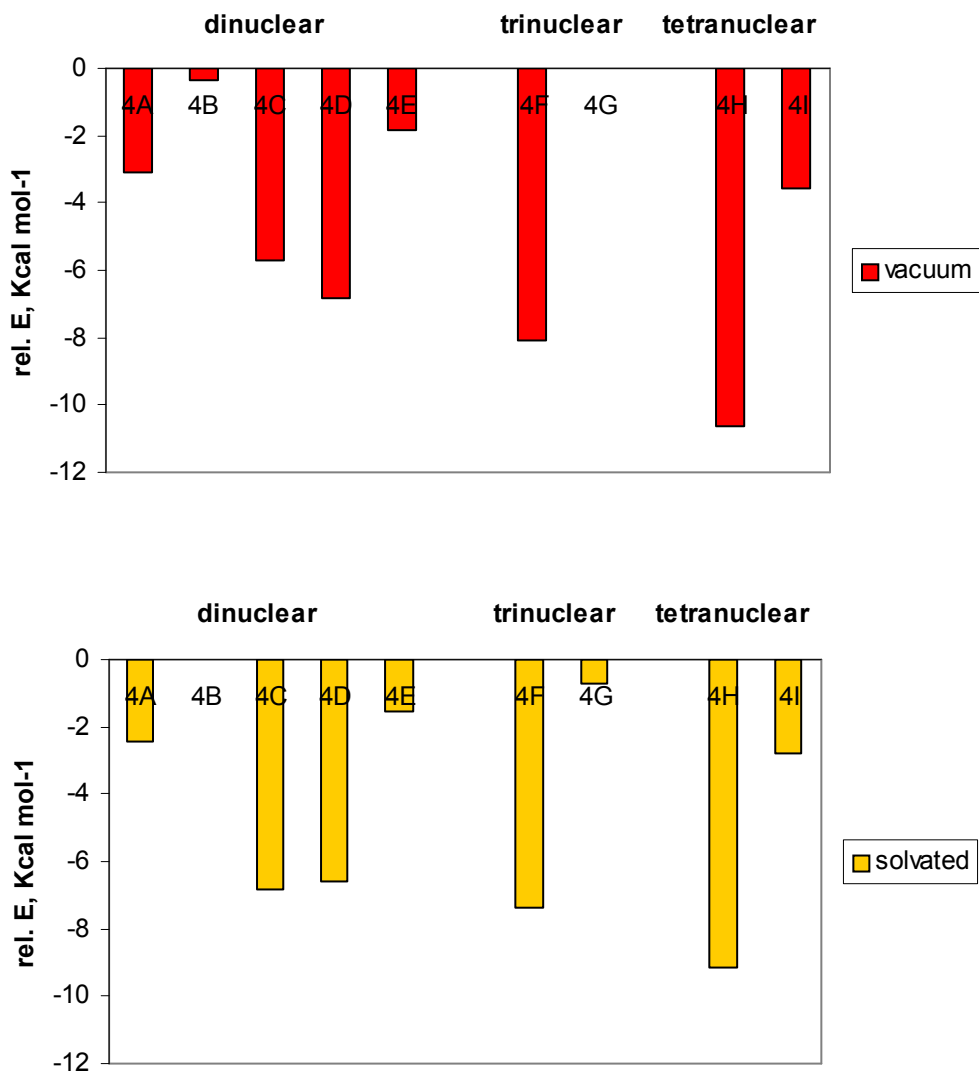
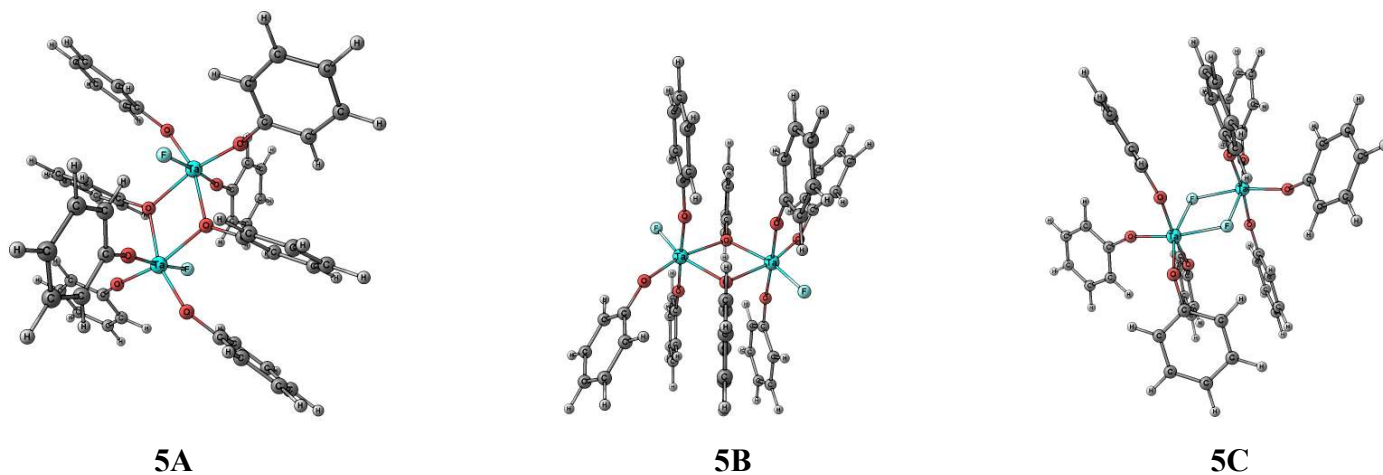
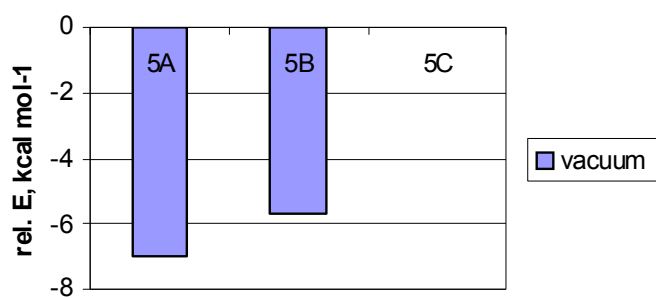


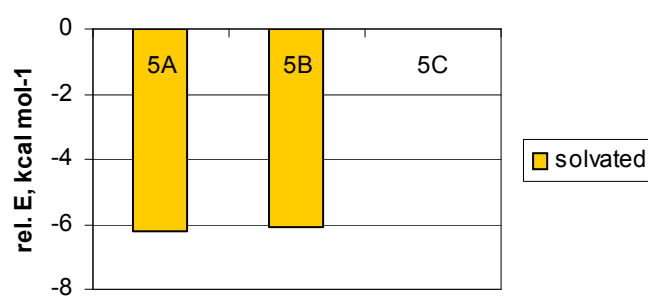
Figure S20. DFT-calculated dinuclear structures of TaF(OPh)₄ (**5**) and relative energy values (Kcal·mol⁻¹), *in vacuo* and with implicit solvation (CH₂Cl₂)



	5A	5B	5C
M06/triple- ζ	-7.0	-5.7	0
M06/triple- ζ /C-PCM	-6.2	-6.1	0



Vacuum



Solvated

Table S2. Selected calculated average bond distances (Å) and angles (deg) for [TaF(OPh)₃(μ-OPh)]₂, **5A**, in the gas phase.

Ta–F	1.935
Ta–O _{terminal, ax.}	1.878
Ta–O _{terminal, eq.}	1.873
Ta–O _{bridging}	2.113
Ta–O _{bridging} –Ta	110.8
O _{bridging} –Ta–O _{bridging}	69.2

Cartesian coordinates (Å) and energies (a.u.) of the gas-phase optimized structures

2bA (-1145.18050392 a.u.)

Ta	-1.70637100	-0.33437500	0.00011700
F	0.24446500	-1.17360500	0.00047700
Ta	1.70637100	0.33437400	0.00005200
F	-0.24446600	1.17360500	-0.00036100
F	2.59300200	1.95032500	-0.00041000
F	-2.59300600	-1.95032400	0.00076200
F	1.46057900	0.39499700	-1.85363900
F	1.46046900	0.39613100	1.85368400
F	-1.46046900	-0.39630300	-1.85352300
F	-1.46058000	-0.39482900	1.85379900
O	3.04821500	-0.86739000	0.00029700
O	-3.04821400	0.86739200	-0.00037300
C	3.87378200	-2.00057500	-0.00088100
H	3.25330900	-2.90006100	-0.00017900
H	4.50264900	-1.98803400	0.89217500
H	4.50040000	-1.98786600	-0.89552200
C	-3.87377200	2.00058300	-0.00105400
H	-3.25329200	2.90006400	0.00057600
H	-4.50300600	1.98738600	0.89173600
H	-4.50002100	1.98854400	-0.89596000

2bB (-1145.18045389 a.u.)

Ta	1.72270000	0.21199700	0.00001200
F	0.00021300	-0.00022500	-1.19871500
Ta	-1.72270800	-0.21200300	0.00000700
F	-0.00020300	0.00001800	1.19873100
F	-2.83515900	-0.49805500	1.43511400
F	2.83515200	0.49820200	-1.43505300
F	-1.19115900	-2.03145500	0.00046300
F	1.19089500	2.03136700	-0.00047800
F	-2.83349100	-0.49813100	-1.43638900
F	2.83341500	0.49825400	1.43642300
O	1.87829700	-1.60350300	-0.00005500
O	-1.87811400	1.60354200	0.00003300
C	1.77579700	-3.00174400	-0.00019900
H	2.26926500	-3.39606300	-0.89225600
H	0.72187800	-3.28436700	-0.00145400
H	2.26711400	-3.39609800	0.89302900
C	-1.77556300	3.00178000	-0.00001800
H	-2.26650100	3.39600800	-0.89351200
H	-0.72162000	3.28436400	0.00161300
H	-2.26938100	3.39626800	0.89177200

2bC (-1145.18254644 a.u.)

Ta	-1.68919400	0.02386200	-0.09965600
Ta	1.68908500	-0.02311800	0.06964700
F	2.77335900	-1.46789500	-0.32449200
F	-2.77731000	-1.38307100	-0.60451100
F	2.77707900	1.38365800	0.57518400
F	-1.73617400	-0.52357800	1.69122100

F	1.73729200	0.52437800	-1.72122600
F	-2.77341400	1.46851000	0.29511700
F	-1.53331100	0.58096300	-1.88241900
F	1.53197500	-0.58022600	1.85229700
O	0.00387800	1.18121700	0.23331700
C	0.02844000	2.58896300	-0.08611200
H	-0.82184100	3.06856600	0.40052500
H	-0.04125600	2.70241500	-1.17148300
H	0.96306400	3.01425800	0.28143600
O	-0.00392000	-1.18034000	-0.26422100
C	-0.02844100	-2.58822000	0.05468200
H	0.82212900	-3.06754400	-0.43172700
H	-0.96283000	-3.01359400	-0.31336000
H	0.04083700	-2.70198300	1.14005000

2bD (-1145.17580815 a.u.)

Ta	1.60046300	0.04663000	-0.18672900
F	-0.32794200	0.43419900	-1.16810200
Ta	-1.87176300	-0.13199000	0.04667700
F	-0.09685300	-0.53055900	1.02317700
F	-2.87436100	-0.72985500	1.45714400
F	2.60536300	0.52918400	-1.66128400
F	-1.73040700	-1.81835000	-0.70989400
F	-1.70597600	1.57516900	0.80127200
F	1.29891100	-1.66733100	-0.91747900
O	2.85064600	-0.55389900	0.99256100
C	3.55761000	-1.66192900	1.49544900
H	3.25234300	-2.57275500	0.97053300
H	3.35154700	-1.76265900	2.56345600
H	4.62734900	-1.49394400	1.34952600
F	-3.15392100	0.42545800	-1.13406600
O	1.38026000	1.76049800	0.44528700
C	0.85151300	3.04554600	0.61283800
H	1.65489800	3.77890200	0.50040600
H	0.07637900	3.23020200	-0.13664300
H	0.40705400	3.13580800	1.60712600

2bE (-1145.17906968 a.u.)

Ta	-1.65142900	-0.23584000	-0.00814900
F	0.00811500	0.85222800	-0.03461400
Ta	1.69449800	-0.23088500	0.01387900
F	0.03042300	-1.32956500	0.04098300
F	3.19964600	-1.27274600	0.06410500
F	1.78783900	-0.13687600	1.85474800
F	1.81422800	-0.27414000	-1.82695300
F	-1.88670000	-0.16043500	1.82400000
F	-1.83851400	-0.29629500	-1.84031200
O	2.56409900	1.34879000	-0.04184800
C	2.80534600	2.74829800	-0.08641700
H	1.84980000	3.28460800	-0.10526100
H	3.38314400	2.94134000	-0.99984800
H	3.38114300	3.00070800	0.81361200
F	-3.06142400	-1.40432800	0.03325400
O	-2.33677900	1.42987600	-0.13477900
C	-3.35455300	2.40170500	0.07053000

H	-2.94221100	3.35040300	-0.29938100
H	-4.24399500	2.10643800	-0.49927700
H	-3.57776400	2.45744800	1.14326600

2bF (-1145.17030487 a.u.)

Ta	-1.64900700	-0.30695800	-0.32506600
F	0.19723400	-1.06009100	-0.29470500
Ta	1.64906600	0.30664000	-0.32549400
F	-0.19717300	1.05980600	-0.29588800
F	2.39978400	1.98792000	-0.27355000
F	-2.39972500	-1.98817700	-0.27118600
F	2.18364200	0.40512300	-2.08778600
F	-2.18368500	-0.40742400	-2.08721400
F	-2.95415500	0.99186000	-0.27332000
F	2.95422800	-0.99211200	-0.27237400
O	-1.90369900	-0.35292800	1.48574200
O	1.90385400	0.35464500	1.48525300
C	-2.61141100	-0.48350000	2.71166700
H	-3.05734900	-1.48432500	2.75663800
H	-1.87182000	-0.34451200	3.50971500
H	-3.38832100	0.28923100	2.75453100
C	2.61167100	0.48658000	2.71097500
H	3.05768900	1.48742300	2.75475800
H	1.87212900	0.34857200	3.50923800
H	3.38852500	-0.28616000	2.75467200

2bG (-1145.17683864 a.u.)

Ta	-1.51495300	-0.12490000	-0.30488200
F	0.05273600	-1.33674200	-0.51469800
Ta	1.81217100	-0.38665700	-0.59827900
F	0.23516900	0.82666100	-0.41336000
F	-2.67932100	-1.55527800	-0.29092700
F	1.83827600	-0.22710800	-2.42694600
F	-2.26618200	0.08319500	-1.97862800
F	-2.38420900	1.47487600	0.00034400
F	3.19068000	-1.59252100	-0.70427000
O	-1.61073600	-0.28329800	1.51055600
C	-2.19237800	-0.38498700	2.80346900
H	-2.88548200	-1.23437500	2.81431500
H	-1.35885100	-0.54675000	3.49946800
H	-2.71879600	0.55032300	3.02619900
F	1.96162600	-0.44644400	1.24789800
O	2.79175000	1.12199700	-0.65769500
C	3.28367400	2.33198800	-0.07891900
H	4.26519900	2.49895900	-0.54229400
H	2.57918200	3.13400000	-0.33058900
H	3.37302200	2.21340400	1.00706100

2bH (-1145.16918935 a.u.)

Ta	-1.41300900	-0.14386300	0.00542500
F	0.19639600	-1.27104700	-0.51662200
Ta	1.83607200	-0.23974300	-0.80596300
F	0.31277500	0.88489500	-0.30544000
F	-2.42804300	-1.71966200	0.08068800
F	1.42883100	-0.04370200	-2.58431600

F	-2.25461500	1.48709200	0.39375400
F	2.85593200	-1.69422000	-1.21894200
O	-1.52480500	-0.31601600	1.83051300
C	-2.40764400	-0.37750800	2.95045200
H	-3.07721800	-1.23847500	2.84291200
H	-1.74608000	-0.49931900	3.81900300
H	-2.97838500	0.55560100	3.01919200
F	2.30148600	-0.43756200	0.95786000
F	3.00954200	1.14987900	-0.94043400
O	-2.35913000	0.05970900	-1.55550400
C	-3.65957400	0.18623700	-2.13020500
H	-3.47794900	0.28204100	-3.20943200
H	-4.24730900	-0.71198600	-1.90901400
H	-4.15036700	1.08226000	-1.73343500

2bI (-1145.16329303 a.u.)

Ta	1.44186500	-0.06354300	0.00016300
F	-0.29276100	1.04248800	0.00153700
Ta	-1.90378200	-0.06180000	-0.00008000
F	-0.27139800	-1.15297600	-0.00144700
F	-3.00546800	-1.51837400	-0.00280600
F	-2.03124300	-0.03098400	-1.82909700
F	-2.03146800	-0.03739100	1.82901200
F	1.64176100	-0.06192100	-1.85158000
F	1.64197200	-0.06438100	1.85182000
O	2.38520500	1.48165200	0.00116400
C	2.26498000	2.91053000	0.00028400
H	3.30110900	3.27351000	0.00159500
H	1.73251200	3.22935900	-0.90327900
H	1.72994000	3.23024200	0.90201300
F	-3.04146600	1.36792100	0.00248200
O	2.80635500	-1.26074500	-0.00019000
C	4.15534500	-1.70665700	-0.00156800
H	4.11087300	-2.80391900	-0.00734300
H	4.65168200	-1.32987600	-0.90334300
H	4.65002100	-1.33920100	0.90497700

2bJ (-1717.79784526 a.u.)

F	-1.50339400	0.33282500	-0.14111200
Ta	-0.68441400	2.25916600	-0.03999400
Ta	-1.57444300	-1.72948700	-0.03656500
F	0.50674200	-1.45999800	-0.02542800
Ta	2.33861400	-0.50013000	-0.00687200
F	1.07120900	1.16948800	-0.00136600
F	2.06910800	-0.36545500	1.83973200
F	3.78769200	0.64691100	-0.00168800
F	2.08122700	-0.35804400	-1.85401400
F	-0.72964700	1.88784900	1.79200700
F	-0.55557800	2.01848000	-1.89029300
F	-2.41092400	2.91606000	-0.09926000
F	-1.35695800	-1.45344000	1.80132600
F	-1.26419600	-3.54909300	0.05210900
F	-1.32624500	-1.62992200	-1.88777200
O	-3.37756100	-1.74828200	-0.04532700
O	3.21560700	-2.07661100	0.00652800

O	0.20380200	3.82703500	0.04694200
C	3.73512800	-3.37340100	0.09285000
H	4.77139900	-3.36734300	-0.25329500
H	3.14324100	-4.04348100	-0.53525400
H	3.69662500	-3.71223000	1.13105100
C	-4.77232800	-1.63613900	-0.02789000
H	-5.20936500	-2.63251700	0.07465800
H	-5.11226400	-1.18167400	-0.96152100
H	-5.07647400	-1.01452200	0.81770800
C	1.00389600	4.97505000	0.04932600
H	1.63100900	4.98317600	-0.84557300
H	1.63444100	4.97681700	0.94154400
H	0.36087300	5.85861500	0.05357500

2bK (-1717.76017209 a.u.)

Ta	-0.91491400	1.97654700	0.17315300
Ta	2.40932500	0.01153500	-0.51360600
Ta	-0.92348100	-1.92661800	0.18107700
F	-0.89338200	-1.24958700	-1.53314200
F	-2.74054000	-2.26358200	0.18116000
F	-0.76456600	-2.32790800	2.01937900
F	-0.88563900	1.29674200	-1.53882600
F	-0.72256100	2.37075900	2.00671600
F	-0.46836500	3.70078200	-0.32666700
F	1.36089700	0.02246400	-2.02874700
F	3.49725600	-1.36618900	-1.09263600
F	3.19447700	0.03557600	1.20146400
F	-0.46213100	-3.64587600	-0.31618300
F	-2.73158200	2.31278100	0.18860300
F	3.54908200	1.33335200	-1.12723500
O	-1.38835900	0.02624300	0.85128100
C	-2.39592400	0.03113000	1.91341700
H	-3.38202300	0.03049600	1.44565300
H	-2.26392300	0.91727200	2.53114600
H	-2.26630700	-0.85102700	2.53706300
O	1.14488500	-1.48932100	0.29395700
C	1.90413500	-2.54439100	0.96914300
H	2.75683100	-2.10275900	1.48156700
H	2.23724300	-3.25910700	0.21502300
H	1.27161000	-3.03301300	1.70667500
O	1.15276700	1.51816900	0.28051900
C	1.88412400	2.46199200	1.12893600
H	2.91045300	2.54072900	0.77347400
H	1.86445700	2.10475400	2.15793900
H	1.41407000	3.44202200	1.05671400

2bL (-1717.80159267 a.u.)

F	-1.67324900	0.23600300	0.09868000
Ta	-0.76719700	2.07491600	-0.29161900
Ta	-1.75151300	-1.84758900	0.06814200
F	0.31349100	-1.60190700	-0.28649600
Ta	2.17846600	-0.72356900	-0.08087200
F	1.01111100	1.00965800	-0.01007800
F	1.73613300	-0.69976000	1.74784900
F	3.72809800	0.21361000	0.26835300

F	-0.61649400	1.22491500	-1.98140200
F	-2.40955500	2.84325200	-0.60983700
F	-1.17852300	-1.58156000	1.83804000
F	-1.55792100	-3.67472700	0.17923600
F	2.91839800	-2.40570000	-0.12462700
F	-3.55381200	-1.76197800	0.41364000
F	0.24772200	3.53876300	-0.76365400
O	-0.71906300	2.20343100	1.52233500
O	2.18977300	-0.35328600	-1.88084900
O	-1.79933500	-1.73941900	-1.75695800
C	-0.48311000	1.55916200	2.75563600
H	-1.20577900	0.74845300	2.88185700
H	0.52622700	1.13795300	2.75752800
H	-0.59168100	2.29057300	3.55856700
C	2.10914300	0.47528100	-3.00842100
H	1.32393200	0.11703200	-3.67948800
H	1.86715500	1.49841500	-2.70438400
H	3.07016600	0.46189000	-3.52927700
C	-1.24549100	-1.53320000	-3.02705800
H	-1.60807200	-0.58807000	-3.43669100
H	-0.15392400	-1.49240500	-2.93973800
H	-1.53301700	-2.36177000	-3.67915700

2bM (-1717.80159267 a.u.)

F	1.57420200	0.15589600	0.02336900
Ta	0.95486100	2.15795500	-0.19528800
Ta	1.39386300	-1.90252900	-0.19645800
F	-0.65042400	-1.43680400	0.01997200
Ta	-2.34456800	-0.25378400	-0.19932300
F	-0.91606200	1.27863600	0.03225100
F	-1.77216200	-0.12809100	-1.96608800
F	-3.69895300	0.95849100	-0.49048000
F	2.67669100	2.73459700	-0.49712500
F	0.99814000	-1.46931100	-1.96264500
F	1.03819600	-3.68544000	-0.48952800
F	-3.33885100	-1.78952100	-0.35708000
F	3.22237500	-1.98682300	-0.34297900
F	0.11494100	3.78388400	-0.34483900
O	-2.38268000	-0.07804900	1.64214000
O	1.24600100	-2.02210900	1.64312300
C	-2.08504700	0.62503100	2.81115600
H	-1.65501700	-0.05252200	3.55654100
H	-1.37193300	1.42947500	2.59368700
H	-3.00123100	1.06089800	3.21975400
C	0.47829000	-2.11972800	2.80559200
H	0.84258300	-1.40933600	3.55549500
H	-0.57303800	-1.90493300	2.57938200
H	0.55645900	-3.13205000	3.21235700
F	0.76179700	1.59590800	-1.95839400
O	1.13043400	2.09588800	1.64565800
C	1.57136300	1.47506100	2.81634600
H	0.75693800	1.43321000	3.54794000
H	1.91562300	0.45826600	2.59396000
H	2.39954200	2.04630600	3.24510200

2bN (-2290.40370180 a.u.)

F	0.12361600	1.59591400	-0.26134900
Ta	-1.81626900	2.21449300	0.03585400
Ta	2.20640500	1.78861500	-0.15287800
F	-2.13913800	0.14314000	0.01465900
F	2.12255400	-0.25228700	0.01915500
Ta	1.80417600	-2.32970800	0.04308900
F	-0.15172500	-1.73601500	-0.25118500
Ta	-2.23612200	-1.90384200	-0.14241400
F	-1.48072800	1.87403200	1.84209800
F	-3.64462500	2.41263200	0.30274100
F	-2.01274700	1.99249300	-1.81337300
F	-2.08223700	-1.63685100	-1.98599900
F	-1.86226900	-1.92400400	1.69030900
F	-2.05944700	-3.75033400	-0.29093700
F	1.46000200	-1.98228200	1.84577100
F	3.62776200	-2.53442700	0.31168000
F	1.99175300	-2.10171100	-1.80537700
F	1.84194100	1.81418100	1.68185400
F	1.92992000	3.62211900	-0.32762700
F	2.07464400	1.49687000	-1.99395400
O	4.00469200	1.75039900	-0.02724200
C	5.35355200	1.40726000	0.14008500
H	5.43365400	0.32211400	0.24851500
H	5.74208100	1.89638000	1.03634200
H	5.92009800	1.73296400	-0.73516900
O	-1.31555000	3.94298500	0.02187000
C	-0.81654500	5.25528500	-0.00830800
H	0.24421400	5.22211900	-0.26458700
H	-0.94775600	5.70897400	0.97683100
H	-1.36783700	5.82857600	-0.75716800
O	-4.02982300	-1.74095600	-0.01788700
C	-5.24348800	-1.04851700	0.13388000
H	-5.03140300	0.02180700	0.22496800
H	-5.74973400	-1.40396400	1.03396500
H	-5.87204700	-1.22941700	-0.74057300
O	1.30934500	-4.06006700	0.02611600
C	0.76966500	-5.35638600	-0.00776200
H	-0.29512300	-5.29004000	-0.24291600
H	0.90587700	-5.82448900	0.96990800
H	1.28866400	-5.93805500	-0.77298500

2bO (-2290.40902523 a.u.)

F	0.05250400	1.68443000	-0.02762600
Ta	-1.99663500	2.10529500	0.02736600
Ta	2.11289200	2.03332300	-0.05094200
F	-2.20943600	0.04037600	-0.13789500
F	2.20952300	-0.04068600	-0.13835500
Ta	1.99652000	-2.10545100	0.02702200
F	-0.05251400	-1.68373200	-0.02717300
Ta	-2.11294600	-2.03353900	-0.05070000
F	-1.72646000	1.60199000	1.83475800
F	-3.82144400	2.29170300	0.17495000
F	-1.81735200	-1.78045300	-1.90927600
F	-1.79336200	-3.84332000	-0.13890200

F	1.72759100	-1.60205200	1.83462400
F	3.82119300	-2.29366600	0.17391400
F	1.79311200	3.84309900	-0.13875800
F	1.81722300	1.78026600	-1.90950700
F	3.94518200	2.11562600	-0.19312400
O	1.97124600	1.83573900	1.75312500
C	1.42720300	1.36636400	2.96150800
H	0.34360300	1.25708600	2.84576700
H	1.64037100	2.09316200	3.74880700
H	1.87595800	0.40098600	3.20828100
F	-1.58283900	3.87721100	0.29877200
O	-1.84808700	2.03135100	-1.78598700
C	-1.32805400	1.40491100	-2.93453900
H	-1.75875400	1.87705300	-3.82001500
H	-1.59180900	0.34220000	-2.91400400
H	-0.24038200	1.52387200	-2.93955100
F	-3.94522800	-2.11522400	-0.19289300
O	-1.97118400	-1.83619000	1.75339500
C	-1.42677100	-1.36628500	2.96141700
H	-0.34320200	-1.25691000	2.84514200
H	-1.63960000	-2.09273300	3.74911900
H	-1.87542100	-0.40075100	3.20792000
F	1.58100600	-3.87696000	0.29846800
O	1.84813500	-2.03147600	-1.78642600
C	1.32785800	-1.40462700	-2.93472600
H	1.75841600	-1.87651800	-3.82039600
H	1.59173200	-0.34195200	-2.91388500
H	0.24020400	-1.52351700	-2.93967800

2bP (-2290.36564449 a.u.)

Ta	0.13803900	-2.50988600	-0.05020300
Ta	-2.51441200	-0.15817600	0.03076100
Ta	-0.16202900	2.48725200	0.12759300
Ta	2.48504900	0.14490900	-0.10438400
F	1.07127300	-0.95957100	1.02628300
F	1.21429900	-3.90307400	-0.64686200
F	0.31339800	-3.31760900	1.60077300
F	-1.23413900	-3.46823400	-0.84030700
F	0.86207300	1.07730400	-1.07259300
F	3.18239900	0.34115100	-1.80204500
F	3.50511500	-1.24023000	0.58095000
F	3.91337300	1.21110300	0.42015600
F	-1.01772800	0.84286200	1.13569000
F	-1.23797100	3.92908600	-0.33743700
F	1.19009800	3.50160400	-0.62855300
F	-0.27271200	3.16739800	1.83907200
F	-3.46594700	1.18739300	0.87467200
F	-3.92585700	-1.23893100	0.57253200
F	-0.94851300	-1.00620200	-1.08488400
F	-3.30854200	-0.24384000	-1.63333800
O	1.49517900	-1.47582900	-1.16511000
C	1.53836600	-1.71943600	-2.57251300
H	2.53022000	-2.07841100	-2.85227500
H	1.30172100	-0.79505800	-3.10434400
H	0.80064500	-2.48443300	-2.83745700

O	-1.49994200	-1.60365500	1.05650800
C	-1.73375600	-1.73450800	2.46065200
H	-2.58783300	-1.11447700	2.75245500
H	-0.84497700	-1.40601300	3.00528500
H	-1.96081100	-2.77452600	2.69817600
O	-1.58981000	1.53779200	-0.97366500
C	-1.69816800	1.84009000	-2.36619000
H	-2.73199400	2.09224400	-2.60580500
H	-1.37403100	0.97106600	-2.94418100
H	-1.06185400	2.69723000	-2.60992900
O	1.52123700	1.49217500	1.08320100
C	1.83948700	1.51932400	2.47564800
H	0.95314600	1.24316000	3.05143500
H	2.18284600	2.51686200	2.75447700
H	2.63986400	0.80171000	2.68574900

2bQ (-2290.38333045 a.u.)

F	-0.02407800	-1.40126600	1.53498200
Ta	-0.04712100	-2.75238000	-0.00642900
Ta	0.19430600	0.32726500	2.80008100
Ta	0.23088900	2.83635400	-0.12288000
F	0.26029900	1.46154900	-1.64140100
Ta	0.11143400	-0.25529600	-2.92798000
F	1.70017800	-3.21663900	0.46129800
F	-0.07471000	-3.82474900	-1.51131500
F	-1.73684900	-2.05552600	-0.36316000
F	-1.61187500	-0.25840900	-2.19596700
F	1.92683500	0.08864200	-3.25050900
F	-0.38642100	0.91877800	-4.27045600
F	1.93968500	2.20891400	0.27228100
F	0.20704300	3.93592400	1.36256300
F	-1.52794000	3.23765100	-0.60114900
F	1.90163900	0.25002600	2.03588200
F	0.69144200	-0.83527000	4.15292000
F	-1.61566400	0.02183200	3.18863000
O	0.39260100	1.88946200	3.66330600
C	0.51601000	3.10699800	4.35740400
H	0.43771500	3.92691900	3.64116300
H	1.48764000	3.13403500	4.85492400
H	-0.28353800	3.17521700	5.09838500
O	-0.00772000	-1.80701400	-3.82440100
C	-0.04122900	-3.02792100	-4.52215700
H	-0.85288800	-2.99536500	-5.25180500
H	-0.20683900	-3.83539900	-3.80656500
H	0.91309000	-3.17004500	-5.03444000
F	-0.72280100	-4.01239700	1.15788700
F	0.87908600	4.09415500	-1.30525200
O	-0.56801800	1.26825800	1.00853000
C	-1.93436500	0.86332400	0.64719300
H	-2.63660400	1.49589800	1.19103100
H	-2.08560200	-0.17835700	0.91063200
H	-2.07255800	0.97459000	-0.42345000
O	0.81852400	-1.20558700	-1.12009900
C	2.18648800	-0.82750300	-0.73941000
H	2.33103000	-1.01282800	0.31889300

H	2.33384500	0.23143700	-0.93128400
H	2.88555000	-1.41938600	-1.33108300

2bR (-2290.39094501 a.u.)

F	0.11276500	1.50156100	-0.27400400
Ta	-1.85959700	2.08235100	0.01074600
Ta	2.17706200	1.75714100	-0.20089200
F	-2.18603900	0.04113600	-0.01509300
F	2.14100100	-0.30214400	0.05660300
Ta	1.83970000	-2.35401500	0.15561200
F	-0.15698500	-1.84691900	-0.16832800
Ta	-2.22758900	-2.04685600	-0.10073200
F	-1.46277100	1.77297700	1.81019000
F	-1.96992400	1.89866500	-1.84837500
F	-2.05324200	-1.78477000	-1.94265700
F	-1.92432300	-1.92326400	1.74041200
F	-2.08121200	-3.88024200	-0.17008100
F	1.39533300	-1.98693100	1.93251000
F	1.95255900	-2.23721600	-1.70697500
F	1.86688500	1.79225000	1.64252000
F	1.87808700	3.55951400	-0.44982900
F	2.06535200	1.32915600	-2.01741100
O	3.98369900	1.80950600	-0.11420600
C	5.37874800	1.85176200	-0.08665700
H	5.71323700	2.87697500	-0.26568300
H	5.78060800	1.19938400	-0.86684800
H	5.73644500	1.52046600	0.89211600
O	-4.03260700	-1.89865000	-0.02509400
C	-5.27256500	-1.26642100	0.09763800
H	-5.11510300	-0.18451200	0.16995000
H	-5.77787900	-1.62282100	0.99879000
H	-5.88564700	-1.48889000	-0.77910000
F	1.27195200	-4.10785300	0.18526400
F	-1.21509000	3.80959400	-0.01645600
O	3.59811700	-2.66211700	0.45307400
C	4.94315700	-2.89201700	0.74785000
H	5.23647800	-2.29143100	1.61344300
H	5.08790500	-3.95094200	0.97734100
H	5.55844700	-2.62220100	-0.11489600
O	-3.61050800	2.48054300	0.26692500
C	-4.92263000	2.90096900	0.49128500
H	-5.28297300	2.49185000	1.43963800
H	-4.95218800	3.99276600	0.53647000
H	-5.56291700	2.55828100	-0.32690900

2bS (-2290.37752945 a.u.)

F	-1.17162300	1.25886700	-0.08974800
Ta	-2.88501500	0.11299100	-0.33856000
Ta	0.07321500	2.94187800	-0.00460600
F	-1.58728100	-1.46571600	0.16691000
F	1.59493900	1.50112900	0.11089900
Ta	2.85525300	-0.08631100	-0.38243100
F	1.13838000	-1.21884000	-0.08061900
Ta	-0.09530900	-2.91501000	-0.05927000
F	-4.25620500	-1.07847700	-0.64067300

F	-0.27137100	-2.48548400	-1.85834500
F	1.37851600	-3.98118500	-0.33290400
F	4.23543700	1.08422200	-0.71920000
F	-1.42584500	3.99634700	-0.14526200
F	0.24085900	2.59289200	-1.82015700
F	1.31459400	4.29609800	0.06198300
O	-0.03032000	2.58426700	1.80903900
C	-0.03690300	1.56209100	2.75364900
H	-0.54321700	0.67751700	2.34324700
H	-0.55735000	1.89494900	3.65725400
H	0.99072500	1.28622500	3.01831000
F	-3.79784000	1.65345800	-0.74633100
F	-1.37021700	-4.23925800	-0.05097200
O	0.10823500	-2.75275600	1.76943600
C	0.30208700	-2.03597000	2.94385500
H	1.05497000	-1.25379700	2.78290100
H	0.64834800	-2.70834800	3.73401900
H	-0.63790700	-1.56878200	3.26480600
F	3.73847500	-1.63414500	-0.83210200
F	2.13102900	0.18160900	-2.07866500
F	-2.19363300	-0.15753400	-2.04573000
O	-3.13782200	0.16585200	1.49253200
O	3.19236500	-0.16009600	1.43604300
C	3.54717900	0.16795100	2.74272700
H	3.22631100	1.18970700	2.97857000
H	3.08402200	-0.52946900	3.45008000
H	4.63350900	0.10745600	2.85721900
C	-3.24743100	-0.25198100	2.81653700
H	-2.86623500	-1.27567500	2.92427900
H	-2.68323200	0.41915200	3.47323700
H	-4.29763900	-0.23443300	3.12258700

2dA (-1223.77577524 a.u.)

Ta	1.62203400	-0.62986900	0.05988800
F	-0.41616100	-0.99283200	0.54063400
Ta	-1.62421500	0.62946900	-0.03175700
F	0.41416000	0.99335000	-0.51366800
F	-2.23472900	2.23524200	-0.70094800
F	2.23158800	-2.23303000	0.73549600
F	-1.14779900	1.39328700	1.60772100
F	-1.63215400	-0.16720900	-1.72983800
F	1.63167000	0.17685500	1.75248100
F	1.13312700	-1.40259400	-1.57266200
O	-3.13505400	-0.18536900	0.51722900
O	3.12920200	0.17172300	-0.51455400
C	-4.10401500	-1.21309700	0.64704300
H	-4.01199600	-1.61790900	1.66012600
H	-5.08563000	-0.73568300	0.56026100
C	4.09706400	1.17232000	-0.77897200
H	3.96067100	1.48804300	-1.81848700
H	5.07887300	0.69477900	-0.69552600
C	-3.89249400	-2.26829800	-0.40682700
H	-2.89958000	-2.71784600	-0.31092900
H	-4.64104500	-3.05779200	-0.29814700
H	-3.97904000	-1.84251100	-1.40976600

C	3.94175000	2.31884600	0.18553500
H	4.67571900	3.09717400	-0.04044500
H	2.94149300	2.75544700	0.10829200
H	4.09537600	1.98844700	1.21606100

2dJ (-1835.69161443 a.u.)

F	-1.63004700	0.19382000	-0.13053100
Ta	-0.92005100	2.15974600	0.03226700
Ta	-1.58918400	-1.86874100	0.07919900
F	0.48696300	-1.52219700	-0.06200000
Ta	2.22619000	-0.43233900	0.08865900
F	0.83595900	1.11803500	0.36498100
F	1.98819900	-0.65789100	1.93002600
F	3.54139900	0.86143700	0.27796700
F	1.91389800	-0.03579600	-1.71502500
F	-1.23227400	1.86357100	1.85194800
F	-0.52590500	1.86979100	-1.77661700
F	-2.63729000	2.76921800	-0.29236100
F	-1.25232400	-1.47489300	1.87393100
F	-1.24193500	-3.67430000	0.25629100
F	-1.43123100	-1.86304700	-1.78722800
O	-3.38982900	-1.90887300	0.14245900
O	3.31301300	-1.84213200	-0.18664200
O	-0.04490600	3.73212000	0.16656100
C	4.31204400	-2.79906500	-0.47122900
H	4.01385300	-3.32499000	-1.38439900
H	4.31922800	-3.52105800	0.35194100
C	-4.75452100	-1.62272800	-0.10339400
H	-5.19878800	-2.52462800	-0.53811700
H	-5.22943300	-1.44257400	0.86660100
C	0.98542700	4.69057800	0.00221500
H	1.03753100	5.27433700	0.92696200
H	0.67647100	5.36047300	-0.80737400
C	5.64340700	-2.11008300	-0.62793200
H	5.91146900	-1.57533600	0.28762500
H	6.42426200	-2.84503400	-0.84099700
H	5.61106700	-1.39084200	-1.45097700
C	-4.87639000	-0.43543100	-1.02335500
H	-4.36271600	-0.62738900	-1.97018000
H	-5.92986700	-0.23488200	-1.23676700
H	-4.44215800	0.45862900	-0.56857500
C	2.28923600	4.00086200	-0.30643800
H	2.19796100	3.38917900	-1.20996600
H	3.07357400	4.74434700	-0.47305000
H	2.59971800	3.35371100	0.51752400

2dN (-2447.60488967 a.u.)

F	-1.08781700	1.26117700	-0.40062700
Ta	-2.60866900	0.48965100	0.77100100
Ta	0.53093800	2.57849400	-0.57700800
F	-1.50427700	-1.24947400	0.38761600
F	1.35500400	1.19721400	0.72810200
Ta	2.49853600	-0.53412300	1.03713600
F	1.09873800	-1.20773000	-0.33664500
Ta	-0.46263100	-2.48855300	-0.89888600

F	-1.37849200	0.68887700	2.15236200
F	-3.81333600	-0.48497200	1.78635700
F	-3.38538100	-0.04937400	-0.86200900
F	-0.72404000	-1.16876600	-2.18764100
F	0.12002200	-3.35376300	0.67222400
F	0.67656100	-3.50724000	-1.95044700
F	1.20496000	-0.92696300	2.31713400
F	3.61806000	0.31429000	2.24038600
F	3.40429700	0.22203500	-0.44074100
F	-0.29311900	3.33039200	0.94183000
F	-0.47027300	3.66779700	-1.69537300
F	1.00777800	1.39243000	-1.93754400
O	2.09373400	3.47678800	-0.52693000
C	3.51146600	3.58739100	-0.51120400
H	3.87098500	2.97780300	0.32735000
H	3.74821700	4.63494700	-0.30101600
O	-3.33893700	2.13454500	0.81495800
C	-3.56833100	3.45698400	0.34652900
H	-2.65818000	4.02777600	0.55991300
H	-4.38572100	3.86967200	0.94570600
O	-2.01386500	-3.38019900	-1.12421200
C	-3.39980100	-3.57507900	-0.86779500
H	-3.91025000	-2.64766100	-1.15027000
H	-3.73762900	-4.37413300	-1.53465200
O	3.25985500	-2.16215700	0.92471600
C	3.45950200	-3.42263600	0.29970000
H	2.50065300	-3.94988800	0.34033200
H	4.18343900	-3.97102900	0.90984900
C	4.08091300	3.11693900	-1.82263700
H	5.17043600	3.21112300	-1.80670300
H	3.82854400	2.06778400	-1.99220200
H	3.69388100	3.71711600	-2.65046200
C	-3.89155700	3.42998400	-1.12448600
H	-4.05274200	4.44763500	-1.48995300
H	-3.06467200	2.99269600	-1.69138700
H	-4.79307000	2.84140300	-1.31504300
C	-3.61399600	-3.91588000	0.58407600
H	-3.26784200	-3.10359800	1.22921700
H	-4.67943800	-4.06979700	0.77580800
H	-3.07703400	-4.82966900	0.85258200
C	3.93338400	-3.22651600	-1.11600000
H	4.08455500	-4.19925400	-1.59206400
H	3.18815700	-2.67953100	-1.70154200
H	4.87708700	-2.67490600	-1.14139000

2fA (-1528.45329535 a.u.)

Ta	-1.26140500	1.18486000	-0.14822500
F	0.80842800	0.85432800	-0.21826100
Ta	1.26129100	-1.18457900	0.14847800
F	-0.80857800	-0.85405800	0.21856400
F	1.24670200	-2.98781600	0.50747500
F	-1.24746200	2.98814000	-0.50702800
F	1.15727100	-0.73201100	1.96189100
F	0.92223800	-1.47111800	-1.66643600
F	-0.92251200	1.47145100	1.66671000

F	-1.15714400	0.73253300	-1.96168800
O	3.02853000	-0.79448700	-0.02701500
O	-3.02860400	0.79444900	0.02703100
C	4.15408800	-0.02203600	-0.03575900
C	5.27261200	-0.47851300	-0.71382700
C	4.14377600	1.19267300	0.63366700
C	6.41384000	0.30769800	-0.71616400
H	5.23248600	-1.43373400	-1.22579100
C	5.29358000	1.96581000	0.61921600
H	3.24303700	1.51600000	1.14705700
C	6.42721500	1.52682000	-0.05190300
H	7.29801800	-0.03551000	-1.24329200
H	5.30145000	2.91957400	1.13651700
H	7.32345000	2.13814900	-0.05862900
C	-4.15387900	0.02160000	0.03541000
C	-5.27268400	0.47757400	0.71336700
C	-4.14307900	-1.19296100	-0.63428100
C	-6.41366200	-0.30899100	0.71535400
H	-5.23293600	1.43269900	1.22554200
C	-5.29264500	-1.96646600	-0.62017200
H	-3.24218400	-1.51590700	-1.14763000
C	-6.42653000	-1.52798700	0.05084400
H	-7.29804200	0.03383900	1.24238800
H	-5.30012700	-2.92010700	-1.13770800
H	-7.32256700	-2.13961000	0.05730000

2fB (-1528.45124807 a.u.)

Ta	0.64379100	1.61138700	-0.14110600
F	0.00080900	-0.00061800	-1.33070300
Ta	-0.64352900	-1.61068400	-0.14181800
F	-0.00045600	0.00118100	1.07156600
F	-0.93396400	-2.76143000	1.26325500
F	0.97601300	2.65427600	-1.61266400
F	1.18663600	-2.03645600	-0.12270900
F	-1.18649400	2.03663000	-0.12449800
F	-0.97498600	-2.65869800	-1.60987400
F	0.93376000	2.76763100	1.25942600
O	2.32604900	0.86042400	-0.05268200
O	-2.32597200	-0.85984900	-0.05603100
C	-3.47835300	-0.17446800	0.16082400
C	-4.49039600	-0.24040100	-0.78481400
C	-3.61816900	0.56470700	1.32671800
C	-5.66976600	0.44846900	-0.54980000
H	-4.34006200	-0.82729800	-1.68462300
C	-4.80277500	1.24649300	1.54712400
H	-2.79333100	0.60353300	2.03063900
C	-5.82910900	1.18976000	0.61307900
H	-6.46930000	0.40499600	-1.28220300
H	-4.92282800	1.83125600	2.45323600
H	-6.75437100	1.72794400	0.79076800
C	3.47799800	0.17383400	0.16275700
C	4.48966900	0.24060700	-0.78326700
C	3.61787600	-0.56718700	1.32742600
C	5.66857200	-0.44963400	-0.55006100
H	4.33931700	0.82924700	-1.68193200

C	4.80202800	-1.25038200	1.54602000
H	2.79367000	-0.60616000	2.03205000
C	5.82787100	-1.19304300	0.61148700
H	6.46780200	-0.40550200	-1.28275700
H	4.92207200	-1.83674700	2.45109000
H	6.75275800	-1.73234200	0.78774100

2fC (-1528.45324608 a.u.)

Ta	-1.69880900	-0.04360000	-0.33599900
Ta	1.70955400	0.04571800	0.07557200
F	2.77334200	-1.45494800	0.04277500
F	-2.81999200	-1.46595000	-0.66969800
F	2.87194800	1.45093800	0.33086000
F	-1.90390000	-0.25610100	1.51543200
F	1.80899100	0.25526500	-1.78275600
F	-2.78014500	1.44595500	-0.33071200
F	-1.35187300	0.14694600	-2.17078000
F	1.45120900	-0.09792000	1.93072100
O	-0.02407900	1.18017900	-0.00994500
O	0.02551300	-1.19497200	-0.17532800
C	-0.00080200	-2.58938400	-0.00721400
C	-0.12148100	-3.38352700	-1.13190100
C	0.08931600	-3.11066500	1.26992000
C	-0.15134500	-4.75970400	-0.96408700
H	-0.19035600	-2.92013200	-2.11171400
C	0.06219300	-4.48981300	1.41751600
H	0.17967200	-2.44566600	2.12281800
C	-0.05768500	-5.31202500	0.30617300
H	-0.24695800	-5.40255000	-1.83274500
H	0.13438000	-4.92148600	2.41030600
H	-0.08015500	-6.38964900	0.43002600
C	-0.00374900	2.58283400	-0.04615600
C	-0.03640800	3.26685600	1.15366000
C	0.05732500	3.21703300	-1.27223200
C	-0.00734000	4.65278000	1.11793100
H	-0.08199700	2.71205400	2.08638600
C	0.08284600	4.60421200	-1.28772900
H	0.08529300	2.62677400	-2.18300400
C	0.05131000	5.31966600	-0.09872100
H	-0.03084400	5.21320100	2.04659100
H	0.12948600	5.12655000	-2.23757900
H	0.07346400	6.40411700	-0.12020100

2fJ (-2292.70903731 a.u.)

F	-1.56442000	0.17576900	-0.18664900
Ta	-0.87620100	2.14174600	-0.06770000
Ta	-1.49207800	-1.89170800	-0.07695200
F	0.56262200	-1.51255800	-0.15078500
Ta	2.32070800	-0.42668900	0.00294200
F	0.94313300	1.14985800	-0.01103500
F	1.92135200	-0.41766400	1.82723100
F	3.66982600	0.82461400	0.14889600
F	2.15086700	-0.25144800	-1.84966200
F	-0.90916300	1.77607500	1.76355100
F	-0.72369700	1.92302800	-1.91726600

F	-2.63981200	2.68814000	-0.12916900
F	-1.20827000	-1.58132600	1.74313200
F	-1.11914500	-3.69741200	0.00977900
F	-1.30845800	-1.78479800	-1.93305200
O	-3.30732100	-1.94817100	-0.02716700
O	3.30247600	-1.95548600	0.01148000
O	-0.04790200	3.75682900	0.02328000
C	0.80656800	4.81910600	0.03900400
C	0.29191200	6.09873200	-0.09392700
C	2.16530600	4.58520200	0.18391400
C	1.16917600	7.17176400	-0.08085700
H	-0.77828500	6.23474600	-0.20579000
C	3.02703900	5.67012800	0.19453500
H	2.52913800	3.56783600	0.28256800
C	2.53379000	6.96128800	0.06313100
H	0.78079200	8.17962900	-0.18501800
H	4.09321100	5.50194000	0.30534600
H	3.21496100	7.80561200	0.07157900
C	3.78084800	-3.22987100	0.09227600
C	5.14536900	-3.42919800	0.22634300
C	2.88557100	-4.28721600	0.04274600
C	5.62086000	-4.72813100	0.31474300
H	5.80938400	-2.57240900	0.26143300
C	3.37929500	-5.57872500	0.13227900
H	1.82370800	-4.08943600	-0.06013600
C	4.74281000	-5.80249600	0.26811400
H	6.68707900	-4.89954600	0.42135500
H	2.68944000	-6.41539800	0.09675400
H	5.12216100	-6.81646800	0.33854200
C	-4.63808400	-1.65077900	-0.00387500
C	-5.55490200	-2.68807900	0.05000000
C	-5.03103300	-0.32138900	-0.03510300
C	-6.90583400	-2.37931400	0.07362700
H	-5.20055600	-3.71284600	0.07240100
C	-6.38627000	-0.03260000	-0.01071300
H	-4.28119300	0.46260400	-0.07867800
C	-7.32348600	-1.05576700	0.04390100
H	-7.63646000	-3.18049700	0.11581200
H	-6.70916700	1.00290400	-0.03448000
H	-8.38238700	-0.82043800	0.06282200

2fK (-2292.65969901 a.u.)

Ta	-0.96519200	2.00890100	0.02326200
Ta	2.41794400	0.01900100	-0.57945500
Ta	-0.98576000	-1.95495600	-0.04528800
F	-0.83680700	-1.18502800	-1.71429100
F	-2.80537200	-2.22079800	-0.18939000
F	-0.91555400	-2.48825600	1.74568100
F	-0.81351200	1.31056600	-1.67632800
F	-0.92341600	2.46469000	1.83640700
F	-0.48329700	3.70552000	-0.51086500
F	1.35877400	0.04533500	-2.08877800
F	3.50885400	-1.31471400	-1.23425200
F	3.21998800	-0.02071500	1.11144800
F	-0.53067500	-3.62953300	-0.66946000

F	-2.78220400	2.29008400	-0.13903500
F	3.49318300	1.39370600	-1.17628800
O	-1.38325700	0.01371000	0.70594400
O	1.09520700	-1.48162700	0.19886100
O	1.10046900	1.48991300	0.26521500
C	1.79020600	2.38713400	1.12900700
C	1.83849600	2.11452100	2.48326400
C	2.39764200	3.50087600	0.58341400
C	2.51789900	2.98546500	3.31594000
H	1.34190400	1.22881900	2.86696800
C	3.07657900	4.36734800	1.42913400
H	2.34401300	3.67796500	-0.48486500
C	3.13828800	4.11169200	2.78992400
H	2.56310000	2.78407300	4.38094800
H	3.55968100	5.24587100	1.01474900
H	3.67155000	4.79207200	3.44564500
C	1.78071500	-2.45144600	0.98404600
C	2.27054000	-3.58178200	0.35880400
C	1.93249000	-2.24209500	2.34232000
C	2.93414600	-4.53077900	1.12397000
H	2.12938000	-3.71270700	-0.70848700
C	2.59799100	-3.19473400	3.09373600
H	1.53580500	-1.34034100	2.79787900
C	3.09878600	-4.33923000	2.48683600
H	3.32279700	-5.42341000	0.64541400
H	2.72523800	-3.04233200	4.16028600
H	3.61924300	-5.08353400	3.08042200
C	-2.21138000	-0.00195700	1.86196200
C	-3.58118300	0.07121700	1.70201100
C	-1.62304900	-0.08781400	3.11040800
C	-4.38318600	0.06029600	2.83545300
H	-4.00615800	0.13817400	0.70675800
C	-2.43287200	-0.10018100	4.23168500
H	-0.54196600	-0.15145600	3.19051100
C	-3.81354300	-0.02520000	4.09587800
H	-5.46079300	0.11796600	2.72522900
H	-1.98371200	-0.16933600	5.21682700
H	-4.44566500	-0.03439800	4.97763200

2fN (-3056.95466852 a.u.)

F	0.03092400	1.20324200	-0.31985500
Ta	-1.70764400	1.89301900	0.56498600
Ta	2.06868000	1.53385300	-0.62674700
F	-2.12639600	-0.14306100	0.48791700
F	2.22110800	-0.36003100	0.16869700
Ta	1.78602600	-2.36773700	0.56538600
F	-0.06035700	-1.81285000	-0.20919100
Ta	-2.13051900	-2.02816800	-0.37400800
F	-0.87380800	1.42156600	2.16614400
F	-3.35385700	2.18723300	1.34914900
F	-2.43098100	1.83793800	-1.16850700
F	-1.84500600	-1.09157900	-1.96209300
F	-1.95501500	-2.63720100	1.39069800
F	-1.88411500	-3.70600500	-1.10288100
F	1.11125200	-1.64707700	2.14980500

F	3.49372200	-2.60347000	1.22262900
F	2.28919300	-2.53454900	-1.22836400
F	1.98481800	2.06934400	1.17214100
F	1.54817400	3.19271900	-1.25706700
F	1.76067300	0.64537100	-2.23482900
O	3.86863700	1.71931000	-0.80592000
O	-1.07886900	3.59927400	0.51028000
O	-3.95042500	-1.93061000	-0.42164300
O	1.15057100	-4.05773500	0.77176900
C	-0.36926400	4.74813200	0.70376100
C	0.42754600	4.85787300	1.83313400
C	-0.46000700	5.76094200	-0.23648100
C	1.14824000	6.02613100	2.02214700
H	0.48062300	4.02856500	2.53116200
C	0.26827900	6.92172900	-0.03121300
H	-1.08716600	5.62257900	-1.11015200
C	1.06989400	7.05681900	1.09480600
H	1.77769700	6.12895200	2.90000500
H	0.21098200	7.72474100	-0.75869200
H	1.63842300	7.96820800	1.24855400
C	5.22227400	1.85013100	-0.79027100
C	5.83765600	2.33400200	0.35457200
C	5.94632500	1.49374500	-1.91782100
C	7.21700600	2.46266900	0.36294700
H	5.22966400	2.59648900	1.21459500
C	7.32486300	1.62994900	-1.89188600
H	5.42309200	1.11540300	-2.78945700
C	7.96135200	2.11282400	-0.75616900
H	7.71348300	2.83746200	1.25205200
H	7.90549000	1.35417700	-2.76607300
H	9.04134600	2.21493600	-0.74232100
C	0.37161700	-5.17601500	0.83133600
C	0.51289400	-6.14570400	-0.14854300
C	-0.55297200	-5.29313900	1.85762400
C	-0.30619500	-7.26185900	-0.09882000
H	1.24517100	-6.00553500	-0.93642500
C	-1.36473900	-6.41544200	1.88975100
H	-0.64264100	-4.49727600	2.58923200
C	-1.24429400	-7.39809000	0.91585100
H	-0.21347100	-8.02748300	-0.86209500
H	-2.09962600	-6.51955400	2.68126700
H	-1.88578500	-8.27270900	0.94606600
C	-5.15144700	-1.29244000	-0.53720500
C	-6.30114800	-1.94184400	-0.11722100
C	-5.18167000	-0.01095900	-1.06825900
C	-7.51482800	-1.28256800	-0.23164500
H	-6.22811100	-2.94358600	0.29194000
C	-6.40462800	0.63331200	-1.17066700
H	-4.25964300	0.46595200	-1.39007700
C	-7.56942100	0.00247000	-0.75523500
H	-8.42445800	-1.77697600	0.09371000
H	-6.44252800	1.63811400	-1.57822100
H	-8.52297600	0.51361400	-0.83791400

2fO (-3056.95594424 a.u.)

F	0.19664100	1.63231700	0.15326000
Ta	-1.77917300	2.21510200	-0.04216500
Ta	2.28139100	1.80551700	0.01794100
F	-2.11168400	0.16352100	-0.22823500
F	2.20212300	-0.24645700	-0.19422300
Ta	1.85929100	-2.29791100	-0.05333100
F	-0.11819800	-1.70992000	0.13171000
Ta	-2.19776900	-1.89202500	-0.01651200
F	-1.88999800	1.76592900	1.78069500
F	-3.58793400	2.56430000	-0.10778300
F	-1.76904000	-1.90528200	-1.84916700
F	-2.06318800	-3.72876600	0.06161500
F	1.92783400	-1.88245400	1.78091200
F	3.66757100	-2.64750400	-0.10197100
F	2.14325100	3.64231400	0.10136900
F	1.86407400	1.81728300	-1.81661400
F	4.10315800	1.69178200	-0.21094200
O	2.18865700	1.58209700	1.84446700
F	-1.19108000	3.93723100	0.22946200
O	-1.57777300	2.11399400	-1.87123400
F	-4.01723400	-1.77101100	-0.26153800
O	-2.12618600	-1.67260400	1.81025200
F	1.26681100	-4.02340900	0.18350600
O	1.66041900	-2.15392000	-1.87822800
C	1.69538900	-1.59955200	-3.12073100
C	0.67322100	-1.87295600	-4.01864500
C	2.77771400	-0.80228400	-3.46586900
C	0.77115800	-1.36662000	-5.30403000
H	-0.17518600	-2.46791700	-3.69913800
C	2.85124700	-0.29304700	-4.75219700
H	3.54986500	-0.59788000	-2.72994000
C	1.85801800	-0.58619600	-5.67592700
H	-0.01596700	-1.58029200	-6.01984500
H	3.69530100	0.32807600	-5.03352300
H	1.92673000	-0.19822100	-6.68773900
C	-1.67517800	1.60529000	-3.12845300
C	-2.76903300	0.81247000	-3.44827900
C	-0.70364700	1.92127800	-4.06670500
C	-2.90209300	0.34785700	-4.74660100
H	-3.50100400	0.57627300	-2.68092800
C	-0.85886600	1.45738600	-5.36235000
H	0.14807900	2.52122500	-3.76673000
C	-1.95646500	0.67979700	-5.70731900
H	-3.75526000	-0.26938300	-5.00841600
H	-0.10764900	1.70016300	-6.10721600
H	-2.07197600	0.32512100	-6.72700900
C	1.64452000	1.63519000	3.09052500
C	0.80246300	2.69221000	3.40767900
C	1.97499400	0.65905400	4.01836000
C	0.29728600	2.78040700	4.69499600
H	0.56618700	3.43603500	2.65119400
C	1.46213400	0.76439300	5.30040200
H	2.61950600	-0.15939900	3.71875100
C	0.63355500	1.82484100	5.64384100
H	-0.35790600	3.60495200	4.95623400

H	1.70891700	0.00622600	6.03673800
H	0.24252800	1.90246600	6.65375100
C	-1.62579700	-1.66933700	3.07480100
C	-0.70895800	-2.64608500	3.43843800
C	-2.07400200	-0.71505200	3.97638800
C	-0.25131700	-2.67748800	4.74623800
H	-0.37285300	-3.37361900	2.70431400
C	-1.61256300	-0.76691800	5.28055500
H	-2.76760300	0.04665500	3.63897800
C	-0.71017600	-1.74853200	5.66971800
H	0.46204000	-3.43919400	5.04366500
H	-1.95927500	-0.03015300	5.99809400
H	-0.35791200	-1.78443300	6.69620200

2fP (-3056.91198435 a.u.)

Ta	-0.02275800	-2.54683900	-0.02800300
Ta	-2.53743700	-0.01907300	0.01915000
Ta	-0.00760500	2.49198000	0.12483800
Ta	2.50151800	-0.03062100	-0.11501200
F	0.97419000	-1.00819700	0.98809500
F	0.94655800	-4.03339300	-0.56429100
F	0.11544100	-3.30678300	1.64315500
F	-1.46062700	-3.40959300	-0.81491200
F	0.88887400	0.95652800	-1.02420200
F	3.14893800	0.12933000	-1.83005800
F	3.41488200	-1.48073700	0.59038400
F	4.02031800	0.92774200	0.34362900
F	-0.93852000	0.87743500	1.08535700
F	-0.98216900	4.01693100	-0.27662200
F	1.39987300	3.39465400	-0.67266400
F	-0.06075500	3.13557600	1.84802600
F	-3.40211400	1.37688400	0.87597200
F	-4.02697200	-1.01251800	0.49719200
F	-0.99266600	-0.94494300	-1.04059700
F	-3.28950000	-0.05320100	-1.66042100
O	1.43859200	-1.65527400	-1.16173000
O	-1.65458000	-1.55537000	1.06586100
O	-1.54159000	1.68228300	-0.97348400
O	1.68166800	1.43011500	1.06989600
C	2.19516800	1.66388700	2.34259500
C	2.98292100	2.78409900	2.54598600
C	1.90660600	0.77168000	3.36065400
C	3.49327100	3.01566000	3.81142800
H	3.18559600	3.44657600	1.70985700
C	2.43314500	1.01409800	4.62318600
H	1.28302800	-0.09372900	3.15777800
C	3.22062600	2.13214400	4.84988000
H	4.11169800	3.88941300	3.98844000
H	2.22119400	0.32218500	5.43190700
H	3.62713900	2.31745600	5.83869600
C	-2.09588000	-1.87122400	2.34772600
C	-2.87084800	-3.00505600	2.52336100
C	-1.74238200	-1.05007800	3.40431300
C	-3.30025900	-3.32441100	3.79974200
H	-3.12197500	-3.61347600	1.65976000

C	-2.18838000	-1.37979300	4.67792100
H	-1.12802600	-0.17339000	3.22435000
C	-2.96197500	-2.51272900	4.87674000
H	-3.90603000	-4.21096800	3.95550600
H	-1.92371900	-0.74526100	5.51753500
H	-3.30474600	-2.76678000	5.87440300
C	1.68784100	-2.09101000	-2.46038200
C	2.80705400	-2.87108400	-2.69585800
C	0.81942800	-1.72549200	-3.47424900
C	3.06258000	-3.29302800	-3.98902200
H	3.45400100	-3.13328100	-1.86432200
C	1.08550900	-2.16381700	-4.76533900
H	-0.04551600	-1.10962900	-3.24876100
C	2.20313000	-2.94206600	-5.02389700
H	3.93706900	-3.90280300	-4.19076700
H	0.41271100	-1.88969300	-5.57148900
H	2.40743900	-3.27870100	-6.03497500
C	-1.84532100	2.19724800	-2.23094700
C	-1.01654000	1.90208100	-3.29985800
C	-2.97422200	2.98658300	-2.37094300
C	-1.33203200	2.42513300	-4.54752300
H	-0.14403100	1.27333900	-3.15156300
C	-3.27900000	3.49371500	-3.62215400
H	-3.58906200	3.18974200	-1.49943700
C	-2.45891800	3.21560700	-4.70995200
H	-0.69101300	2.20729900	-5.39561400
H	-4.16081000	4.11291200	-3.74937300
H	-2.70177000	3.61911400	-5.68750400

2fQ (-3056.93835579 a.u.)

F	-0.58986800	-1.27363200	1.41629600
Ta	-1.29882400	-2.54531000	-0.04374400
Ta	0.19033500	0.46305200	2.30514000
Ta	-1.34484400	2.58293800	-0.56229300
F	-0.62871100	0.87697700	-1.45092800
Ta	0.22412800	-0.37702500	-2.89029700
F	-0.05465700	-3.72444700	0.67174600
F	-1.86199800	-3.63968300	-1.40736700
F	-2.26695800	-1.02661500	-0.51537900
F	-1.49030800	-1.08437800	-3.14368800
F	1.81148100	0.31736400	-2.17598900
F	-0.05908200	1.03168100	-4.04967300
F	0.42250000	2.97143100	-0.07457500
F	-1.95497900	4.11794600	0.24816400
F	-3.04586100	1.91022600	-0.88336800
F	1.09731500	0.47192400	0.67059500
F	1.49246100	-0.57532500	3.11206100
F	-1.08978100	0.05433600	3.60025300
O	0.67951200	2.08340300	2.97496400
O	1.08999300	-1.48904500	-4.04802000
F	-2.60807600	-3.08660600	1.14094000
F	-1.16822300	3.34432100	-2.22983800
O	-1.41179600	1.47010000	1.23024500
O	0.25935900	-1.83197100	-1.26712700
C	0.52803800	3.31516900	3.53832400

C	0.84198600	4.44013300	2.79217700
C	0.01687500	3.40042700	4.82537500
C	0.62105400	5.68767800	3.35702000
H	1.23286700	4.31906600	1.78758700
C	-0.19476800	4.65525900	5.37269000
H	-0.22323900	2.49091800	5.36762500
C	0.10303800	5.79802500	4.64055200
H	0.85412800	6.57982400	2.78526900
H	-0.59789100	4.73992100	6.37664600
H	-0.06768500	6.77816600	5.07343600
C	2.09218400	-2.17720500	-4.66052900
C	1.76344700	-3.17949100	-5.55970500
C	3.40796800	-1.87467700	-4.34430300
C	2.78729400	-3.89926500	-6.15558500
H	0.71890800	-3.37895500	-5.77489600
C	4.41826100	-2.60607000	-4.94678400
H	3.61575600	-1.08737800	-3.62610500
C	4.11226400	-3.61683600	-5.84924300
H	2.54737800	-4.68554800	-6.86392100
H	5.45322000	-2.38554600	-4.70614600
H	4.90950200	-4.18432700	-6.31798000
C	-2.63449200	1.61991300	1.93695900
C	-3.60662800	0.64281600	1.83325800
C	-2.80392400	2.73991200	2.73243400
C	-4.77346800	0.78935000	2.56662600
H	-3.45882500	-0.20244300	1.17206400
C	-3.97656600	2.87065000	3.46218400
H	-2.03930700	3.51009300	2.76574700
C	-4.95904100	1.89548700	3.38469500
H	-5.54428900	0.02938000	2.49327200
H	-4.11809900	3.74521800	4.08902100
H	-5.87535400	2.00023500	3.95644200
C	1.45642300	-2.58715100	-1.28580800
C	1.47630900	-3.77162600	-2.00230400
C	2.55432400	-2.13737200	-0.57777300
C	2.64047400	-4.52379600	-2.01577200
H	0.58706000	-4.09298700	-2.53914600
C	3.71091700	-2.90497100	-0.59734600
H	2.49641200	-1.20049800	-0.03644200
C	3.75749400	-4.09261300	-1.31368300
H	2.67014000	-5.45234300	-2.57682900
H	4.58016400	-2.56868500	-0.04154100
H	4.66541700	-4.68683100	-1.32226700

Ta₄F₁₉(OMe) (Is1: -2244.65724731 a.u.)

F	-0.68778500	-2.25002400	0.27148300
Ta	-2.49464500	-1.36036700	0.56990800
Ta	1.28052600	-2.23576700	-0.51638900
F	-1.54472800	0.28731200	-0.30771200
F	1.33485000	-0.41740200	0.57732400
Ta	2.32128800	1.35894800	0.71157900
F	0.46698100	2.11953700	0.25318600
Ta	-1.40307000	2.31168300	-0.65198900
F	-2.80787700	-1.86815300	-1.18686000
F	-3.98608400	-0.30510300	0.67164600

F	-3.19667200	-2.85426200	1.34250300
F	-1.70346000	-0.67082600	2.09655400
F	-1.99367200	2.37296100	1.10498200
F	-3.05354500	2.29409000	-1.42426400
F	-0.45052200	1.79635000	-2.14900400
F	-1.09155700	4.10277500	-0.81771200
F	2.47069700	1.15860000	-1.13832000
F	3.86339700	0.41842700	1.03161700
F	1.73407000	1.38344600	2.46380100
F	3.03955600	3.04103500	0.73562200
F	0.41740900	-1.13098500	-1.74775500
F	0.94624600	-3.82158500	-1.37821200
F	1.64249400	-2.97052300	1.15706500
O	2.97019400	-1.94286500	-1.04560400
C	4.25327000	-1.59153800	-1.50596200
H	4.17309200	-0.69867500	-2.12943300
H	4.65576500	-2.42438600	-2.08627400
H	4.89259000	-1.39407300	-0.64409200

Ta₄F₁₉(OMe) (Is2: -2244.65456766 a.u.)

F	-0.21968900	1.56639200	1.37716300
Ta	-0.51403400	0.19679400	2.88715500
Ta	0.07400100	3.09295800	-0.09715300
F	0.13971000	-1.19477600	1.44407100
F	-0.22471100	1.45874300	-1.45103700
Ta	-0.54682300	-0.00041400	-2.86953200
F	0.11065600	-1.31074400	-1.35233500
Ta	0.91020900	-2.58025300	0.09233200
F	1.36371700	0.43034500	3.14218200
F	-0.65702400	-1.21745200	4.11517600
F	-1.05990800	1.54700700	4.06434400
F	-2.19763600	-0.09861300	2.06726000
F	-0.83861300	-3.31213700	0.14999200
F	1.59351300	-3.57433400	1.52789700
F	2.35961200	-1.33895600	0.02294900
F	1.55314600	-3.70554000	-1.26251100
F	1.33034000	0.19741800	-3.15551800
F	-1.09345500	1.28591500	-4.11557300
F	-2.22273400	-0.23541000	-2.01537200
F	-0.71780500	-1.48261800	-4.01118300
F	0.17522400	4.38001500	1.27695600
F	-1.84388400	3.02802200	-0.09375900
F	0.17373300	4.27793000	-1.56095300
O	1.84987400	2.57452800	-0.08028500
C	3.15468600	1.97092100	-0.05898500
H	3.25355300	1.30826200	-0.92227800
H	3.26598500	1.39949000	0.86592700
H	3.89759900	2.77191800	-0.10491400

Ta₄F₁₉(OMe) (Is3: -2244.63468331 a.u.)

Ta	-1.96631100	-1.60845300	1.34433800
Ta	-2.29611200	2.04097300	0.26492900
F	-0.33590400	-2.03061000	0.03923000
F	-0.22037200	1.88773300	0.54656000
Ta	1.87033000	1.91378900	0.48615300

F	1.64432100	-0.08098600	-0.13401800
Ta	1.48874800	-2.00477500	-0.94440000
F	-0.66397600	-0.42715300	2.06392600
F	-1.38022100	-3.08219600	2.36711400
F	-3.42536800	-1.17133700	2.43474500
F	-2.92084900	-2.74367900	0.13964400
F	0.45540400	-1.11257400	-2.28119800
F	1.19434100	-3.72897400	-1.61780400
F	2.18667800	-2.55581100	0.73172000
F	3.14838400	-1.73552200	-1.77575100
F	1.78518200	1.18694900	2.23365500
F	1.85918700	3.71131100	1.01613000
F	1.58264900	2.25561500	-1.36403900
F	3.72956100	1.73417600	0.31963200
F	-4.13797800	2.14726900	-0.11248600
F	-1.77802400	2.16359800	-1.56824600
F	-2.08539700	3.88208800	0.62250100
F	-2.47929600	1.54739900	2.09237000
O	-2.36475300	-0.07032000	-0.06891400
C	-2.78794800	-0.41894900	-1.48379000
H	-3.64327500	0.20951200	-1.73850700
H	-3.07378700	-1.46775900	-1.50062600
H	-1.93997800	-0.22146000	-2.13837800

3eA (-1939.11254036 a.u.)

F	-0.30757500	-3.18165100	0.57925800
F	0.53019500	1.02077400	-2.19446400
F	-0.62520600	-1.08817200	2.24616600
F	0.30161700	3.18276800	-0.60023200
F	1.12390200	1.71331300	1.50055500
F	-1.05268900	-1.63488000	-1.49677400
O	-0.99743300	0.67580300	0.09667400
O	1.00283500	-0.65571600	0.00364600
O	-2.78311100	-1.50071300	0.54428300
O	2.76791200	1.48808400	-0.61788600
C	4.06141300	1.25315700	-0.28522100
C	4.91898200	0.72744800	-1.24179400
C	4.49161300	1.53676900	1.00603000
C	6.23539800	0.47658700	-0.89105800
H	4.53501800	0.51102500	-2.23319100
C	5.81128400	1.28169400	1.33804400
H	3.78366000	1.93887300	1.72387600
C	6.68279800	0.75120800	0.39480100
H	6.91570100	0.06006200	-1.62691500
H	6.16169600	1.49745300	2.34228400
H	7.71544300	0.55240600	0.66278100
C	-2.15252200	1.43505400	0.16328900
C	-2.92211100	1.58149200	-0.97903800
C	-2.51613100	2.00111000	1.37387800
C	-4.09846500	2.31196700	-0.89820800
H	-2.58997500	1.11577900	-1.90361900
C	-3.69258600	2.73430700	1.43579800
H	-1.87689700	1.85536600	2.23986300
C	-4.48421900	2.88703800	0.30507000
H	-4.71894700	2.42697100	-1.78133900

H	-3.99112600	3.18919000	2.37518800
H	-5.40466500	3.45947900	0.36089900
C	2.15561600	-1.42069500	-0.02845100
C	2.88132100	-1.58118700	1.13980900
C	2.55208700	-1.99108400	-1.22671300
C	4.04286400	-2.33881200	1.10149300
H	2.52420800	-1.11059900	2.05228300
C	3.71535200	-2.74676400	-1.24756500
H	1.94173800	-1.83720400	-2.11222800
C	4.45906600	-2.92226500	-0.08759800
H	4.62566000	-2.47169000	2.00752200
H	4.03902500	-3.20628500	-2.17630000
H	5.36695500	-3.51639500	-0.11049400
C	-4.05755900	-1.26189300	0.14672100
C	-4.94862400	-0.69051400	1.04451200
C	-4.43311500	-1.58266400	-1.15283800
C	-6.24329600	-0.43145100	0.62607100
H	-4.60831300	-0.44862600	2.04593600
C	-5.73192700	-1.31811000	-1.55310200
H	-3.70046300	-2.02098900	-1.82292800
C	-6.63674300	-0.74339300	-0.66893200
H	-6.94882400	0.01955300	1.31652900
H	-6.04029400	-1.56310100	-2.56444200
H	-7.65300100	-0.53935200	-0.99035700
Nb	0.92786300	1.42782700	-0.38233400
Nb	-0.93453100	-1.42233700	0.40136700

3eB (-2908.70455787 a.u.)

F	0.75280400	-1.31105700	0.35983100
F	-1.71989200	-0.22145000	0.19824800
F	0.59640700	1.33020100	-0.09028600
F	-1.54264800	1.60452500	-1.72540400
F	-1.04134600	1.55253200	1.98607000
F	2.21747100	-0.18843000	-1.57732200
F	1.81000800	0.49384600	2.10981600
F	-0.60705300	-1.30707300	-1.89470900
F	-1.28985300	-2.48285900	1.60184100
O	-0.10354900	-3.71406400	-0.66453200
O	-3.26661900	2.09102300	0.40637400
O	3.47356700	1.53741100	0.08408000
O	-0.83303700	3.62153500	0.12915700
O	-2.80862700	-2.56860500	-0.74620200
O	3.38724100	-1.29732500	0.76094400
C	-4.04151900	-2.06948400	-1.01540400
C	-5.15977500	-2.75532500	-0.55874200
C	-4.15784100	-0.88319500	-1.73269800
C	-6.41645800	-2.22788800	-0.80814400
H	-5.02316100	-3.68101200	-0.00978900
C	-5.42344800	-0.37379700	-1.97416600
H	-3.26271300	-0.37665800	-2.08541900
C	-6.55175800	-1.03734100	-1.50974800
H	-7.29758400	-2.75088000	-0.44912600
H	-5.52653700	0.55487300	-2.52673800
H	-7.53816100	-0.62387100	-1.69413200
C	1.09215700	-4.20802200	-1.08092500

C	1.44789500	-5.49746700	-0.70736100
C	1.92583300	-3.42409800	-1.87199600
C	2.66008100	-6.01062100	-1.13834400
H	0.77091800	-6.07125300	-0.08336200
C	3.13406500	-3.95639600	-2.29406900
H	1.62622300	-2.41728900	-2.14857400
C	3.50338400	-5.24532500	-1.93333800
H	2.94826400	-7.01638900	-0.84821600
H	3.78993900	-3.35188900	-2.91306100
H	4.45111000	-5.65403400	-2.27007900
C	3.44217600	-2.51886200	1.35251500
C	2.50796200	-2.87116400	2.32308800
C	4.45365400	-3.39204600	0.97429800
C	2.60341700	-4.11863200	2.91830600
H	1.72239800	-2.17505000	2.59812400
C	4.53196400	-4.63519100	1.57948500
H	5.15433400	-3.08224500	0.20611800
C	3.61241900	-5.00048200	2.55363000
H	1.87921300	-4.40046000	3.67589600
H	5.31626000	-5.32533000	1.28336100
H	3.67983000	-5.97500400	3.02669800
C	3.91388600	2.65232500	-0.54257200
C	5.13033100	3.20523700	-0.16296600
C	3.14159200	3.22116400	-1.54952200
C	5.57912900	4.34540000	-0.81006100
H	5.70201600	2.73031100	0.62728800
C	3.60532200	4.36118200	-2.18358200
H	2.19522200	2.76101300	-1.81928700
C	4.82142200	4.92520600	-1.81947700
H	6.53103700	4.78239000	-0.52479900
H	3.00671500	4.81505900	-2.96736900
H	5.17952000	5.81728100	-2.32338300
C	0.22230500	4.45595000	0.29764300
C	0.33991400	5.56851200	-0.52573400
C	1.15949400	4.18321200	1.28825600
C	1.42640200	6.41167100	-0.36002300
H	-0.41762600	5.74808800	-1.28126700
C	2.24105100	5.03648500	1.43659400
H	1.02123600	3.31413800	1.92513100
C	2.38005800	6.14680100	0.61469200
H	1.53156600	7.28151300	-1.00117100
H	2.98366900	4.82769200	2.20036900
H	3.23677700	6.80306400	0.72964400
C	-4.50549300	1.69025500	0.77558500
C	-4.66656400	0.52192900	1.51311800
C	-5.59475600	2.46918000	0.40567400
C	-5.94697600	0.13240300	1.87009400
H	-3.79472200	-0.06085700	1.79776500
C	-6.86713400	2.06563500	0.77599900
H	-5.42346900	3.37621800	-0.16433000
C	-7.04719400	0.89733600	1.50428700
H	-6.08438100	-0.78117300	2.44022200
H	-7.72386900	2.66979600	0.49422500
H	-8.04591700	0.58376000	1.79098600
Nb	-1.05611100	-2.16630200	-0.25774000

Nb	-1.43950600	1.86002900	0.15554000
Nb	2.27744700	0.12820100	0.30260400

3eC (-2908.70536343 a.u.)

F	-0.14457600	1.48679100	0.28018800
F	-0.84502300	-0.69782700	-1.05146800
F	1.46410600	-0.74682000	0.32578700
F	-0.48581400	-2.23813300	1.14577900
F	1.48946400	-3.70127500	0.10623700
F	2.39899100	1.72954000	-0.20857600
F	1.58549100	2.80550100	2.12089600
F	-2.31606500	0.86141800	-2.98127200
F	0.27477300	1.22206800	-2.36466300
O	-1.45129400	3.15637500	-1.43816200
O	-0.96328500	-3.28517300	-1.39004000
O	3.15741500	0.38731700	2.11965700
O	0.34109600	0.42198100	2.64092700
O	-2.87157800	0.94212100	-0.32736900
O	1.57495900	-1.99540600	-1.97730700
C	-2.32359800	-3.28857600	-1.49352800
C	-3.05830400	-4.18051300	-0.72500200
C	-2.94160300	-2.37300400	-2.33509500
C	-4.44186900	-4.14118100	-0.79711300
H	-2.53589900	-4.87944900	-0.07975600
C	-4.32596800	-2.33325500	-2.37735600
H	-2.34044300	-1.68563900	-2.92019800
C	-5.07820100	-3.21382700	-1.61166300
H	-5.02809900	-4.83183200	-0.19851500
H	-4.81502200	-1.60296000	-3.01463700
H	-6.16207700	-3.17404700	-1.64544700
C	2.81338400	-1.58431000	-2.34940200
C	3.80315300	-2.54274400	-2.53958200
C	3.07307900	-0.22955900	-2.50890700
C	5.07564000	-2.12978500	-2.90135100
H	3.55929100	-3.59064600	-2.39617900
C	4.35466600	0.16430800	-2.86168200
H	2.28249300	0.49228700	-2.33711800
C	5.35551200	-0.77797800	-3.06262700
H	5.85390700	-2.87089300	-3.05741900
H	4.56878300	1.22227500	-2.97651400
H	6.35443300	-0.45983500	-3.34418800
C	4.32362300	-0.30018500	2.03553400
C	5.01623300	-0.58798600	3.20446700
C	4.79545000	-0.70294300	0.79175900
C	6.20750300	-1.28952200	3.12031600
H	4.61190500	-0.25487300	4.15423500
C	5.98570400	-1.40979800	0.72832600
H	4.23413100	-0.45883200	-0.10629600
C	6.69327300	-1.70333800	1.88636500
H	6.75889900	-1.51773100	4.02690200
H	6.35607300	-1.72989700	-0.24096100
H	7.62496300	-2.25668700	1.82852300
C	-0.90183700	0.30058700	3.15494500
C	-1.77717500	1.38223200	3.11333000
C	-1.27409000	-0.90063900	3.74973100

C	-3.03223100	1.25705500	3.68814200
H	-1.45730200	2.30976400	2.64807800
C	-2.52849000	-1.00581400	4.32447400
H	-0.57587500	-1.72959600	3.73306600
C	-3.40939200	0.06912500	4.29830900
H	-3.72092600	2.09569200	3.65666700
H	-2.82504900	-1.93993700	4.79223200
H	-4.39619400	-0.02463400	4.74052500
C	-0.81349300	4.34999000	-1.31621600
C	-1.57144500	5.51315200	-1.35585700
C	0.56657400	4.38378300	-1.14663800
C	-0.93105700	6.73452400	-1.22743300
H	-2.64536000	5.43934200	-1.48951800
C	1.18707000	5.61546800	-1.01254200
H	1.13680800	3.45995400	-1.11574700
C	0.44609700	6.78879800	-1.05379300
H	-1.51268800	7.65027700	-1.26022000
H	2.26222900	5.65351600	-0.87139800
H	0.94175100	7.74838000	-0.94827800
Nb	-1.37916900	1.30296300	-1.40790300
Nb	1.59406100	1.07169600	1.40101000
Nb	0.39728200	-2.32694000	-0.55622000
C	-3.84009100	0.24661700	0.30616300
C	-3.54306400	-0.95735800	0.93315700
C	-5.13299800	0.76077400	0.31112800
C	-4.56268400	-1.65210100	1.56198400
H	-2.51911300	-1.31735200	0.95760000
C	-6.13977600	0.05156500	0.94518700
H	-5.32635200	1.70555000	-0.18628500
C	-5.85988200	-1.15790200	1.56980600
H	-4.33054300	-2.58908200	2.06010700
H	-7.15087200	0.44713800	0.95032400
H	-6.65186900	-1.70976700	2.06625600

3eD (-3878.27687177 a.u.)

F	-1.23370300	0.98337900	-0.33384000
F	-1.46378100	-1.73352800	0.17701500
F	1.42045900	1.76797100	-0.23988400
F	1.16815000	-1.01173700	-0.20875700
F	-4.16875900	-1.64743400	-0.24483700
F	-2.42722300	-0.68579500	-2.04389900
F	0.45286600	-2.00928800	2.09960600
F	1.97087900	-3.63668800	0.62754600
F	4.13361100	1.56241800	-0.66113000
F	2.33734100	0.35938500	-2.24422900
F	-0.15923600	1.67581300	1.89588600
F	-2.01162000	3.37191600	0.90961600
O	0.73503900	4.19768800	0.88417300
O	-4.09570900	1.10863200	-0.66939700
O	-0.82959500	-4.23677600	0.90556500
O	3.98650800	-1.22921500	-0.65747600
O	2.89476500	0.33575800	1.46047600
O	0.33031400	-3.10992300	-1.46329100
O	-2.86899500	-0.05560300	1.62493000
O	-0.56906100	3.19334900	-1.45903700

C	0.99945400	-2.79419500	-2.59925500
C	2.27993400	-3.30747200	-2.77085400
C	0.40946800	-1.97340200	-3.55116700
C	2.98575500	-2.99325700	-3.92013300
H	2.70693400	-3.92992000	-1.98966600
C	1.13010800	-1.67734900	-4.69761800
H	-0.58383100	-1.57168700	-3.36814300
C	2.41035500	-2.18089000	-4.88780700
H	3.99121900	-3.38377700	-4.05128000
H	0.68315500	-1.04633900	-5.45934200
H	2.96121200	-1.93554600	-5.79018900
C	-1.94495800	-4.82539200	1.39194900
C	-1.86834300	-5.55620800	2.57086100
C	-3.14894800	-4.65793200	0.71798900
C	-3.02526700	-6.11909000	3.08569200
H	-0.90889400	-5.66034500	3.06666600
C	-4.29749600	-5.21716800	1.25451100
H	-3.17609800	-4.06635200	-0.19137700
C	-4.24064100	-5.94669600	2.43543300
H	-2.97727500	-6.69173500	4.00671100
H	-5.24513100	-5.07499500	0.74527200
H	-5.14450000	-6.38169300	2.84911800
C	-5.04845100	1.75614200	-1.37119000
C	-5.72861200	1.08924400	-2.38401900
C	-5.32622100	3.08163100	-1.05994300
C	-6.70221700	1.77110000	-3.09552000
H	-5.48590900	0.05196100	-2.59616700
C	-6.29414900	3.75164600	-1.79041300
H	-4.76571000	3.55657900	-0.26033000
C	-6.98318700	3.10051800	-2.80675700
H	-7.24352400	1.25976200	-3.88528300
H	-6.51603600	4.78902600	-1.56117100
H	-7.74388000	3.62924700	-3.37183700
C	-2.51689800	-0.53630100	2.83971300
C	-2.70621500	-1.88650700	3.12051200
C	-2.00074900	0.32855200	3.79677200
C	-2.34839900	-2.37585500	4.36560600
H	-3.13241400	-2.53930400	2.36358100
C	-1.65370200	-0.17700300	5.03875100
H	-1.85967900	1.37246400	3.54275000
C	-1.81832100	-1.52572900	5.32695300
H	-2.49101200	-3.43121900	4.57984500
H	-1.25390800	0.49586100	5.79164200
H	-1.54104100	-1.91161600	6.30281300
C	1.83229600	4.95388900	1.11470200
C	1.80034400	5.90428000	2.12636800
C	2.97095900	4.75046500	0.34371200
C	2.93505100	6.66259400	2.36776800
H	0.89218200	6.02943900	2.70615500
C	4.09976200	5.50924100	0.60726200
H	2.96573600	3.98756400	-0.42853300
C	4.08622400	6.46510400	1.61552600
H	2.91995500	7.41215100	3.15274400
H	4.99652600	5.34926700	0.01741800
H	4.97232200	7.05932600	1.81306500

C	4.94122400	-2.04306900	-1.15235400
C	5.75687900	-1.57781600	-2.17791400
C	5.07653300	-3.32693000	-0.63877700
C	6.73208000	-2.41770200	-2.68970100
H	5.60779500	-0.56964000	-2.55410500
C	6.04978500	-4.15669700	-1.17238700
H	4.40055600	-3.65263400	0.14553400
C	6.87935300	-3.70669700	-2.19260300
H	7.37931100	-2.06402400	-3.48619200
H	6.16279200	-5.16424800	-0.78482500
H	7.64201900	-4.36202000	-2.60063800
C	-1.07545800	2.72017000	-2.62495300
C	-2.39281700	3.02282300	-2.94153200
C	-0.28836200	1.93606600	-3.45692200
C	-2.93476400	2.53589000	-4.12010300
H	-2.97279800	3.63268000	-2.25508700
C	-0.84466000	1.46712800	-4.63673000
H	0.72501600	1.68397800	-3.15758100
C	-2.15980500	1.76122600	-4.97264800
H	-3.96712500	2.76675900	-4.36742400
H	-0.23795900	0.85944500	-5.30050800
H	-2.58159100	1.38247200	-5.89812800
C	2.69405100	0.99377800	2.62471500
C	3.24843700	2.26069600	2.76779200
C	1.94589600	0.40875000	3.63791500
C	3.03559400	2.96358300	3.94233900
H	3.83495900	2.67558100	1.95308200
C	1.75450500	1.12195300	4.80976000
H	1.49747900	-0.56667000	3.47617800
C	2.29094100	2.39441200	4.96733900
H	3.45646700	3.95947500	4.05089500
H	1.17130700	0.67533000	5.60933300
H	2.12783900	2.94247200	5.89018400
Nb	2.84421300	0.20430100	-0.40798900
Nb	0.27274100	-2.83884900	0.39350800
Nb	-2.90195500	-0.24411700	-0.24586000
Nb	-0.31454900	2.76756300	0.35150200

3bA (-1175.66073602 a.u.)

Ta	-1.75102900	-0.04294100	0.02352400
F	0.06403300	-1.19380600	0.17971900
Ta	1.74185100	0.04572600	0.01238100
F	-0.07465100	1.19547100	-0.15435500
F	1.48930100	-0.25601800	-1.83480500
F	1.47888600	0.26645000	1.86810100
F	-1.51010000	-0.25889600	-1.83823200
F	-1.52357800	0.20577100	1.87857300
O	3.05229400	-1.20649200	0.18405500
O	-3.06788600	1.21084300	-0.09937600
C	4.01427700	-2.21065800	0.24551200
H	3.98735900	-2.80801500	-0.67094200
H	3.81911900	-2.85901000	1.10461900
H	5.00748500	-1.76416000	0.35311900
C	-4.01724900	2.21031200	0.10281700
H	-3.91614700	2.62276300	1.11169700

H	-5.02179400	1.79333500	-0.01616700
H	-3.87381100	3.00918800	-0.63032000
O	2.66638700	1.60747400	-0.20786900
O	-2.66259300	-1.63129200	0.14355300
C	2.73323900	2.98754000	-0.41509500
H	1.72419200	3.40809300	-0.47531900
H	3.26987700	3.45686600	0.41451700
H	3.26452600	3.19257100	-1.34908200
C	-2.58418100	-2.95706700	-0.30675800
H	-1.76458800	-3.47291900	0.20328700
H	-3.52572700	-3.46874900	-0.09237900
H	-2.39758100	-2.96907200	-1.38688400

3bB (-1175.66661986 a.u.)

Ta	1.72173600	-0.11478800	-0.24434400
F	-0.20241300	-0.23942600	-1.16787800
Ta	-1.71826400	0.11487100	0.24484000
F	0.20383600	0.24098500	1.16769800
F	-2.53528900	0.34595900	1.89632400
F	2.54170900	-0.34926800	-1.89396300
F	-1.46535100	-1.75312600	0.58228800
F	1.46751200	1.75158600	-0.58688700
O	1.60718800	-1.89397400	0.19027500
O	-1.61066800	1.89372000	-0.18981500
C	1.23577800	-3.17926400	0.59238600
H	1.40914100	-3.88110000	-0.22906400
H	0.17654000	-3.18381300	0.86223800
H	1.84157900	-3.48046100	1.45265300
C	-1.26906800	3.18237000	-0.60294800
H	-2.00150800	3.53573400	-1.33539000
H	-0.27176500	3.16845000	-1.04789400
H	-1.27181700	3.85564700	0.25958100
O	3.13717000	0.30820600	0.84512400
O	-3.13634200	-0.30863000	-0.84145900
C	-3.89730200	-1.38019600	-1.33176200
H	-3.86248700	-1.38021300	-2.42438100
H	-3.50441500	-2.32926600	-0.95099900
H	-4.93533900	-1.25971400	-1.00938400
C	3.89690200	1.37976000	1.33754700
H	3.50579700	2.32881100	0.95490200
H	3.85816400	1.38033000	2.43003100
H	4.93600800	1.25852700	1.01895700

3bC (-1175.65682819 a.u.)

Ta	1.73285000	-0.01805200	0.17110600
F	0.06478600	-0.00185300	-1.21822900
Ta	-1.73294100	0.01804100	-0.17120800
F	-0.06480600	0.00203700	1.21829300
F	-3.03326900	0.02309100	1.17475200
F	3.03342000	-0.02314800	-1.17462100
F	-2.72273300	0.03036100	-1.72682600
F	2.72253800	-0.03067500	1.72678800
O	1.55920600	-1.85396300	-0.08846500
O	-1.55936100	1.85395000	0.08832500
C	1.33938000	-2.82795700	-1.06796400

H	1.92419700	-2.59103200	-1.96508500
H	0.27489800	-2.86092700	-1.32844200
H	1.65021000	-3.80516200	-0.68699600
C	-1.33948400	2.82772700	1.06809200
H	-1.65127200	3.80486100	0.68775300
H	-0.27484800	2.86121300	1.32782600
H	-1.92347500	2.59002600	1.96554200
O	1.59507600	1.82451600	-0.08076000
O	-1.59486000	-1.82446600	0.08088900
C	1.47328800	2.81421900	-1.06089000
H	0.45905900	2.81394200	-1.47591300
H	1.67911200	3.79347100	-0.61810500
H	2.19238400	2.62867200	-1.86768800
C	-1.47249500	-2.81376000	1.06138500
H	-1.67966000	-3.79308300	0.61940100
H	-0.45769400	-2.81399000	1.47499300
H	-2.19032000	-2.62723300	1.86908100

3bD (-1175.67213234 a.u.)

Ta	1.66364200	0.30487800	-0.16625200
Ta	-1.66365900	-0.30488900	0.16614200
F	-2.39291400	-2.01144300	0.38420600
F	1.46276800	0.10947200	-2.02854900
F	-1.46266200	-0.10986200	2.02846600
F	2.39303200	2.01135100	-0.38459500
F	1.68756600	0.48679800	1.72341400
F	-1.68751600	-0.48651300	-1.72350400
O	-0.24225100	1.19959600	0.03746400
C	-0.41607900	2.45331200	0.70782500
H	0.37926000	3.13330000	0.39751400
H	-0.37087000	2.29352600	1.78916000
H	-1.38778500	2.87196000	0.43508300
O	0.24228500	-1.19961300	-0.03739100
C	0.41623600	-2.45340100	-0.70757900
H	-0.37897900	-3.13345700	-0.39711100
H	1.38803600	-2.87185500	-0.43487600
H	0.37093500	-2.29377600	-1.78894000
O	-3.11189400	0.81514600	0.02733300
O	3.11184000	-0.81512900	-0.02702400
C	-3.97263300	1.50916300	-0.83491500
H	-5.00518900	1.21915100	-0.62441200
H	-3.86721400	2.58614200	-0.67237600
H	-3.72567400	1.26739400	-1.87438400
C	3.97237700	-1.50881600	0.83573800
H	3.86621700	-2.58588800	0.67431000
H	5.00504000	-1.21964300	0.62464500
H	3.72579100	-1.26584700	1.87500900

3bE (-1175.67098923 a.u.)

Ta	1.67899500	-0.20311700	-0.05639600
Ta	-1.68625100	0.19826500	0.07058100
F	-2.82830000	0.76768500	-1.29371000
F	2.75369400	-0.20105800	-1.57898800
F	-2.74395300	0.15695600	1.60237200
F	2.79713100	-0.74196900	1.33841300

F	1.24430700	-2.03695000	-0.35880400
F	-1.23835800	2.02585800	0.38312400
O	0.00504600	-0.29470900	1.20680500
C	-0.07662100	-1.24685700	2.27356400
H	0.81815100	-1.16311000	2.89335100
H	-0.13764100	-2.25920800	1.86080800
H	-0.96479400	-1.03211000	2.87127900
O	-0.01077800	0.28491600	-1.19840100
C	0.08056700	1.24080300	-2.26025800
H	-0.76519800	1.10467600	-2.93694600
H	1.01460500	1.08018500	-2.80276100
H	0.05690400	2.25542300	-1.84944800
O	-1.88664000	-1.58136300	-0.35359700
O	1.89117200	1.58801800	0.30817200
C	-1.70302100	-2.81488100	-0.98311700
H	-2.66892600	-3.19637000	-1.32665100
H	-1.02749600	-2.69507700	-1.83576300
H	-1.25530700	-3.52720000	-0.28424400
C	1.76734000	2.88584400	0.80703200
H	1.13984000	2.88002900	1.70312300
H	2.75839200	3.27658900	1.05591200
H	1.30047400	3.53131800	0.05701000

3bF (-1763.51228459 a.u.)

F	-1.00358300	1.19636200	0.28356600
Ta	-2.32042000	-0.42155500	0.03934900
Ta	0.79353200	2.22245600	-0.00853000
F	1.55913500	0.27833500	0.11862000
Ta	1.54499900	-1.79660100	0.00851400
F	-0.51060000	-1.43260700	-0.13714700
F	1.52051100	-1.43518100	-1.84191200
F	1.21498400	-1.61749200	1.85625700
F	-2.02506300	-0.08843500	-1.79160800
F	-1.99570100	-0.69480800	1.87607900
F	0.45417100	1.72866500	-1.79384500
F	0.85231100	2.13191300	1.87544600
O	0.01674300	3.87108200	-0.10809700
O	3.36100600	-1.92232600	0.16222900
O	-3.29596100	-1.94560400	-0.21508900
C	4.72175400	-1.92799900	0.44691300
H	5.09317400	-2.95732600	0.46193200
H	4.90244800	-1.47014900	1.42501100
H	5.26596900	-1.36765600	-0.32054100
C	-0.55204800	5.12872500	-0.27081000
H	0.23466300	5.87798100	-0.40457300
H	-1.14184800	5.38851500	0.61397800
H	-1.20156300	5.13427800	-1.15193300
C	-4.11873200	-3.02533500	-0.51218500
H	-3.97485800	-3.81859900	0.22861300
H	-3.88176300	-3.41477800	-1.50768600
H	-5.16739300	-2.71142800	-0.49503200
O	1.07770800	-3.56999700	-0.11973300
O	2.55766300	2.68440300	-0.25140900
O	-3.67305000	0.79870100	0.25354200
C	0.03177300	-4.48502300	-0.26590300

H	-0.00523400	-5.14405700	0.60658100
H	-0.92302700	-3.95245000	-0.35617100
H	0.19396100	-5.08848600	-1.16382900
C	-4.17252600	2.07890400	0.48494800
H	-3.34814100	2.78376200	0.64195100
H	-4.76482300	2.40577900	-0.37525300
H	-4.80837700	2.07321400	1.37536200
C	3.86162500	2.19814100	-0.38037600
H	4.51106500	2.69408700	0.34713200
H	3.88140700	1.11507600	-0.20406400
H	4.23279000	2.40304200	-1.38902900

3bG (-1763.52641755 a.u.)

F	0.78676700	1.34863600	0.21771700
Ta	2.38768200	-0.02835400	0.04774800
Ta	-1.12863300	2.05184300	-0.18172200
F	-1.59093400	0.01429800	0.11366900
Ta	-1.18794200	-2.02435800	-0.01706400
F	0.77767000	-1.31009100	-0.23249700
F	-0.74384300	-1.71047700	1.82010200
F	-0.47424100	-3.74603000	0.04938000
F	2.07807200	0.31396600	-1.79376200
F	3.58980500	1.39578000	0.14249500
F	-2.91368000	2.37658600	-0.61915300
F	-0.80556500	1.34457900	-1.90762000
O	-0.47412100	3.72810900	-0.43897000
O	-2.94143500	-2.43989300	0.25055700
O	3.57096900	-1.39278200	-0.17636500
C	-4.31165200	-2.60931500	0.42677700
H	-4.50652500	-3.59546500	0.85850100
H	-4.82576300	-2.52959800	-0.53593600
H	-4.69714600	-1.84077800	1.10391100
C	0.21329400	4.93349500	-0.57247700
H	-0.34639100	5.59958900	-1.23510800
H	1.20320200	4.74946500	-0.99970200
H	0.32410400	5.40854900	0.40691000
C	4.31237900	-2.54206200	-0.44051800
H	4.00830700	-2.97079500	-1.39996300
H	4.15143300	-3.27950600	0.35136700
H	5.37512000	-2.28685200	-0.48360300
O	2.10520900	-0.16104800	1.87035900
O	-1.43183500	2.09268700	1.65281900
O	-1.18386400	-1.83849500	-1.84539500
C	1.38970900	0.14903300	3.02820200
H	0.83461400	1.08465100	2.88265900
H	0.68215000	-0.65557900	3.24939200
H	2.08669600	0.27290600	3.86302900
C	-1.89753000	1.41918900	2.78412500
H	-1.64346700	0.35383600	2.73095200
H	-1.44948200	1.85415200	3.68393700
H	-2.98615900	1.52465600	2.85279700
C	-0.61799700	-1.36160600	-3.03844000
H	-1.32247700	-0.68671900	-3.52966800
H	0.30353100	-0.81195300	-2.82405600
H	-0.40758400	-2.21335900	-3.69272300

3bH (-1763.51187371 a.u.)

F	0.80588800	1.42970800	-0.11580200
Ta	2.39837100	0.12090300	0.00750000
Ta	-1.23906900	2.06022400	-0.06031700
F	-1.59513300	0.00556600	-0.03644300
Ta	-1.10729000	-2.04757500	0.04386000
F	0.80479300	-1.30671200	0.07641200
F	-0.36248200	-3.74001100	0.12674600
F	3.52339600	1.58437000	-0.05626000
F	-3.06804000	2.32174000	-0.02830000
F	-2.90914000	-2.54278900	-0.00405500
F	-0.74302800	3.84967300	-0.09322400
F	3.69190500	-1.22298800	0.13441500
O	2.14708100	-0.00710000	1.84963500
O	-0.94112000	1.90572200	1.76706600
O	-1.30283900	-1.70312400	1.87063100
C	-0.16599100	1.86222700	2.92630200
H	-0.29283300	0.89303000	3.42442400
H	0.89458600	1.99327300	2.68934200
H	-0.48842100	2.65473200	3.60888500
C	1.92911500	-0.92216000	2.88501600
H	2.20105500	-0.46234300	3.84038600
H	0.87456000	-1.22354700	2.91174200
H	2.54917900	-1.81336200	2.72937900
C	-2.19635100	-1.11534500	2.77341200
H	-1.81608200	-1.23200300	3.79384500
H	-2.31469400	-0.04845600	2.54859000
H	-3.17392400	-1.60637300	2.69927100
O	2.24696700	-0.26445800	-1.80867500
O	-1.17561100	-1.82114300	-1.81360100
O	-1.01535200	1.84705000	-1.89355700
C	-2.03066500	-1.33909000	-2.81180700
H	-2.24404100	-0.27577300	-2.64845800
H	-1.55896900	-1.46591800	-3.79212700
H	-2.97310900	-1.89881200	-2.79351900
C	2.14539200	-1.31432800	-2.72861900
H	1.13817000	-1.74904000	-2.70312800
H	2.35173700	-0.93683900	-3.73491500
H	2.87746900	-2.09351800	-2.48426400
C	-0.17672900	1.52163700	-2.96151600
H	0.74931500	2.10462800	-2.91305800
H	0.08372300	0.45745900	-2.91780300
H	-0.68969700	1.73329300	-3.90489500

3bI (-1763.49054510 a.u.)

Ta	-1.88665500	-1.22588600	0.01391900
Ta	-0.17397900	2.32152200	-0.02191900
Ta	2.04657800	-0.95580900	-0.15575100
F	1.35247600	-0.69108500	-1.85595400
F	2.41017100	-2.76414600	-0.50530000
F	2.49466200	-1.20525200	1.68921900
F	-1.36391200	-0.64472700	-1.67319800
F	-2.22814200	-1.49515700	1.86653600
F	-3.64757400	-0.62780300	-0.25897000

F	-0.07325800	1.54967200	-1.71181400
F	1.09944900	3.63306500	-0.40767600
F	-0.11364300	2.81500600	1.81104300
O	0.12409200	-1.69352800	0.47456600
C	0.22214200	-2.90240900	1.27090000
H	0.31226600	-3.76066900	0.60001100
H	-0.66005200	-3.00007800	1.90289100
H	1.09904100	-2.84372000	1.91431600
O	1.46053900	0.98076700	0.42968600
C	2.48289400	1.65412600	1.20964400
H	2.03664300	2.45692700	1.79372600
H	3.22859200	2.06908700	0.52597400
H	2.94118900	0.94282600	1.89730300
O	-1.47524800	0.78053600	0.64664800
C	-2.34881800	1.22129800	1.71842700
H	-2.47191300	2.30364300	1.67250100
H	-1.91128500	0.94670700	2.67874400
H	-3.32630300	0.75152900	1.60807300
O	-1.69272900	3.23666000	-0.49550000
O	3.75061500	-0.38159100	-0.49746200
O	-2.19523700	-2.96459200	-0.43753400
C	-2.84284400	3.06367300	-1.28616700
H	-3.67575500	2.73909000	-0.65321400
H	-3.09961200	4.01099800	-1.76556100
H	-2.64917400	2.29953500	-2.04822100
C	5.09995600	-0.25044800	-0.15955200
H	5.22464700	-0.38515100	0.92159400
H	5.68511300	-1.00875500	-0.68743600
H	5.45713500	0.74185600	-0.45003900
C	-2.42310800	-4.32262200	-0.65052900
H	-2.35267100	-4.86310600	0.29960700
H	-3.42233000	-4.46544500	-1.07160100
H	-1.67910400	-4.71652400	-1.34941500

3bJ (-1763.49530246 a.u.)

Ta	2.17851100	-0.71706400	-0.00014400
Ta	-0.43242800	2.21228200	0.21911900
Ta	-1.63449200	-1.53000900	-0.14001200
F	-1.50298200	-3.39006200	-0.16732300
F	-2.11690500	-1.46457900	-1.99469500
F	2.66803100	-0.48843200	-1.83972600
F	3.80336700	0.04618100	0.51886800
F	-1.98110400	3.08444700	0.78817700
F	-3.47818100	-1.49381000	0.21643800
F	2.84248000	-2.45997800	-0.09544300
F	0.59302100	3.66689900	0.77464600
O	0.35394100	-1.50244700	-0.78827700
C	0.59040400	-2.42276000	-1.90486400
H	0.84494700	-3.39881900	-1.48841900
H	1.41366200	-2.04197100	-2.50584200
H	-0.30865500	-2.48670000	-2.51434000
O	-1.70976600	0.60068200	-0.34238600
C	-2.93050700	1.05045500	-0.98970000
H	-2.84760000	2.09920200	-1.27125800
H	-3.75752300	0.93562200	-0.28597300

H	-3.11252700	0.44461300	-1.87720700
O	1.40074500	1.23825800	-0.27207200
C	2.29008400	2.08769600	-1.04931300
H	2.05207100	3.13398400	-0.86362400
H	2.19393800	1.84719400	-2.10835100
H	3.31743500	1.90540700	-0.73224200
O	-1.35262600	-1.32039000	1.66841500
O	1.56159600	-0.88248500	1.70692600
C	1.30670700	-1.06013700	3.06675400
H	0.66855800	-0.25027800	3.42436200
H	0.81235300	-2.02323300	3.22280800
H	2.25556500	-1.04690700	3.61139400
C	-1.97667700	-0.93742500	2.86601800
H	-1.67726300	-1.61600100	3.67008500
H	-1.68897700	0.08611200	3.11926100
H	-3.06340500	-0.99365300	2.73471700
F	-0.23089800	1.23237900	1.81863700
O	-0.50035600	2.62729200	-1.58246500
C	-0.48164800	2.14797100	-2.89754800
H	-0.31245400	1.06205300	-2.90255200
H	-1.44048100	2.36005100	-3.38126400
H	0.31426900	2.64360800	-3.46123600

3bK (-2351.36607327 a.u.)

F	0.35986100	1.83830400	-0.23991100
Ta	-1.39577100	2.30909500	0.78871700
Ta	2.32066600	1.37449600	-0.79266900
F	-2.08239600	0.59268800	-0.18602100
F	2.01734100	-0.29079100	0.44498200
Ta	1.34759600	-2.23716500	0.81410400
F	-0.29590200	-1.47681000	-0.21363700
Ta	-2.28103300	-1.37122000	-0.83824500
F	-0.71936700	1.04023300	1.99882400
F	-1.88999200	3.12509400	-0.85146800
F	-1.51874700	-0.68327600	-2.41241600
F	-2.62041300	-1.73087400	0.99765200
F	0.50498700	-1.47956200	2.30988800
F	1.97244300	-2.59417900	-0.94865500
F	2.74176900	2.19981100	0.86666700
F	1.47433900	0.25337300	-2.04105800
O	3.99475200	0.72810900	-1.17561500
C	4.69828100	-0.45816800	-1.43561600
H	3.99628300	-1.29783100	-1.50574000
H	5.41623300	-0.64184000	-0.62982000
H	5.24404800	-0.35882900	-2.37786300
O	-0.56209300	3.77523900	1.48905500
C	0.56548700	4.57390800	1.72008200
H	1.46474500	4.04933100	1.37920300
H	0.65321800	4.77832900	2.79068400
H	0.45612600	5.52163300	1.18398700
O	-4.01787700	-0.95795300	-1.26245200
C	-4.97999700	0.04279500	-1.43656400
H	-4.55282300	1.01972100	-1.17567700
H	-5.84333800	-0.16186800	-0.79597200
H	-5.30699000	0.06263600	-2.47991800

O	0.47648300	-3.83898000	1.03955400
C	-0.68041900	-4.41866800	1.59186100
H	-1.43226400	-3.64394600	1.77932700
H	-0.42334100	-4.91632400	2.53127800
H	-1.08512500	-5.15970700	0.89565600
O	-2.12985400	-3.12093000	-1.38527900
O	2.96657000	-2.53858500	1.62460200
O	2.27920400	2.92068300	-1.77565600
O	-3.03977900	2.37041800	1.61388500
C	1.52109700	3.99713300	-2.25619200
H	1.50688300	3.97465200	-3.34917400
H	0.49207800	3.92973200	-1.88311700
H	1.97278800	4.93716100	-1.92524100
C	4.21147800	-2.05195700	2.02890900
H	5.00663100	-2.64658400	1.56807300
H	4.31832100	-1.00223100	1.72759600
H	4.30013800	-2.12100300	3.11690100
C	-1.21172300	-3.97382000	-2.02668400
H	-0.19244100	-3.58650500	-1.90729500
H	-1.27509700	-4.97290800	-1.58586200
H	-1.45413500	-4.03565600	-3.09144700
C	-3.98681500	1.48604300	2.15298700
H	-4.23162800	0.70709300	1.42055700
H	-3.57377700	1.00302000	3.04501800
H	-4.89185200	2.03808700	2.41854800

3bL (-2351.38300124 a.u.)

F	-1.65020500	-0.35033100	-0.12576700
Ta	-1.61359700	-2.42632900	-0.02086600
Ta	-2.44744000	1.59230000	0.01024600
F	0.44784100	-2.09834700	0.26892600
F	-0.45111200	2.11308900	0.18669300
Ta	1.63084500	2.41919700	-0.01194700
F	1.62297600	0.34639400	-0.18565000
Ta	2.43533500	-1.58164500	0.02280200
F	-1.21721500	-4.25465100	-0.03169700
F	-1.03434000	-2.20999200	-1.82834300
F	2.27043000	-1.07978700	1.86041800
F	4.15871400	-0.84465200	-0.04495700
F	1.25915200	4.25095900	0.01512200
F	1.14778600	2.27056000	-1.85463800
F	-2.23313600	1.18539000	1.86585700
F	-4.16072400	0.82907400	-0.00455400
O	-2.88560000	3.34883100	0.21477800
C	-2.69960900	4.73474800	0.20390000
H	-1.62897900	4.95834000	0.14836100
H	-3.11436500	5.16754600	1.11824600
H	-3.20563800	5.16839000	-0.66339100
O	-3.40171500	-2.51323900	-0.33867000
C	-4.79366500	-2.38254200	-0.26207300
H	-5.05276800	-1.32098600	-0.23984500
H	-5.15839700	-2.86712700	0.64844000
H	-5.25067600	-2.85829100	-1.13381600
O	2.83983400	-3.34150200	0.28313100
C	2.52969400	-4.70663100	0.23972900

H	1.44143000	-4.83208100	0.22496400
H	2.94350400	-5.20339000	1.12104300
H	2.95835300	-5.15392800	-0.66191800
O	3.42976800	2.48975700	-0.26062300
C	4.82177600	2.35763400	-0.21452300
H	5.07969700	1.29627500	-0.18460700
H	5.20796700	2.85395700	0.68058600
H	5.26006900	2.82057200	-1.10291300
O	1.59037200	2.14124700	1.80738900
O	2.15661300	-1.60141400	-1.79762300
O	-1.63719500	-2.19874000	1.80705400
O	-2.17711100	1.54767600	-1.81055300
C	-1.06154600	-1.62391700	2.94863200
H	0.00767300	-1.44910000	2.77898300
H	-1.55935400	-0.67399700	3.16493000
H	-1.18566200	-2.30609000	3.79487400
C	0.98104800	1.57893300	2.93723800
H	-0.08002500	1.39563200	2.73197900
H	1.48038700	0.63767500	3.18063700
H	1.07237300	2.27455100	3.77697600
C	-1.53358300	1.00050000	-2.92911100
H	-0.71428800	1.65765400	-3.23239500
H	-1.13545100	0.00943600	-2.68051200
H	-2.25539100	0.90470500	-3.74593100
C	1.63217900	-1.03632700	-2.96724900
H	0.70355200	-1.55051100	-3.22934900
H	1.43239400	0.02969100	-2.80629600
H	2.35912300	-1.15073100	-3.77719500

3bM (-2351.35753421 a.u.)

F	-1.60104100	0.34581400	-0.08030800
Ta	-2.43675900	-1.51057000	-0.34650000
Ta	-1.54741700	2.44637900	0.42508600
F	-0.40125600	-2.07581200	-0.08367800
F	0.38939900	2.37261100	-0.27362700
Ta	2.37208800	1.65238800	-0.47300600
F	1.46768100	-0.12712300	0.25663400
Ta	1.60482000	-2.21364300	0.30743700
F	-2.97012400	-3.28946500	-0.57672000
F	3.42551300	-2.13366300	0.71843000
F	2.98627400	3.29017900	-1.07346500
F	-3.30232700	2.25409100	1.03065300
F	-1.32243100	4.24197600	0.79098500
O	-0.91045700	1.72312900	2.02388600
C	-0.98960000	0.61778800	2.87249500
H	-0.36246900	-0.19974200	2.48966100
H	-2.02624600	0.26530200	2.93302100
H	-0.64568400	0.90103400	3.87390500
F	-4.07793700	-0.68141400	-0.56058900
O	-1.88587200	-1.52066400	-2.13606000
C	-1.23119300	-2.31997800	-3.08066600
H	-1.65004300	-3.33312100	-3.06325200
H	-0.15736800	-2.37420000	-2.85905100
H	-1.37018800	-1.89418600	-4.07945900
F	1.41222200	-4.06105800	0.28894600

O	1.26731400	-2.04650600	2.15078800
C	1.75344000	-1.93642900	3.45049200
H	2.83005400	-1.72396900	3.43777900
H	1.58593900	-2.87252600	3.99538400
H	1.23727100	-1.12786200	3.98490400
F	3.96491800	0.71595800	-0.64007500
O	1.66548400	1.08994200	-2.10130000
C	0.50035000	0.72638400	-2.77675400
H	0.75593300	0.31609800	-3.76018000
H	-0.14690100	1.60130200	-2.90982300
H	-0.04412500	-0.03236700	-2.20483100
O	-2.15609900	2.54478600	-1.32807700
O	-2.46652400	-1.80007900	1.49077500
O	2.05152500	-2.06987100	-1.49640400
O	2.49660300	2.02976300	1.33315700
C	-3.00093900	1.95440400	-2.27427400
H	-2.54144300	1.04680700	-2.68673600
H	-3.95138900	1.68205600	-1.80048100
H	-3.18864500	2.66280300	-3.08578500
C	3.00303600	-1.82419100	-2.49292300
H	2.79650200	-0.86601200	-2.98101000
H	4.00179600	-1.77241300	-2.04392400
H	2.97634600	-2.62964900	-3.23352200
C	-2.11768900	-2.69467400	2.50729000
H	-1.03298500	-2.67746200	2.67149800
H	-2.63126800	-2.41372100	3.43219900
H	-2.42096200	-3.71014800	2.22527800
C	2.11962000	1.94248000	2.67121200
H	1.27473200	2.60836700	2.87464400
H	1.81778300	0.91337200	2.90586500
H	2.96798900	2.22024600	3.30364900

3bN (-2351.34030647 a.u.)

Ta	-1.32658700	2.12670300	-0.51124000
Ta	-2.13318700	-1.20951900	0.42496900
Ta	1.13585800	-2.29120500	-0.39869200
Ta	2.26452800	1.37763000	0.39143000
F	-1.65446400	0.24806600	-1.23776100
F	-1.29381600	2.87518000	-2.23264000
F	-3.15266600	2.60016800	-0.59683200
F	0.74862200	1.50598800	1.56192900
F	2.40953400	3.25643200	0.22583300
F	3.43428000	1.50560600	1.84273700
F	1.17347300	-0.97080800	-1.76165800
F	0.88595800	-3.78623700	-1.49773000
F	2.94735600	-2.71098700	-0.70084600
F	-2.16610600	-1.23693000	2.30444700
F	-0.14313000	-0.91178500	0.69529700
F	-2.75219200	-2.96876300	0.70880700
O	0.67386800	1.60830300	-0.99782600
C	1.03007400	1.67917500	-2.40172300
H	0.21305400	1.28808200	-3.00522400
H	1.90956000	1.07223700	-2.58489500
H	1.21914000	2.72421600	-2.65896000
O	-1.93795400	0.93327300	1.00096900

C	-2.28079800	1.41995900	2.29581600
H	-3.15457400	0.88328000	2.66967600
H	-2.52196500	2.48530300	2.23329900
H	-1.44010200	1.26319500	2.97612400
O	-1.02319600	-2.25521800	-0.91465500
C	-1.62967800	-3.00125800	-1.96292100
H	-2.60902500	-2.56927600	-2.19715000
H	-1.75556700	-4.04420800	-1.66311500
H	-0.99840900	-2.94528000	-2.85149800
O	2.28309100	-0.69281200	0.72638300
C	3.33548400	-1.20453300	1.55314300
H	4.31229800	-0.98628300	1.10713500
H	3.24420700	-2.28641900	1.65516900
H	3.28443500	-0.74121300	2.54100600
O	-0.82261900	3.51462300	0.52373500
O	-3.80152000	-0.76896900	-0.16835000
O	3.50477600	1.01442700	-0.91716400
O	0.91035100	-3.16669800	1.20900600
C	0.50370300	-3.15240600	2.54927200
H	-0.52320300	-3.52458800	2.62566400
H	1.16633300	-3.79372800	3.13756000
H	0.53697800	-2.12762000	2.93671600
C	-4.75856800	0.05923100	-0.77197400
H	-5.70176300	-0.48855800	-0.84074200
H	-4.89284000	0.96619300	-0.17727300
H	-4.42247000	0.34495000	-1.77341600
C	-0.27610000	4.37866800	1.48685600
H	0.75285500	4.61003100	1.20722300
H	-0.87803500	5.28971100	1.52476900
H	-0.28164600	3.87891900	2.45917300
C	4.27605600	0.20449400	-1.75785900
H	4.18715200	0.55283500	-2.79226800
H	5.32535900	0.27094200	-1.45486200
H	3.93646000	-0.83501000	-1.69084600

3bO (-2351.33327730 a.u.)

Ta	0.29314700	-2.51693000	0.18171800
Ta	2.88387300	0.33824800	0.05915100
Ta	-0.29120000	2.51918300	-0.19817800
Ta	-2.88440100	-0.33564700	-0.04807500
F	0.49458700	-3.57484900	-1.39740700
F	-0.91091700	-3.76489000	0.85047500
F	1.79755000	-3.37244400	0.88600500
F	-2.61499500	-1.27765800	1.56654300
F	-4.01469000	-1.66805000	-0.73806700
F	0.91510800	3.76425900	-0.86695900
F	-1.79646200	3.36863800	-0.90692900
F	2.70792200	-0.55433500	1.71256600
F	4.00939400	1.66506800	0.76727800
O	-1.31512000	-1.58583300	-0.86368000
C	-1.68554200	-2.15695400	-2.14403500
H	-0.79366000	-2.39005500	-2.72275400
H	-2.30236600	-1.44819300	-2.69602600
H	-2.24645500	-3.07882800	-1.97118200
O	1.67304700	-1.16621500	-0.80501900

C	2.20880900	-1.59435000	-2.08121800
H	2.61384200	-0.73445600	-2.61647800
H	1.42697600	-2.05539100	-2.68045400
H	2.99739500	-2.33074800	-1.90249100
O	1.30993400	1.59015300	0.85968900
C	1.66552600	2.15393800	2.14709700
H	2.23072500	3.07528200	1.98614900
H	2.27329600	1.44064000	2.70336300
H	0.76680200	2.38594900	2.71558200
O	-1.66695400	1.16993000	0.79973900
C	-2.18499000	1.59657600	2.08339800
H	-2.97024700	2.33933000	1.91669600
H	-1.39303300	2.04901200	2.67599900
H	-2.59067000	0.73794400	2.61997900
O	0.12525100	-1.35350200	1.57694200
C	0.03992800	-0.85781600	2.87929800
H	-0.85791000	-1.26693100	3.35135700
H	0.93621900	-1.15172400	3.43243300
H	-0.02389400	0.23191500	2.85478500
F	2.62957200	1.28244500	-1.55571700
F	-2.73123400	0.55196600	-1.70638900
F	-0.49756100	3.58532900	1.37413900
O	-0.12354700	1.34878400	-1.58809200
C	-0.05180500	0.81530400	-2.87589800
H	-0.97151500	1.05966200	-3.41414000
H	0.81660800	1.23918900	-3.38793100
H	0.05181200	-0.27030300	-2.81714700
O	4.38992500	-0.56027400	-0.46131200
O	-4.38580200	0.56156400	0.48739000
C	5.78701000	-0.65755000	-0.42764400
H	6.07911100	-1.53256100	0.15875000
H	6.17289200	-0.75672100	-1.44567100
H	6.19685500	0.24874100	0.03200700
C	-5.78334900	0.65630600	0.46841200
H	-6.15835800	0.75852000	1.49018300
H	-6.08321100	1.52876400	-0.11787300
H	-6.19661700	-0.25228700	0.01639200

4A (-1206.13520746 a.u.)

Ta	1.74995000	-0.01017500	0.08407900
F	-0.02633900	-1.20419700	-0.09653800
Ta	-1.75423800	0.01664100	-0.08417200
F	0.02309500	1.20899000	0.08847700
F	-1.50503100	-0.18709000	1.81505500
F	1.50713000	0.19367000	-1.81557200
O	1.59355000	0.05548900	1.92842500
O	-1.59072200	-0.06661700	-1.92861800
C	1.16648400	0.45438400	3.19136600
H	1.45504000	-0.29716600	3.93418800
H	0.07848700	0.56226400	3.19758800
H	1.63425800	1.40894200	3.45919500
C	-1.11927200	-0.54336900	-3.14903900
H	-1.75531200	-1.36642000	-3.49510500
H	-0.08828700	-0.89167400	-3.03956100

H	-1.14065900	0.25783700	-3.89481200
O	3.03575300	1.32770800	-0.02943900
O	-3.04290900	-1.31832300	0.03425000
C	-3.68917800	-2.09556700	1.00070700
H	-3.57488500	-3.15671000	0.75694600
H	-3.26370200	-1.90445100	1.99302100
H	-4.75764700	-1.85546700	1.01398400
C	3.67743100	2.10979100	-0.99518800
H	3.25191600	1.91824800	-1.98737900
H	3.55842700	3.16996400	-0.74936100
H	4.74702400	1.87473000	-1.00983600
O	-2.71491700	1.58115400	0.05120500
O	2.71285400	-1.57274200	-0.06561500
C	-2.81102400	2.96307900	0.19305500
H	-3.44529100	3.37475800	-0.59875200
H	-3.25311200	3.21032000	1.16380800
H	-1.81751700	3.42116900	0.12814700
C	2.81263200	-2.95197200	-0.22516400
H	3.25825400	-3.18594300	-1.19771300
H	3.44525200	-3.37323300	0.56302500
H	1.81975300	-3.41297200	-0.16944200

4B (-1206.12924414 a.u.)

Ta	-1.70770500	-0.16704200	-0.33417600
F	-0.25132500	0.05994200	1.19919600
Ta	1.71363600	0.16270700	0.34099800
F	0.25373300	-0.05927300	-1.19341400
F	2.36852200	0.29924500	2.07757900
F	-2.35963700	-0.33753500	-2.06901800
O	-1.42413000	-1.98012700	0.05422600
O	1.42527200	1.97864100	-0.02546300
C	-1.32743100	-2.87246200	1.12080100
H	-2.17904200	-2.73681000	1.80012800
H	-0.39633600	-2.70721100	1.67697400
H	-1.33708700	-3.90118900	0.74456200
C	1.33407700	2.88374500	-1.08102400
H	1.30750900	3.90652100	-0.68972100
H	0.42267500	2.70383500	-1.66465300
H	2.20669800	2.77997700	-1.73908800
O	-1.72650100	1.71114700	-0.22822000
O	1.73088600	-1.71379900	0.19414300
C	-1.60487700	2.80904500	0.62430800
H	-0.58192400	2.88392600	1.00884600
H	-1.85045500	3.72749100	0.07970800
H	-2.28977200	2.71445300	1.47744800
C	1.54620800	-2.76635700	-0.70642800
H	1.91863300	-3.69734700	-0.26528600
H	0.48245100	-2.87902200	-0.94583700
H	2.09071200	-2.57730500	-1.64143800
O	-3.27964300	-0.22809300	0.67085400
O	3.28394900	0.23908500	-0.66577100
C	-4.32155600	0.62016600	1.05842700
H	-4.32330500	0.73381700	2.14785500
H	-4.22196300	1.60895900	0.59296300

H	-5.27800000	0.18273300	0.75525900
C	4.31230800	-0.61325400	-1.07995100
H	4.18609700	-1.61870700	-0.65847200
H	4.32311800	-0.67926600	-2.17312300
H	5.27434300	-0.20994300	-0.74819100

4C (-1206.14480877 a.u.)

Ta	1.71372500	-0.00604800	0.00564700
Ta	-1.71537300	0.00166800	0.00072200
F	1.57239400	0.34129100	-1.86186000
F	-1.67215400	-0.34980600	1.87276600
F	1.65643800	-0.35236600	1.87905200
F	-1.56132500	0.34332200	-1.86767000
O	0.00476800	1.14817100	0.42463400
C	0.01044700	2.13097800	1.45464700
H	0.80367100	2.85788200	1.25823500
H	0.18425200	1.65004700	2.42209900
H	-0.95738300	2.63910400	1.47468300
O	-0.00688500	-1.17926100	-0.35280200
C	-0.01313000	-2.17904700	-1.36719300
H	-0.81578100	-2.89416500	-1.16699200
H	0.94881000	-2.69840500	-1.36865600
H	-0.17154100	-1.70986600	-2.34314900
O	-2.80628300	1.49887000	0.13749300
O	2.83225800	-1.47623000	-0.18269000
C	-3.23008200	2.65311000	-0.52412300
H	-4.31189900	2.76967900	-0.40822700
H	-2.73697400	3.53456900	-0.09730500
H	-2.98375000	2.58862200	-1.59055500
C	3.34693100	-2.60830600	0.45127000
H	2.87731000	-3.51286500	0.04697400
H	4.42587100	-2.67059300	0.27939100
H	3.15336200	-2.55751100	1.52932500
O	-2.87236200	-1.43605000	-0.19039900
O	2.84574700	1.45714000	0.14540300
C	-3.47291500	-2.52172100	0.44929500
H	-3.11221000	-3.46130800	0.01565500
H	-3.23592600	-2.50604700	1.51978600
H	-4.55855900	-2.47409100	0.31905400
C	3.37720900	2.56416700	-0.51847800
H	3.09432400	2.53976500	-1.57755100
H	3.00135500	3.48997700	-0.06817200
H	4.46845900	2.55675100	-0.43573400

4D (-1206.15055931 a.u.)

Ta	-1.68211700	0.09296700	-0.28386500
Ta	1.68209000	-0.09299700	0.28394900
F	2.44088600	-0.23735700	2.00118200
F	-2.44090900	0.23732400	-2.00110400
F	-1.48129300	-1.81155300	-0.56082400
F	1.48137200	1.81155100	0.56082600
O	0.23187500	0.11743500	-1.21102900
C	0.42979900	-0.41326000	-2.51666700
H	-0.26999200	0.06319000	-3.20651700

H	0.24659800	-1.49360900	-2.51370700
H	1.45696800	-0.21831700	-2.83812000
O	-0.23189600	-0.11734800	1.21111300
C	-0.42979500	0.41354100	2.51668000
H	0.27012300	-0.06269600	3.20654800
H	-1.45691000	0.21849700	2.83824500
H	-0.24675700	1.49391700	2.51351500
O	3.11737900	0.31414800	-0.82520200
O	-3.11737300	-0.31424500	0.82527800
C	3.77600600	1.41607300	-1.38227900
H	4.84574600	1.35180700	-1.16168500
H	3.64549200	1.41414400	-2.47041200
H	3.37317800	2.34836000	-0.96976100
C	-3.77594000	-1.41616500	1.38243800
H	-3.64532300	-1.41420900	2.47055800
H	-4.84570000	-1.35191300	1.16194400
H	-3.37314000	-2.34845700	0.96990600
O	-1.67105100	1.91285400	0.03423000
O	1.67095900	-1.91288100	-0.03420900
C	-1.33778200	3.24535500	0.26409100
H	-0.25876100	3.32873600	0.42572200
H	-1.62677900	3.85508400	-0.59834400
H	-1.87026200	3.61410000	1.14811600
C	1.33794000	-3.24526400	-0.26509000
H	1.62737800	-3.85564600	0.59673300
H	0.25888500	-3.32876600	-0.42643100
H	1.87021400	-3.61313000	-1.14960700

4E (-1206.13485687 a.u.)

Ta	-1.60238100	0.03636300	0.17106600
Ta	1.80843200	-0.04342900	-0.06172000
F	2.78444700	-0.29180100	-1.64040100
F	-2.90301400	0.01004600	-1.22487500
F	3.08797600	0.04659300	1.30961400
F	-2.52368400	0.10098800	1.80792300
O	0.15370000	0.19329100	1.26698500
C	0.23910100	1.03899400	2.41568500
H	-0.51498200	0.72847600	3.14182500
H	0.04936300	2.07799700	2.12445800
H	1.23544600	0.95492500	2.85478500
O	-0.00551500	-0.09749400	-1.18404700
C	-0.09890400	-0.92601800	-2.34012200
H	0.61366500	-0.57561000	-3.09053800
H	-1.11342200	-0.87272400	-2.74425200
H	0.14273900	-1.96404700	-2.08012300
O	1.77466500	1.81627900	-0.22855500
O	-1.72688500	-1.84057400	0.07403800
C	1.31192700	3.09825600	-0.48116500
H	2.15567600	3.76698300	-0.68271600
H	0.64596000	3.09739900	-1.35338100
H	0.75228400	3.48743900	0.37864400
C	-2.35540500	-2.93111000	-0.51686800
H	-2.92546100	-3.49307900	0.23133000
H	-3.04393700	-2.59257200	-1.30248800

H	-1.61363500	-3.60437100	-0.96530000
O	1.57301600	-1.87815100	0.19919500
O	-1.68455100	1.90868200	-0.05222800
C	1.08599000	-3.05786400	0.74495400
H	1.86468200	-3.54145700	1.34499600
H	0.21467900	-2.85160500	1.37709300
H	0.78306200	-3.74827400	-0.05238100
C	-2.18477700	2.87845000	-0.91728800
H	-1.71570900	2.78918200	-1.90718800
H	-3.26797700	2.76590300	-1.04194200
H	-1.97870200	3.87828900	-0.51969600

4F (-1809.22849191 a.u.)

F	-1.57840900	0.30140300	0.35731400
Ta	-1.53132500	-1.81113300	0.16931000
Ta	-0.87207500	2.23785200	0.01333000
F	0.98243300	1.20133200	0.17846100
Ta	2.33978400	-0.33796100	-0.09933000
F	0.52878000	-1.43178200	0.02243600
F	1.80162800	-0.10352100	-1.91966700
F	-1.08378900	-1.68232400	2.03694100
F	-0.81486600	1.52991000	-1.76416400
O	-2.55987000	2.96720800	-0.20680000
O	3.78619800	0.81362100	-0.15913400
O	-1.28275200	-3.64952400	0.10769200
C	4.70056000	1.55832200	0.58122900
H	5.72133800	1.28052900	0.29907900
H	4.56439000	1.37606500	1.65492500
H	4.56334900	2.62648600	0.38094900
C	-3.50005200	3.38832600	-1.14844200
H	-3.40333200	4.46661800	-1.31590900
H	-4.51022000	3.18263000	-0.78069500
H	-3.35122500	2.86649100	-2.10187900
C	-1.03850400	-4.70711400	-0.76464900
H	-0.12285200	-5.23212500	-0.46997400
H	-0.92730700	-4.34137000	-1.79532200
H	-1.86988200	-5.41958800	-0.73309400
O	3.11559400	-1.96559800	-0.56736500
O	0.18089100	3.69322900	-0.45473100
O	-3.36214600	-1.71961500	0.40993300
C	2.79627700	-3.01499800	-1.42844300
H	3.51324200	-3.83124900	-1.29911300
H	1.78649200	-3.39254300	-1.21195300
H	2.82415900	-2.67526700	-2.47184100
C	-4.50129100	-0.92901200	0.54285500
H	-4.23513200	0.13429200	0.49922100
H	-5.20852200	-1.15314600	-0.26297400
H	-4.98738000	-1.13184500	1.50291000
C	1.31018300	3.98741900	-1.22524400
H	2.11849600	4.34350400	-0.57708600
H	1.65421900	3.09865800	-1.76980200
H	1.07098200	4.77407400	-1.94810600
O	-0.74775000	2.28542600	1.87105700
C	-0.33019500	1.50812700	2.95511200

H	-0.72260000	0.48740300	2.86579600
H	0.76635500	1.45810500	2.98015700
H	-0.68794000	1.95512000	3.88785500
O	2.37757600	-0.56538200	1.75222900
C	1.96991300	-1.15802500	2.94690000
H	2.06721800	-0.44373000	3.77312400
H	0.92686400	-1.48424100	2.87387500
H	2.60311500	-2.02576100	3.16590000
O	-1.46986600	-1.57906400	-1.66870300
C	-0.81184000	-1.33048800	-2.87921600
H	-0.74668800	-0.25280300	-3.04816300
H	0.20842200	-1.73126800	-2.84081800
H	-1.36689500	-1.80736700	-3.69469400

4G (-1809.19300201 a.u.)

Ta	-1.72861200	-1.49957900	0.00614400
Ta	-0.46598200	2.27106600	0.00729400
Ta	2.15767200	-0.69116900	-0.24390700
F	1.44050800	-0.48085300	-1.94484800
F	2.74213000	-0.86445400	1.60168000
F	-1.19892300	-1.01243600	-1.71936000
F	-1.98452400	-1.84709200	1.87976300
F	-0.30244900	1.50994100	-1.69277500
F	-0.51750700	2.72577300	1.87154000
O	0.37249300	-1.65940800	0.45184800
C	0.65511200	-2.81566500	1.26451900
H	0.78899600	-3.68678400	0.61436700
H	-0.16444900	-2.99072900	1.96203400
H	1.56099300	-2.64351500	1.84532900
O	1.31385800	1.15530200	0.44935700
C	2.22485400	1.93327400	1.24980600
H	1.66656100	2.57246400	1.93484700
H	2.84967100	2.54439600	0.58922000
H	2.85108200	1.26714600	1.84364600
O	-1.56879900	0.54070800	0.66731800
C	-2.47191300	0.84702400	1.74814500
H	-2.81362600	1.88060400	1.66490000
H	-1.96315700	0.71708700	2.70472000
H	-3.33777800	0.18359200	1.71310700
O	-2.14481500	2.94730700	-0.45028300
O	3.73289600	0.24279300	-0.57345000
O	-1.76123500	-3.32793400	-0.29632500
C	-3.24741400	2.53122300	-1.19870300
H	-4.04450200	2.17769200	-0.53123400
H	-3.63547500	3.36905200	-1.78622000
H	-2.96278300	1.71692800	-1.87929900
C	5.04140600	0.41983800	-0.13411300
H	5.16098900	0.00630800	0.87692700
H	5.74059300	-0.08370100	-0.81167800
H	5.29263300	1.48640600	-0.11294400
C	-2.04625200	-4.61007700	0.15909800
H	-2.08811900	-4.62290500	1.25629000
H	-3.01254300	-4.94483900	-0.23446800
H	-1.27319700	-5.30956900	-0.17734900

O	2.88488200	-2.37544400	-0.54703600
O	-3.51771800	-1.16852100	-0.32634900
O	0.51904300	3.80641100	-0.29297500
C	1.03604100	5.01635000	0.15996600
H	0.99385500	5.05829300	1.25614300
H	2.07671400	5.12377600	-0.16374500
H	0.45422000	5.84913300	-0.24868600
C	-4.77138500	-0.76518100	-0.75315600
H	-5.10668300	0.10766900	-0.17692100
H	-4.74442100	-0.49420400	-1.81516800
H	-5.49933200	-1.57218200	-0.61442200
C	3.81810800	-3.30243500	-0.09365800
H	3.39702200	-4.31314700	-0.13647500
H	4.71454700	-3.27736700	-0.72432000
H	4.10418600	-3.07853000	0.94340100

4H (-2412.32484123 a.u.)

F	-1.35468500	-0.61888100	0.09454500
Ta	-2.66717500	1.03205900	0.10094800
Ta	-1.04998200	-2.67248100	-0.17690300
F	-0.89709900	2.01393000	-0.38395100
F	0.91738400	-1.99130800	-0.26106500
Ta	2.69456400	-1.00067900	0.20217400
F	1.38963400	0.62751100	0.09926100
Ta	1.09097000	2.67418300	-0.26006500
F	-1.94273400	1.26700400	1.87037300
F	1.10106900	2.02304200	-2.06942300
F	1.92664400	-1.11358300	1.96740900
F	-0.99298300	-2.13665300	-2.02782500
O	-0.32801500	-4.34863600	-0.53624400
C	0.62501300	-4.91805100	-1.38546700
H	1.57069100	-4.36193300	-1.32149900
H	0.27540700	-4.89220300	-2.42448600
H	0.80344800	-5.95791400	-1.09532500
O	-3.95930000	-0.13565100	0.75603100
C	-4.17559900	-0.97210900	1.86139300
H	-3.69102400	-1.94177100	1.69133400
H	-5.25021100	-1.12739600	1.99681700
H	-3.75912100	-0.51546900	2.76810300
O	0.40789700	4.35612400	-0.61803000
C	-0.73435500	5.15594900	-0.66289300
H	-1.62928100	4.55921800	-0.44338400
H	-0.84146800	5.59719700	-1.65914400
H	-0.65220200	5.96412500	0.07171300
O	4.04882700	0.13508300	0.77058200
C	4.39214700	1.01455400	1.80572600
H	3.88187000	1.97461600	1.65916200
H	5.47361000	1.18067100	1.80001500
H	4.09976000	0.59577100	2.77670000
O	2.85934700	-0.80823000	-1.63782700
O	0.93521800	2.68539000	1.59379800
O	-2.80516400	0.75260300	-1.72590400
O	-0.95492100	-2.67016800	1.67832600
C	-2.10455400	0.62592200	-2.93372300

H	-1.05795700	0.92554900	-2.79422900
H	-2.12950800	-0.41374000	-3.26874200
H	-2.56677800	1.26932900	-3.68937500
C	2.16780800	-0.73966000	-2.85526000
H	1.10696200	-0.97638500	-2.70092100
H	2.24105700	0.26937800	-3.27021800
H	2.59893600	-1.46098500	-3.55794800
C	-0.82492400	-1.97579700	2.88274700
H	0.16832900	-2.14710200	3.30581500
H	-0.95007400	-0.89742900	2.71602600
H	-1.59119000	-2.32333700	3.58586100
C	0.83451400	1.98801400	2.80025900
H	-0.12244400	2.20920600	3.27985400
H	0.89745000	0.90617400	2.62768100
H	1.65307300	2.29250200	3.46389800
O	3.46566900	-2.68522800	0.41576600
C	3.22031600	-3.82546400	1.18960800
H	3.58828000	-3.68305600	2.21220900
H	2.14111100	-4.03299800	1.23435700
H	3.72894100	-4.68724600	0.74614600
O	2.91953900	2.98242100	-0.37882500
C	4.01428400	2.76353200	-1.22639700
H	4.31649100	1.70978700	-1.18451100
H	3.75824500	3.01987800	-2.26054000
H	4.85354900	3.38675700	-0.90163200
O	-2.87442900	-2.98613100	-0.33528700
C	-3.95440400	-2.79207600	-1.20485300
H	-4.53355600	-1.91915800	-0.88075700
H	-3.59304600	-2.62074100	-2.22617900
H	-4.59677200	-3.67829700	-1.19674100
O	-3.60805400	2.63778100	0.22255200
C	-4.18330000	3.42399600	1.22531300
H	-3.45002000	3.63830200	2.01315200
H	-4.53776200	4.36740200	0.79855600
H	-5.03597500	2.90103900	1.67687700

4I (-2412.28463266 a.u.)

Ta	-0.11879000	2.48223300	-0.12336700
Ta	2.94196000	0.15089600	-0.04742300
Ta	0.11432400	-2.48665200	0.13488600
Ta	-2.94356800	-0.15555400	0.02980200
F	-0.05360500	3.44170400	1.53584300
F	-2.91266100	1.05981600	-1.44991600
F	2.65419700	1.12930800	-1.64100300
O	-1.59431900	1.27592400	0.92721800
C	-1.86788600	1.45388700	2.32535400
H	-1.33392300	2.32458200	2.70244700
H	-1.56841900	0.55653600	2.87385000
H	-2.94309900	1.60489400	2.47018600
O	1.41907800	1.23562800	0.87011300
C	1.51526600	1.33657800	2.30199500
H	2.28234400	0.66008500	2.67554400
H	0.56686200	1.04317900	2.74927600
H	1.75946400	2.36517500	2.57675800

O	1.60544700	-1.30988500	-0.92578500
C	1.89987100	-1.53129000	-2.31312800
H	2.96833200	-1.74356400	-2.43007600
H	1.66211800	-0.63166700	-2.88726500
H	1.32896500	-2.37896000	-2.68705900
O	-1.40190800	-1.22718100	-0.87423500
C	-1.47416000	-1.31238500	-2.30823800
H	-1.74066300	-2.33177900	-2.59719300
H	-0.51064400	-1.03922300	-2.73561500
H	-2.21342600	-0.60968500	-2.69001700
F	2.91033800	-1.04790000	1.44340600
F	-2.68542700	-1.15453300	1.61694700
F	0.02010000	-3.46364600	-1.51160200
O	4.11485700	1.39512900	0.71856500
O	-4.10777700	-1.38378300	-0.76853000
C	5.45785900	1.74874700	0.78384600
H	5.59654500	2.76907200	0.40545600
H	5.81048700	1.71464300	1.82058500
H	6.07032000	1.06748400	0.17774800
C	-5.45108500	-1.71191200	-0.91090200
H	-5.75155400	-1.63716500	-1.96190700
H	-5.62346400	-2.74185200	-0.57552500
H	-6.08121700	-1.03907100	-0.31276900
O	4.38118500	-0.81187300	-0.75150800
O	-4.38117700	0.80794800	0.73638700
F	-0.11857200	1.12132500	-1.42564800
F	0.09550500	-1.10250100	1.41547000
O	1.48079400	-3.48015600	0.85115100
O	-1.28124000	-3.48000500	0.80384000
O	1.26812800	3.47043500	-0.80853700
O	-1.49665900	3.50538900	-0.78136500
C	2.54328600	4.01962200	-0.69715900
H	3.20508700	3.55120100	-1.43255600
H	2.49884800	5.09839300	-0.87800800
H	2.94329800	3.83410500	0.30876900
C	-2.79838900	3.97050200	-0.62302400
H	-2.88977300	4.97229100	-1.05450600
H	-3.48976900	3.28908200	-1.12780400
H	-3.04979500	4.02160000	0.44602100
C	-5.35292600	1.79163300	0.61016400
H	-5.45992100	2.09306700	-0.44084400
H	-6.31940400	1.42587700	0.97543200
H	-5.07668800	2.67578200	1.20016900
C	5.37946700	-1.76900200	-0.62625700
H	6.35020000	-1.35594700	-0.92371300
H	5.44493000	-2.12221900	0.41199500
H	5.16362600	-2.62757800	-1.27649800
C	2.80851800	-3.87900200	0.95143100
H	3.24322300	-3.48927800	1.87625500
H	2.86877000	-4.97217600	0.94382100
H	3.37930400	-3.47788700	0.10472000
C	-2.53895700	-4.03420100	0.57045600
H	-3.31059400	-3.36918300	0.97298100
H	-2.69521900	-4.15722600	-0.51019100
H	-2.60703300	-5.01175300	1.05778500

5A (-2769.74763900 a.u.)

C	-1.26285800	2.27632300	-0.18707700
C	-1.36530200	3.09806400	0.92396700
H	-0.88855000	2.79195600	1.85238500
C	-2.06441800	4.29084000	0.81033900
H	-2.13778700	4.95224000	1.66831600
C	-2.65673400	4.64338900	-0.39596500
H	-3.21031800	5.57354700	-0.47712200
C	-2.54713700	3.80269600	-1.49689400
H	-3.02308800	4.06791400	-2.43619500
C	-1.84264700	2.61110200	-1.40033300
H	-1.74514600	1.92395700	-2.23780600
C	-4.20202300	0.67875900	-0.23299500
C	-4.84627500	1.71706100	0.42855700
H	-4.53119500	1.97173800	1.43604600
C	-5.85404000	2.41242400	-0.21984300
H	-6.34945200	3.23327400	0.29023000
C	-6.22214400	2.07284000	-1.51555900
H	-7.01775500	2.61541500	-2.01617500
C	-5.56884800	1.03456200	-2.16737300
H	-5.84849100	0.76761200	-3.18216400
C	-4.55405700	0.33379700	-1.53420000
H	-4.00619700	-0.45757500	-2.03644400
C	-1.99502500	-3.83386300	0.05814300
C	-2.94035000	-4.02751100	-0.94345800
H	-3.51871300	-3.17700900	-1.29358600
C	-3.12050100	-5.29721900	-1.46859400
H	-3.86281500	-5.45287200	-2.24549700
C	-2.35817100	-6.36390500	-1.00835200
H	-2.49825700	-7.35495300	-1.42787900
C	-1.41739300	-6.15694400	-0.00735100
H	-0.81381300	-6.98441300	0.35478400
C	-1.23534200	-4.89550100	0.53590600
H	-0.50262200	-4.71055500	1.31594900
C	-1.17146400	-0.35329600	3.56950100
C	-2.21643700	-0.86374800	4.33477000
H	-3.05032600	-1.34423500	3.83153000
C	-2.16871300	-0.74484500	5.71457100
H	-2.97818000	-1.15014800	6.31441200
C	-1.09172000	-0.11971000	6.32991000
H	-1.06288900	-0.02245700	7.41056600
C	-0.05500300	0.38428300	5.55478700
H	0.79113000	0.87089000	6.03107300
C	-0.08401000	0.27127900	4.17313500
H	0.71384400	0.65081000	3.54084700
F	-1.66850000	-0.97901600	-1.51641900
O	-0.58185300	1.08201100	-0.07675800
O	-3.20556200	0.02233500	0.40059200
O	-1.80732500	-2.60106900	0.57176200
O	-1.21534000	-0.47058500	2.23218500
Ta	-1.50242200	-0.76243600	0.39957000
C	1.24676400	-2.21551500	0.17024700
C	1.35319000	-3.02490300	-0.95022800

H	0.88248000	-2.70891600	-1.87856000
C	2.05094800	-4.21950400	-0.84765200
H	2.12734500	-4.87066300	-1.71314400
C	2.63861000	-4.58691900	0.35642000
H	3.19119800	-5.51840300	0.42863200
C	2.52588000	-3.75903100	1.46636700
H	2.99872700	-4.03501700	2.40415500
C	1.82269200	-2.56583400	1.38103400
H	1.72496400	-1.88943800	2.22689500
C	4.18176700	-0.62366900	0.22798400
C	4.83342100	-1.64869700	-0.44689900
H	4.52918200	-1.88383200	-1.46246100
C	5.83457800	-2.35630800	0.19843800
H	6.33553600	-3.16710200	-0.32218500
C	6.18919400	-2.04159400	1.50420200
H	6.97979200	-2.59357100	2.00247900
C	5.52911000	-1.01587700	2.16893400
H	5.79844500	-0.76817800	3.19136600
C	4.52049400	-0.30338300	1.53897600
H	3.96732800	0.47855900	2.05014100
C	1.97237400	3.90046600	-0.06708400
C	2.90912500	4.09814600	0.94179700
H	3.48381800	3.24889100	1.30100100
C	3.08537700	5.37018100	1.46262700
H	3.82090500	5.52896000	2.24532800
C	2.32790700	6.43521100	0.99063100
H	2.46493500	7.42808600	1.40683400
C	1.39586800	6.22420300	-0.01767700
H	0.79616100	7.05039000	-0.38907100
C	1.21769000	4.96032500	-0.55655100
H	0.49181900	4.77214000	-1.34219600
C	1.22092300	0.21663000	-3.54209700
C	2.29421600	0.62455100	-4.32961600
H	3.10166400	1.18486000	-3.86754100
C	2.30804000	0.30184500	-5.67730600
H	3.13991600	0.62521700	-6.29592900
C	1.26424500	-0.42310300	-6.23799900
H	1.28389200	-0.67991600	-7.29241300
C	0.19792900	-0.82098600	-5.44166100
H	-0.62319800	-1.38346800	-5.87627700
C	0.16520100	-0.50386300	-4.09213700
H	-0.65802400	-0.79350300	-3.44552100
F	1.65154200	1.03951500	1.51346100
O	0.56698700	-1.01870700	0.07242400
O	3.19112500	0.04451800	-0.40225900
O	1.78888900	2.66562500	-0.57720000
O	1.20555700	0.52615300	-2.23526100
Ta	1.48662600	0.82686800	-0.40313300

5B (-2769.74617165 a.u.)

C	-1.04696200	1.55129000	-1.81827900
C	-2.26792600	1.21456800	-2.38104100
H	-2.77674000	0.31125300	-2.05249900
C	-2.80921700	2.04043000	-3.35559200

H	-3.76643400	1.78688400	-3.80049100
C	-2.13603100	3.18559300	-3.75841500
H	-2.56195400	3.82526300	-4.52478500
C	-0.91508800	3.51055100	-3.18113600
H	-0.38545300	4.40501500	-3.49466200
C	-0.36353900	2.69314700	-2.20493100
H	0.59037100	2.91638200	-1.73327500
C	3.16632000	-2.79019600	-0.87250400
C	4.10466800	-2.38634800	-1.81529100
H	3.77400200	-1.83544800	-2.69161400
C	5.44292200	-2.68218200	-1.60829000
H	6.17908500	-2.36240600	-2.33914900
C	5.84320400	-3.37139900	-0.47095000
H	6.89323600	-3.59428000	-0.31039900
C	4.89356600	-3.78043800	0.45638000
H	5.19713600	-4.32299300	1.34712100
C	3.55105500	-3.50163100	0.25643700
H	2.79274800	-3.81053000	0.96953800
C	-1.94312200	-2.73633600	-1.54565200
C	-2.42590400	-3.75783600	-0.73278800
H	-1.89116900	-4.00256900	0.18025900
C	-3.57936800	-4.43291800	-1.09435300
H	-3.95739800	-5.22275400	-0.45198200
C	-4.25781900	-4.09663800	-2.25870100
H	-5.16255200	-4.62805100	-2.53641900
C	-3.76482900	-3.08378500	-3.07048100
H	-4.28063300	-2.82521400	-3.99060400
C	-2.60804500	-2.40293400	-2.72388400
H	-2.19556000	-1.62321300	-3.35779200
O	-0.49927500	0.73983000	-0.84711400
O	1.85700700	-2.47493600	-1.03877100
O	-0.83212200	-2.07308800	-1.19459000
Ta	0.72095600	-0.99008300	-1.20930700
C	1.07987100	-1.45416700	1.82061600
C	2.28936800	-1.06463000	2.37280200
H	2.75557200	-0.14413300	2.03045800
C	2.86936500	-1.85769400	3.35268500
H	3.81702200	-1.55938800	3.79051600
C	2.24635800	-3.02685700	3.76720400
H	2.70083600	-3.64176800	4.53743900
C	1.03842300	-3.40865900	3.19550500
H	0.54964400	-4.32360100	3.51604700
C	0.44854400	-2.62293000	2.21592900
H	-0.49580000	-2.89107700	1.74921800
C	-3.22946000	2.83085100	0.68599600
C	-4.30120200	2.25295300	1.35632500
H	-4.10869100	1.52119500	2.13562400
C	-5.59304500	2.61202400	1.00424000
H	-6.43202500	2.15869100	1.52321600
C	-5.81491200	3.53902800	-0.00560800
H	-6.82849800	3.81432600	-0.27909900
C	-4.73463700	4.11279800	-0.66312800
H	-4.89973400	4.83483500	-1.45751500
C	-3.43777500	3.76687100	-0.31877600
H	-2.57963100	4.18920700	-0.83384200

C	1.88640700	2.71641700	1.66390700
C	2.50807900	2.38063500	2.86460400
H	2.02899900	1.65999200	3.52095500
C	3.71023800	2.98338700	3.20209200
H	4.19208000	2.72333700	4.14004200
C	4.29188900	3.92021500	2.35795000
H	5.23272100	4.38931000	2.62769000
C	3.65653100	4.26047300	1.17065600
H	4.10177200	4.99392400	0.50522900
C	2.45653800	3.66524300	0.82023000
H	1.94638500	3.92072800	-0.10313100
O	0.49334500	-0.66498700	0.85423200
O	-1.95874800	2.47380700	1.00035800
O	0.73158500	2.12963700	1.31676000
Ta	-0.79873600	1.01952900	1.21257200
O	2.22942700	0.15950800	-1.20060300
F	0.51794000	-0.70875900	-3.06033600
F	-0.68847300	0.70258500	3.06822500
O	-2.25944400	-0.19529700	1.11811300
C	3.26688700	0.99228100	-1.34460900
C	3.26922000	1.92507900	-2.37860600
C	4.34551500	0.90918600	-0.46670600
C	4.35023600	2.78237100	-2.52007400
H	2.42495900	1.94661900	-3.06353700
C	5.41434400	1.77609300	-0.61617900
H	4.33237400	0.14707800	0.30938700
C	5.42196900	2.71658600	-1.63966800
H	4.35643900	3.50529300	-3.33060600
H	6.25101200	1.71515200	0.07325200
H	6.26487000	3.39057800	-1.75515000
C	-3.19513200	-1.11088100	1.40446300
C	-4.31711600	-1.22802900	0.58770600
C	-3.05495900	-1.92377900	2.52725200
C	-5.28973200	-2.16556300	0.89206400
H	-4.40930000	-0.57262700	-0.27337400
C	-4.03545800	-2.86109700	2.81736100
H	-2.18338900	-1.79457800	3.16261700
C	-5.15382400	-2.98769900	2.00385000
H	-6.15906200	-2.25905300	0.24813400
H	-3.92789300	-3.49102200	3.69546000
H	-5.91926600	-3.72083700	2.23767400

5C (-2769.73798031 a.u.)

C	2.90454800	-0.33626900	-2.82869300
C	4.21965700	0.11019100	-2.86306200
H	4.43330200	1.13967000	-2.58931800
C	5.22451200	-0.76556900	-3.24449600
H	6.25349900	-0.42059500	-3.27113000
C	4.92055900	-2.07541400	-3.59127000
H	5.70964600	-2.75738500	-3.89092600
C	3.60122900	-2.50767500	-3.55584200
H	3.35741700	-3.52963200	-3.83049800
C	2.58688700	-1.64331600	-3.17176100
H	1.54814200	-1.95777100	-3.12752000

C	-1.06362900	3.07254500	-1.22484800
C	-1.74822600	3.58400400	-2.32168500
H	-1.65394500	3.08007800	-3.27855300
C	-2.54861700	4.70282400	-2.16334600
H	-3.08764800	5.09739300	-3.01971500
C	-2.67558600	5.31095500	-0.92101200
H	-3.30593500	6.18660600	-0.80354000
C	-1.99432300	4.78950000	0.17058600
H	-2.09232700	5.25561500	1.14661900
C	-1.18655700	3.67175700	0.02721000
H	-0.65222400	3.24611300	0.87162900
O	1.91969500	0.51355300	-2.43495300
O	-0.27297200	1.99457000	-1.38391200
Ta	1.14172700	0.89765500	-0.76925800
C	-3.16633500	-0.35501300	3.18529900
C	-4.42377500	-0.25296400	2.59955200
H	-4.56035800	-0.56303400	1.56687500
C	-5.47798000	0.26175000	3.33905200
H	-6.45928700	0.34254200	2.88135400
C	-5.28490800	0.67178400	4.65098600
H	-6.11364500	1.07392100	5.22442900
C	-4.02569000	0.56149700	5.22616000
H	-3.86717400	0.87799600	6.25254900
C	-2.96403500	0.04688400	4.50007300
H	-1.97225500	-0.04948500	4.92920600
C	1.15369900	-2.97958400	1.25638500
C	1.46877700	-3.46949400	-0.00783300
H	0.90756500	-3.12244200	-0.87186600
C	2.51840500	-4.36450900	-0.14663800
H	2.76644000	-4.74524200	-1.13317200
C	3.25082600	-4.77353900	0.95916500
H	4.07160800	-5.47389200	0.84135400
C	2.92920600	-4.27758800	2.21613200
H	3.50499800	-4.58087700	3.08543600
C	1.88321200	-3.38415400	2.37000200
H	1.62529100	-2.96845400	3.33870500
O	-2.11961700	-0.85184200	2.48708600
O	0.14595600	-2.10322700	1.42003500
Ta	-1.29697100	-1.04145000	0.81876200
O	2.37044100	-0.22191900	0.14191400
O	-2.50746500	0.12326400	-0.05718800
C	3.24547700	-0.53776400	1.11252900
C	3.04496900	-0.07259400	2.40867600
C	4.36425100	-1.29808500	0.79261400
C	3.98615900	-0.35724500	3.38460700
H	2.15673800	0.51788500	2.61804900
C	5.29324000	-1.58018000	1.78127900
H	4.48484100	-1.65061200	-0.22900000
C	5.11193700	-1.11077200	3.07604700
H	3.84040100	0.01512400	4.39414100
H	6.16851900	-2.17491700	1.53662900
H	5.84748700	-1.33075200	3.84332100
C	-3.28225800	0.71006100	-0.98817400
C	-4.21463500	1.66341500	-0.59083500
C	-3.16165500	0.35652100	-2.32894300

C	-5.03364600	2.25298300	-1.54032500
H	-4.26951600	1.93475000	0.45912800
C	-3.99528600	0.94567600	-3.26520600
H	-2.42554500	-0.38808600	-2.61692900
C	-4.93233100	1.89535000	-2.87803500
H	-5.75368000	3.00452300	-1.23020900
H	-3.91123400	0.65595300	-4.30867500
H	-5.58144100	2.35516200	-3.61666100
F	-0.04169400	0.64350800	1.00886900
F	-0.10997400	-0.78650600	-0.96472500
O	2.05727600	2.41698800	-0.16972600
O	-2.13566800	-2.53085600	0.03449200
C	-2.96301500	-2.82994700	-0.99302400
C	-4.33731100	-2.69623700	-0.84156000
C	-2.41962500	-3.25276100	-2.20050600
C	-5.16900600	-2.96941400	-1.91539600
H	-4.73158100	-2.37201900	0.11765000
C	-3.26223400	-3.52143800	-3.26780200
H	-1.33993000	-3.34745200	-2.28002200
C	-4.63711600	-3.37728800	-3.13148800
H	-6.24272300	-2.85697700	-1.80210200
H	-2.84068000	-3.84635000	-4.21423500
H	-5.29307800	-3.58598500	-3.97021100
C	3.07658700	3.06958200	0.42861000
C	4.35679200	2.52481000	0.44405600
C	2.82293400	4.30046000	1.02310000
C	5.37857100	3.21122300	1.08012300
H	4.53511900	1.56081700	-0.02415600
C	3.85612900	4.97851100	1.65007500
H	1.81491300	4.70252100	0.97746300
C	5.13445900	4.43749500	1.68476400
H	6.37405300	2.77842100	1.10449300
H	3.66011700	5.94024400	2.11432700
H	5.93932800	4.97059600	2.18023000