Supporting Information for

Geometries, Electronic Structures, Bonding Properties, and Stability Strategy of Endohedral Metallofullerenes $TM@C_{28}$ ($TM = Sc^-, Y^-, La^-, Ti, Zr, Hf, V^+, Nb^+, Ta^+$)

Dong Liu, Yuan Shui and Tao Yang *

MOE Key Laboratory for Non-Equilibrium Synthesis and Modulation of Condensed Matter, School of Physics, Xi'an Jiaotong University, Xi'an 710049, Shaanxi, China; dliu_sd@stu.xjtu.edu.cn (D.L.); f24270216f@stu.xjtu.edu.cn (Y.S.)

* Correspondence: taoyang1@xjtu.edu.cn

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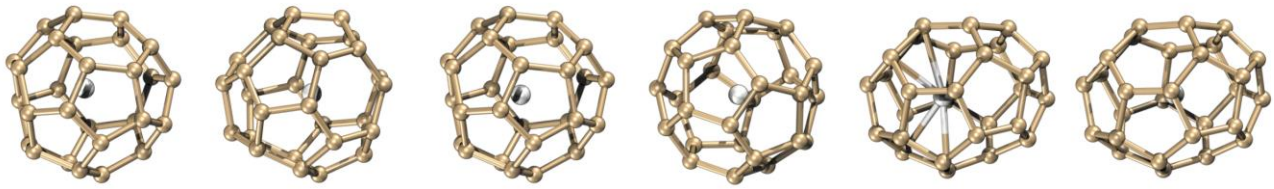
I. The Necessity of Clustering Algorithms

In our conformational search strategy, the generation of an extensive set of structures necessitates the implementation of clustering algorithms. While smaller fullerene cages, such as the ones we studied, are often considered to have limited conformational possibilities due to their inherent symmetry, the process of randomly placing transition metal (TM) atoms can disrupt this symmetry. To effectively manage this, we employed the ISOSTAT module of the Molclus software for clustering purposes. This module categorizes structures as identical if they exhibit an energy difference less than 0.25 kcal/mol and a geometric deviation smaller than 0.1 Ångström.

Although strict symmetry constraints would theoretically consolidate most structures into a single category, our research methodology rigorously validates this assumption from another perspective. By allowing for the perturbation of symmetry through the random placement of TM atoms and subsequently clustering the resulting structures, our approach not only adheres to the principles of thoroughness but also provides a robust framework for analyzing the nuanced variations in structural configurations, even within the constraints of presumed symmetry.

$[Sc@C_{28}]^-$



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$[Y@C_{28}]^-$

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$[La@C_{28}]^-$

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$[Ti@C_{28}]$

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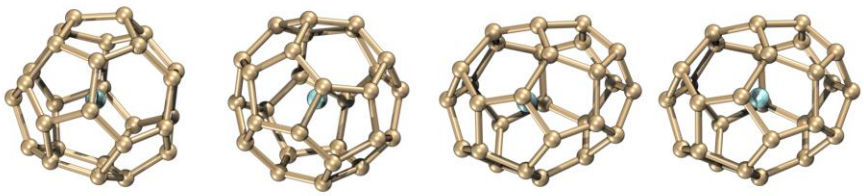
$[Zr@C_{28}]$



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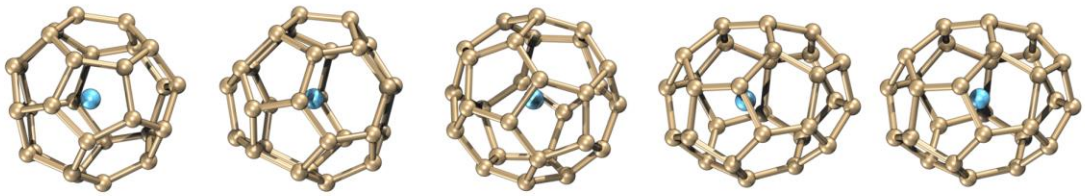
Hf@C_{28}



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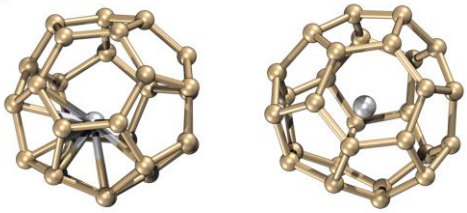
```

$[V@C_{28}]^+$



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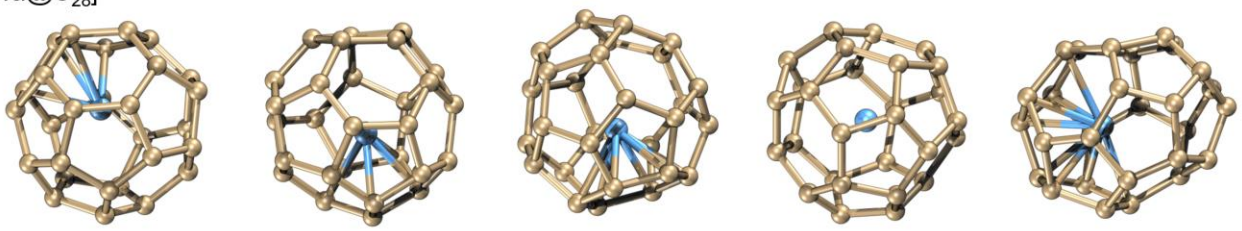
$[Ta@C_{28}]^+$



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#    5 Count:    2  E=  -1122.238304 a.u.  DGmin=   0.46  DE=   61.83 kcal/mol
```

II. Atomic Multiplicity

Table S1. The atomic (ionic) energies (in eV) calculated using PBE-D3(BJ)/def2-TZVPPD, with red indicating the ground state.

	Singlet	Triplet	Quintet	Septet
Sc^-	0.89	0.00	3.61	27.25
Y^-	0.73	0.00	0.88	24.18
La^-	0.71	0.00	0.67	17.87
Ti	2.07	0.39	0.00	29.84
Zr	1.18	0.05	0.00	26.11
Hf	1.06	0.00	1.00	29.15
V^+	2.90	1.15	0.00	33.64
Nb^+	2.45	0.98	0.00	29.34
Ta^+	2.28	0.88	0.00	31.84

III. The Energy relationship of $[V@C_{28}]^{+}$- $(CF_3)_{n=1,2}$

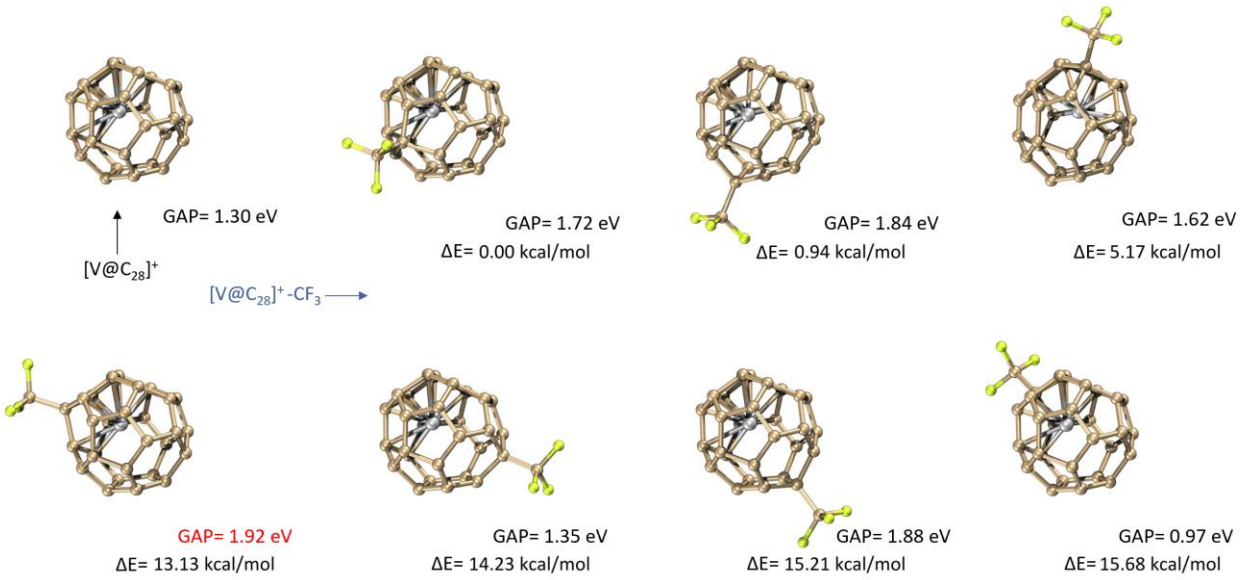

Figure S1. The HOMO-LUMO GAP after attaching a CF_3 group to $[V@C_{28}]^{+}$ and the energy differences between different isomers, at the PBE-D3(BJ)/def2-SVP level.

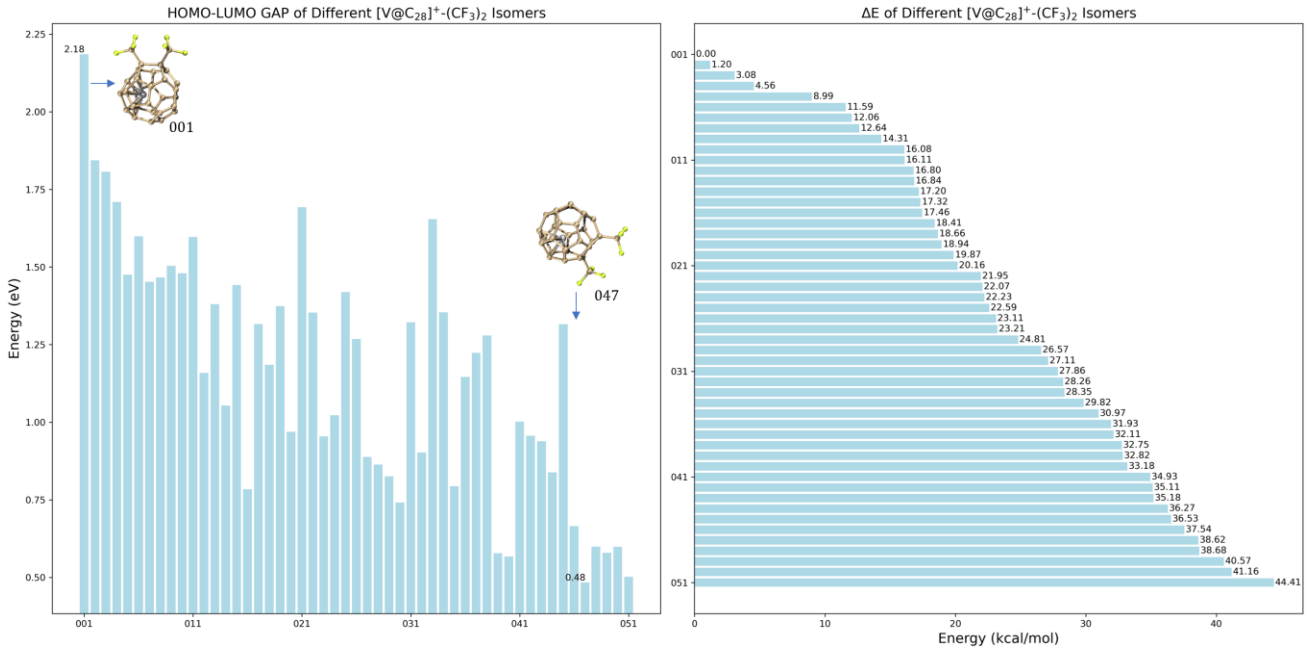

Figure S2. After the addition of two CF_3 groups, the HOMO-LUMO GAP and the energy relationships among different isomers, at the PBE-D3(BJ)/def2-SVP level.

IV. EDA analysis

Table S2. The EDA results (in kcal/mol) of the [TM@C_{28}] with TM^{m+} and C_{28}^{n-} as interacting fragments at the BP86-D3(BJ)/TZ2P+ level.

[Sc@C_{28}]$^-$	Sc $4s^23d^1$ +$[C_{28}]^-$	$Sc^+4s^03d^2$ +$[C_{28}]^{2-}$	$Sc^+4s^13d^1$ + $[C_{28}]^{2-}$	$Sc^{2+}4s^03d^1$ + $[C_{28}]^{3-}$	$Sc^{2+}4s^13d^0$ + $[C_{28}]^{3-}$	$Sc^{3+}4s^03d^0$ + $[C_{28}]^{4-}$
ΔE_{int}	–274.95	–552.31	–513.62	–994.28	–1074.63	–1843.12
ΔE_{Pauli}	1345.90	472.26	783.90	284.84	624.06	248.45
ΔE_{disp}[a]	–2.79	–2.79	–2.79	–2.79	–2.79	–2.79
ΔE_{elstat}[a]	–715.99	–363.65	–509.97	–533.37	–699.82	–983.46
ΔE_{orb}	–902.08	–658.14	–784.77	–742.96	–996.11	–1105.33

[Ti@C_{28}]	Ti $4s^23d^2$ +$[C_{28}]$	Ti^+ $4s^23d^1$ +$[C_{28}]^-$	$Ti^+4s^13d^2$ + $[C_{28}]^-$	$Ti^{2+}4s^13d^1$ + $[C_{28}]^{2-}$	$Ti^{2+}4s^23d^0$ + $[C_{28}]^{2-}$	$Ti^{3+}4s^13d^0$ + $[C_{28}]^{3-}$	$Ti^{4+}4s^03d^0$ + $[C_{28}]^{4-}$
ΔE_{int}	–1873.80	–461.08	–422.99	–895.60	–1091.93	–1586.78	–2543.15
ΔE_{Pauli}	1502.98	1205.46	908.53	723.86	1012.79	615.20	313.90
ΔE_{disp}[a]	–5.69	–5.69	–5.69	–5.69	–5.69	–5.69	–5.69
ΔE_{elstat}[a]	–747.18	–594.45	–464.52	–547.78	–668.21	–908.21	–1354.69
ΔE_{orb}	–2623.88	–1066.32	–861.29	–1065.92	–1430.67	–1287.96	–1496.59

[V@C_{28}]$^+$	V^+ $4s^13d^3$ +$[C_{28}]$	V^+ $4s^23d^2$ +$[C_{28}]$	$V^{2+}4s^03d^3$ + $[C_{28}]^-$	$V^{2+}4s^13d^2$ + $[C_{28}]^-$	$V^{3+}4s^03d^2$ + $[C_{28}]^{2-}$	$V^{4+}4s^03d^1$ + $[C_{28}]^{3-}$	$Ti^{4+}4s^13d^0$ + $[C_{28}]^{3-}$
ΔE_{int}	–768.30	–833.54	–851.46	–1007.04	–1366.04	–2997.75	–2569.33
ΔE_{Pauli}	1145.45	1071.78	831.14	756.73	404.47	638.23	378.76
ΔE_{disp}[a]	–5.36	–5.36	–5.36	–5.36	–5.36	–5.36	–5.36
ΔE_{elstat}[a]	–513.34	–427.78	–463.13	–397.26	–495.70	–1052.89	–957.98
ΔE_{orb}	–1394.99	–1472.17	–1214.05	–1361.14	–1269.46	–2577.63	–1984.72

V. Cartesian coordinates of optimized structures

PBE-D3(BJ)/def2-TZVPPD

Singlet

$[Sc@C_{28}]^-$

29

symmetry C_{2v}

C	–1.178620000	2.127919000	–0.063358000
C	–2.016975000	–0.297859000	1.313513000
C	–1.192432000	0.688451000	2.004264000
C	–0.750534000	1.895681000	1.313513000
C	0.000000000	2.396107000	–0.875955000
C	0.750534000	1.895681000	1.313513000
C	1.178620000	2.127919000	–0.063358000
C	0.000000000	0.000000000	2.516373000
C	0.000000000	1.440024000	–1.985520000
C	–1.256854000	0.725645000	–1.979039000
C	–1.247097000	–0.720012000	–1.985520000
C	1.256854000	0.725645000	–1.979039000
C	1.247097000	–0.720012000	–1.985520000
C	0.000000000	–1.451290000	–1.979039000
C	2.005774000	1.158034000	–0.755831000
C	–1.253522000	–2.084674000	–0.063358000
C	–2.075089000	–1.198053000	–0.875955000
C	–1.266441000	–1.597822000	1.313513000
C	0.000000000	–2.316069000	–0.755831000
C	–2.432142000	–0.043245000	–0.063358000
C	–2.005774000	1.158034000	–0.755831000
C	1.253522000	–2.084674000	–0.063358000
C	2.075089000	–1.198053000	–0.875955000
C	1.192432000	0.688451000	2.004264000
C	2.016975000	–0.297859000	1.313513000
C	2.432142000	–0.043245000	–0.063358000
C	1.266441000	–1.597822000	1.313513000
C	0.000000000	–1.376902000	2.004264000
Sc	0.000000000	0.000000000	0.216841000

$[Y@C_{28}]^-$

29

symmetry T_d

C	–0.050963000	1.733201000	–1.733201000
C	2.336744000	0.534178000	–0.534178000
C	1.733201000	–0.050963000	–1.733201000
C	0.534178000	0.534178000	–2.336744000
C	–1.470004000	1.470004000	–1.470004000
C	–0.534178000	–0.534178000	–2.336744000
C	–1.733201000	0.050963000	–1.733201000
C	1.470004000	–1.470004000	–1.470004000
C	–1.733201000	1.733201000	–0.050963000
C	–0.534178000	2.336744000	0.534178000
C	0.050963000	1.733201000	1.733201000
C	–2.336744000	0.534178000	0.534178000
C	–1.733201000	–0.050963000	1.733201000
C	–0.534178000	0.534178000	2.336744000
C	–2.336744000	–0.534178000	–0.534178000
C	1.733201000	0.050963000	1.733201000
C	1.470004000	1.470004000	1.470004000
C	2.336744000	–0.534178000	0.534178000
C	0.534178000	–0.534178000	2.336744000
C	1.733201000	1.733201000	0.050963000
C	0.534178000	2.336744000	–0.534178000
C	–0.050963000	–1.733201000	1.733201000
C	–1.470004000	–1.470004000	1.470004000
C	0.050963000	–1.733201000	–1.733201000
C	–0.534178000	–2.336744000	–0.534178000
C	–1.733201000	–1.733201000	0.050963000
C	0.534178000	–2.336744000	0.534178000
C	1.733201000	–1.733201000	–0.050963000
Y	0.000000000	0.000000000	0.000000000

$[La@C_{28}]^-$

29

symmetry T_d

C	0.052141000	1.754154000	1.754154000
C	–2.368086000	0.540369000	0.540369000
C	–1.754154000	–0.052141000	1.754154000
C	–0.540369000	0.540369000	2.368086000
C	1.477880000	1.477880000	1.477880000
C	0.540369000	–0.540369000	2.368086000
C	1.754154000	0.052141000	1.754154000
C	–1.477880000	–1.477880000	1.477880000
C	1.754154000	1.754154000	0.052141000
C	0.540369000	2.368086000	–0.540369000
C	–0.052141000	1.754154000	–1.754154000
C	2.368086000	0.540369000	–0.540369000
C	1.754154000	–0.052141000	–1.754154000

C	0.540369000	0.540369000	–2.368086000
C	2.368086000	–0.540369000	0.540369000
C	–1.754154000	0.052141000	–1.754154000
C	–1.477880000	1.477880000	–1.477880000
C	–2.368086000	–0.540369000	–0.540369000
C	–0.540369000	–0.540369000	–2.368086000
C	–1.754154000	1.754154000	–0.052141000
C	–0.540369000	2.368086000	0.540369000
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C	1.477880000	–1.477880000	–1.477880000
C	–0.052141000	–1.754154000	1.754154000
C	0.540369000	–2.368086000	0.540369000
C	1.754154000	–1.754154000	–0.052141000
C	–0.540369000	–2.368086000	–0.540369000
C	–1.754154000	–1.754154000	0.052141000
La	0.000000000	0.000000000	0.000000000

[Ti@C_{28}]

29

symmetry C_{3v}

C	0.000000000	1.438208000	–2.031167000
C	0.000000000	–1.447157000	–2.021421000
C	–1.245524000	–0.719104000	–2.031167000
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C	0.000000000	2.377145000	–0.907087000
C	–1.991596000	1.149848000	–0.800244000
C	–1.173967000	2.115308000	–0.103086000
C	–2.058668000	–1.188573000	–0.907087000
C	1.173967000	2.115308000	–0.103086000
C	1.991596000	1.149848000	–0.800244000
C	2.418894000	–0.040969000	–0.103086000
C	0.748504000	1.877518000	1.274582000
C	1.207311000	0.697042000	2.007470000
C	2.000230000	–0.290535000	1.274582000
C	–0.748504000	1.877518000	1.274582000
C	1.244927000	–2.074339000	–0.103086000
C	2.058668000	–1.188573000	–0.907087000
C	0.000000000	–2.299697000	–0.800244000
C	1.251726000	–1.586983000	1.274582000
C	1.245524000	–0.719104000	–2.031167000
C	1.253275000	0.723579000	–2.021421000
C	0.000000000	–1.394083000	2.007470000
C	0.000000000	0.000000000	2.520804000
C	–2.418894000	–0.040969000	–0.103086000
C	–2.000230000	–0.290535000	1.274582000
C	–1.207311000	0.697042000	2.007470000
C	–1.251726000	–1.586983000	1.274582000
C	–1.244927000	–2.074339000	–0.103086000
Ti	0.000000000	0.000000000	0.465699000

[Zr@C_{28}]

29

symmetry C_{2v}

C	0.000000000	2.440740000	–0.069731000
C	0.000000000	0.751661000	2.315902000
C	1.258670000	1.185905000	1.713254000
C	1.267648000	2.018750000	0.516471000
C	0.000000000	2.078128000	–1.482645000
C	2.016102000	1.265705000	–0.545624000
C	1.179906000	1.254071000	–1.737122000
C	2.072917000	0.000000000	1.452970000
C	–1.179906000	1.254071000	–1.737122000
C	–2.016102000	1.265705000	–0.545624000
C	–2.436998000	0.000000000	0.034641000
C	–0.750719000	0.000000000	–2.332528000
C	–1.179906000	–1.254071000	–1.737122000
C	–2.016102000	–1.265705000	–0.545624000
C	0.750719000	0.000000000	–2.332528000
C	–1.258670000	–1.185905000	1.713254000
C	–2.072917000	0.000000000	1.452970000
C	0.000000000	–0.751661000	2.315902000
C	–1.267648000	–2.018750000	0.516471000
C	–1.258670000	1.185905000	1.713254000
C	–1.267648000	2.018750000	0.516471000
C	0.000000000	–2.440740000	–0.069731000
C	0.000000000	–2.078128000	–1.482645000
C	2.436998000	0.000000000	0.034641000
C	2.016102000	–1.265705000	–0.545624000
C	1.179906000	–1.254071000	–1.737122000
C	1.267648000	–2.018750000	0.516471000
C	1.258670000	–1.185905000	1.713254000
Zr	0.000000000	0.000000000	0.056229000

[Hf@C_{28}]

29

symmetry T_d

C	0.052547000	1.725710000	1.725710000
C	–2.322286000	0.530640000	0.530640000
C	–1.725710000	–0.052547000	1.725710000
C	–0.530640000	0.530640000	2.322286000
C	1.468633000	1.468633000	1.468633000

C	0.530640000	–0.530640000	2.322286000
C	1.725710000	0.052547000	1.725710000
C	–1.468633000	–1.468633000	1.468633000
C	1.725710000	1.725710000	0.052547000
C	0.530640000	2.322286000	–0.530640000
C	–0.052547000	1.725710000	–1.725710000
C	2.322286000	0.530640000	–0.530640000
C	1.725710000	–0.052547000	–1.725710000
C	0.530640000	0.530640000	–2.322286000
C	2.322286000	–0.530640000	0.530640000
C	–1.725710000	0.052547000	–1.725710000
C	–1.468633000	1.468633000	–1.468633000
C	–2.322286000	–0.530640000	–0.530640000
C	–0.530640000	–0.530640000	–2.322286000
C	–1.725710000	1.725710000	–0.052547000
C	–0.530640000	2.322286000	0.530640000
C	0.052547000	–1.725710000	–1.725710000
C	1.468633000	–1.468633000	–1.468633000
C	–0.052547000	–1.725710000	1.725710000
C	0.530640000	–2.322286000	0.530640000
C	1.725710000	–1.725710000	–0.052547000
C	–0.530640000	–2.322286000	–0.530640000
C	–1.725710000	–1.725710000	0.052547000
Hf	0.000000000	0.000000000	0.000000000

$[V@C_{28}]^+$

29

symmetry C_{3v}

C	1.174706000	2.108405000	–0.121545000
C	1.991061000	–0.284050000	1.248310000
C	2.413286000	–0.036877000	–0.121545000
C	1.996670000	1.152778000	–0.826469000
C	0.000000000	2.367138000	–0.922406000
C	1.254512000	0.724293000	–2.031961000
C	0.000000000	1.440521000	–2.045654000
C	2.050001000	–1.183569000	–0.922406000
C	–1.174706000	2.108405000	–0.121545000
C	–0.749536000	1.866335000	1.248310000
C	–1.211076000	0.699215000	2.004377000
C	–1.996670000	1.152778000	–0.826469000
C	–2.413286000	–0.036877000	–0.121545000
C	–1.991061000	–0.284050000	1.248310000
C	–1.254512000	0.724293000	–2.031961000
C	0.000000000	–1.398430000	2.004377000
C	0.000000000	0.000000000	2.530408000
C	1.241525000	–1.582284000	1.248310000
C	–1.241525000	–1.582284000	1.248310000
C	1.211076000	0.699215000	2.004377000
C	0.749536000	1.866335000	1.248310000
C	–1.238579000	–2.071528000	–0.121545000
C	–2.050001000	–1.183569000	–0.922406000
C	1.247528000	–0.720260000	–2.045654000
C	0.000000000	–1.448586000	–2.031961000
C	–1.247528000	–0.720260000	–2.045654000
C	0.000000000	–2.305556000	–0.826469000
C	1.238579000	–2.071528000	–0.121545000
V	0.000000000	0.000000000	0.567481000

$[Nb@C_{28}]^+$

29

symmetry C_{2v}

C	0.000000000	2.471755000	–0.183196000
C	0.000000000	0.768666000	2.313883000
C	1.264600000	1.213547000	1.664881000
C	1.249234000	2.002799000	0.429609000
C	0.000000000	2.080373000	–1.561391000
C	1.984063000	1.249175000	–0.620459000
C	1.173456000	1.244296000	–1.821153000
C	2.039919000	0.000000000	1.370435000
C	–1.173456000	1.244296000	–1.821153000
C	–1.984063000	1.249175000	–0.620459000
C	–2.415370000	0.000000000	–0.045854000
C	–0.754108000	0.000000000	–2.408036000
C	–1.173456000	–1.244296000	–1.821153000
C	–1.984063000	–1.249175000	–0.620459000
C	0.754108000	0.000000000	–2.408036000
C	–1.264600000	–1.213547000	1.664881000
C	–2.039919000	0.000000000	1.370435000
C	0.000000000	–0.768666000	2.313883000
C	–1.249234000	–2.002799000	0.429609000
C	–1.264600000	1.213547000	1.664881000
C	–1.249234000	2.002799000	0.429609000
C	0.000000000	–2.471755000	–0.183196000
C	0.000000000	–2.080373000	–1.561391000
C	2.415370000	0.000000000	–0.045854000
C	1.984063000	–1.249175000	–0.620459000
C	1.173456000	–1.244296000	–1.821153000
C	1.249234000	–2.002799000	0.429609000
C	1.264600000	–1.213547000	1.664881000
Nb	0.000000000	0.000000000	0.353679000

$[Ta@C_{28}]^{+}$

29

symmetry C_{3v}

C	–1.178949000	2.128886000	–0.164796000
C	–2.017964000	–0.295975000	1.222279000
C	–1.211044000	0.699196000	1.943244000
C	–0.752660000	1.895596000	1.222279000
C	0.000000000	2.383466000	–0.966293000
C	0.752660000	1.895596000	1.222279000
C	1.178949000	2.128886000	–0.164796000
C	0.000000000	0.000000000	2.448880000
C	0.000000000	1.437161000	–2.087952000
C	–1.253792000	0.723877000	–2.078939000
C	–1.244618000	–0.718580000	–2.087952000
C	1.253792000	0.723877000	–2.078939000
C	1.244618000	–0.718580000	–2.087952000
C	0.000000000	–1.447754000	–2.078939000
C	1.999795000	1.154582000	–0.859589000
C	–1.254195000	–2.085443000	–0.164796000
C	–2.064142000	–1.191733000	–0.966293000
C	–1.265304000	–1.599621000	1.222279000
C	0.000000000	–2.309165000	–0.859589000
C	–2.433144000	–0.043443000	–0.164796000
C	–1.999795000	1.154582000	–0.859589000
C	1.254195000	–2.085443000	–0.164796000
C	2.064142000	–1.191733000	–0.966293000
C	1.211044000	0.699196000	1.943244000
C	2.017964000	–0.295975000	1.222279000
C	2.433144000	–0.043443000	–0.164796000
C	1.265304000	–1.599621000	1.222279000
C	0.000000000	–1.398393000	1.943244000
Ta	0.000000000	0.000000000	0.275738000

PBE-D3(BJ)/def2-SVP

Doublet

[V@C28]$^-$ - CF_3

33

Isomer: 1

C	1.19334400	2.06587600	–0.05544400
C	2.02252800	–0.31946800	1.23100000
C	2.47783600	–0.05857500	–0.13539600
C	2.01682200	1.14070100	–0.80620000
C	-0.00827300	2.30022200	-0.83121600
C	1.26451500	0.74050700	-2.02825000
C	-0.00826600	1.43742600	-2.01150700
C	2.09016500	-1.18471000	-0.94949800
C	-1.16626800	2.07145200	-0.02730500
C	-0.73674900	1.83218600	1.34142900
C	-1.18482100	0.64811200	2.10883800
C	-2.19349900	1.26779200	-0.83257700
C	-2.37692800	-0.04174600	-0.05740200
C	-1.97001900	-0.32050000	1.31076500
C	-1.26196500	0.75123400	-2.03729700
C	0.05640200	-1.44408200	1.99431700
C	0.05237000	-0.06717400	2.56512100
C	1.28292500	-1.61043800	1.21265000
C	-1.20496000	-1.62257900	1.26908600
C	1.24908200	0.63764900	2.02396800
C	0.77387500	1.83140600	1.31824400
C	-1.17824600	-2.07363500	-0.11429500
C	-1.97868500	-1.13903900	-0.88011400
C	1.27395100	-0.70106400	-2.07747100
C	0.02516000	-1.42272600	-2.05900300
C	-1.21999600	-0.67759600	-2.04158000
C	0.04552900	-2.30009300	-0.85508800
C	1.30491400	-2.10580400	-0.16448200
V	-0.07512400	0.03382600	0.60973400
C	-3.48118700	2.01100900	-1.23432400
F	-3.17519300	3.10660400	-1.94548200
F	-4.26283900	1.20796600	-1.97160100
F	-4.14980900	2.37880700	-0.12561400

[V@C28]$^-$ - CF_3

33

Isomer: 2

C	1.17797900	2.05844300	-0.11743300
C	1.98429100	-0.30773400	1.22323500
C	2.43811100	-0.09627400	-0.15474600
C	1.95637700	1.09280700	-0.83371200
C	-0.00068300	2.51038900	-0.98951500
C	1.20937900	0.67607800	-2.05364400
C	-0.01846500	1.40607900	-2.08361600
C	2.04150000	-1.23250900	-0.94361900
C	-1.16176500	2.06825800	-0.08925800
C	-0.73104600	1.89596900	1.29622800
C	-1.19115700	0.70034500	2.04350900
C	-1.96515600	1.10917000	-0.78648100
C	-2.44040300	-0.07588800	-0.09601400
C	-1.95538400	-0.29127300	1.27070200
C	-1.25129800	0.68635500	-2.02401200
C	0.01873000	-1.40056800	1.98360000
C	0.03106600	-0.00740000	2.52489500
C	1.24282800	-1.60408200	1.23158100
C	-1.22479400	-1.59377300	1.26130300
C	1.24720900	0.69012600	2.01410400
C	0.77928800	1.88963000	1.27801800
C	-1.25691600	-2.12040300	-0.09569500
C	-2.07245300	-1.21532500	-0.89410900
C	1.21575600	-0.77349400	-2.06788200
C	-0.03009500	-1.49856600	-2.03892500
C	-1.27016800	-0.76310600	-2.03795800
C	-0.01877800	-2.34284100	-0.80499700
C	1.23789500	-2.13084000	-0.12572500
V	0.00794100	0.15749500	0.55541900
C	-0.00012300	3.97871500	-1.45130100
F	0.01615000	4.78673700	-0.37389400
F	1.08636700	4.22311000	-2.19854000
F	-1.10218400	4.23217200	-2.17227400

[V@C28]$^-$ - CF_3

33

Isomer: 3

C	1.15574000	2.28391700	-0.14972800
C	2.10184800	-0.19891400	1.36812300
C	2.47686600	0.08222500	-0.03090800
C	1.98017400	1.24341900	-0.76003800
C	-0.02340000	2.44713700	-0.96884500
C	1.25334100	0.76687800	-1.96152800
C	-0.00288600	1.47077800	-2.06016200
C	2.07701100	-1.10213600	-0.80639500
C	-1.21869800	2.16160200	-0.17234200
C	-0.76755300	1.91514900	1.17636000
C	-1.17255800	0.72605200	1.87590900

C	-2.00963400	1.15089900	-0.84500400
C	-2.41953100	-0.05818200	-0.16181400
C	-1.91805000	-0.28950700	1.16707900
C	-1.23723600	0.71204400	-2.04434600
C	0.04674700	-1.34197000	2.01007400
C	0.00687500	0.07411000	2.40796700
C	1.39101600	-1.57006500	1.41210300
C	-1.18005300	-1.54835600	1.23697000
C	1.19797700	0.80891200	1.95488800
C	0.71430300	1.96273900	1.20558300
C	-1.34863100	-2.32501000	-0.07603900
C	-2.08196400	-1.23731300	-0.94632400
C	1.28529000	-0.67045700	-1.94041500
C	0.04035900	-1.40215600	-1.87376500
C	-1.22735000	-0.73556000	-2.01298600
C	0.05799400	-2.25163200	-0.68539500
C	1.33353500	-2.07304200	0.01200500
V	0.42375000	-0.28691400	0.31977700
C	-1.99702400	-3.71830400	0.01613000
F	-3.22080000	-3.62045500	0.55426100
F	-2.08786500	-4.26408000	-1.20479100
F	-1.23532300	-4.50941500	0.79620700

$[V@C28]^-$ - CF_3

33

Isomer: 4

C	1.24167700	2.06150100	-0.09637600
C	1.94881100	-0.36046800	1.27577100
C	2.42185400	-0.11659000	-0.09149700
C	2.03095500	1.07394800	-0.80000900
C	0.10134400	2.32528100	-0.93125000
C	1.34270400	0.69164800	-2.07275600
C	0.11106400	1.44471500	-2.11092500
C	2.03956100	-1.23403100	-0.93078900
C	-1.10033000	2.11266700	-0.14868100
C	-0.73058400	1.85282200	1.23668900
C	-1.38068500	0.79150800	2.17059900
C	-1.92001500	1.20597600	-0.91090100
C	-2.37954800	0.03784200	-0.20424700
C	-2.01387200	-0.22893700	1.18077600
C	-1.16495800	0.77337600	-2.13667700
C	-0.09206300	-1.40470900	1.96273900
C	-0.07529100	-0.02204600	2.50488100
C	1.16612000	-1.63010300	1.24170200
C	-1.30923300	-1.53228900	1.17236600
C	1.16497800	0.63415300	2.01777500
C	0.75033400	1.80900400	1.26210100
C	-1.28187600	-2.03231400	-0.20581700
C	-2.01044100	-1.10024600	-1.02282200
C	1.31197400	-0.75387800	-2.11844300
C	0.03391400	-1.43153500	-2.12946200
C	-1.19133300	-0.66816100	-2.16728500
C	-0.02838600	-2.26683200	-0.88919200
C	1.19347900	-2.10902200	-0.14467800
V	0.01987700	-0.02562500	0.49411000
C	-2.24418100	1.29203900	3.33947700
F	-3.30654700	1.95921700	2.85816100
F	-2.67005100	0.24782600	4.06935900
F	-1.52161500	2.11254700	4.11976000

$[V@C28]^-$ - CF_3

33

Isomer: 5

C	1.07500300	2.16102500	-0.12499600
C	1.99031000	-0.21813300	1.20223100
C	2.37868500	0.01910200	-0.19113900
C	1.87341100	1.18136300	-0.88244600
C	-0.11878500	2.36321900	-0.88624600
C	1.15934100	0.77563900	-2.06736800
C	-0.11355700	1.44418600	-2.03194700
C	2.06398800	-1.14030500	-0.98241900
C	-1.27501100	2.10177600	-0.04826200
C	-0.80269100	1.88021100	1.31871300
C	-1.20719100	0.69486800	2.10000800
C	-2.08520600	1.12435000	-0.74019300
C	-2.45685300	-0.06754400	-0.01093700
C	-1.99481100	-0.30798800	1.35635500
C	-1.35586700	0.70558600	-1.98515000
C	0.06073600	-1.37539100	2.03406500
C	0.04262300	0.02209900	2.57224200
C	1.28098100	-1.52017100	1.22465000
C	-1.20505500	-1.58731400	1.31968600
C	1.21859500	0.74991500	1.99749500
C	0.69977400	1.90908700	1.25952100
C	-1.23316000	-2.07574000	-0.05211200
C	-2.06145900	-1.20269800	-0.82491100
C	1.31248700	-0.75342800	-2.28857100
C	-0.05171400	-1.44739500	-2.02913700
C	-1.30319900	-0.73946700	-1.99440300
C	0.01182900	-2.23566000	-0.82365900

C	1.27218700	-2.01191900	-0.15618100
V	-0.05215600	0.04016500	0.62187000
C	1.99521900	-1.14780500	-3.61687500
F	3.19877200	-0.55908600	-3.70780500
F	2.15368100	-2.47989400	-3.67518700
F	1.23281700	-0.75040000	-4.64924800

$[V@C28]^-$ - CF_3

33

Isomer: 6

C	1.14531200	2.11215600	-0.14586700
C	1.97151900	-0.25346900	1.23253400
C	2.40260300	-0.00078100	-0.14586100
C	1.96092400	1.16688900	-0.86328600
C	-0.03076500	2.33157800	-0.95800600
C	1.24370600	0.74017000	-2.11317300
C	-0.01902500	1.43985800	-2.12918500
C	2.03458800	-1.13914600	-0.95800600
C	-1.20062500	2.08110600	-0.14586100
C	-0.76624900	1.83412000	1.23253400
C	-1.20948600	0.67719600	2.01085700
C	-1.99101800	1.11476600	-0.86328600
C	-2.40183700	-0.06420900	-0.14586700
C	-1.96417500	-0.30535700	1.23253100
C	-1.26285900	0.70699600	-2.11317300
C	0.01827400	-1.38604400	2.01085700
C	0.00000000	0.00000000	2.76055100
C	1.24653400	-1.54834700	1.23253100
C	-1.20527000	-1.58065100	1.23253400
C	1.19121200	0.70884800	2.01085700
C	0.71764100	1.85370400	1.23253100
C	-1.20197800	-2.08032500	-0.14586100
C	-2.00382300	-1.19243200	-0.95800600
C	1.25646600	-0.70345300	-2.12918500
C	0.01915300	-1.44716600	-2.11317300
C	-1.23744100	-0.73640500	-2.12918500
C	0.03009300	-2.28165500	-0.86328600
C	1.25652500	-2.04794700	-0.14586700
V	0.00000000	0.00000000	0.49136500
C	0.00000000	0.00000000	4.29775400
F	-0.01645100	1.26496700	4.74870500
F	-1.08726800	-0.64673000	4.74870500
F	1.10371900	-0.61823700	4.74870500

$[V@C28]^-$ - CF_3

33

Isomer: 7

C	1.18010200	2.06149500	-0.15161600
C	1.99363700	-0.30465400	1.22918600
C	2.37426800	-0.05005500	-0.16570600
C	2.03577500	1.15672700	-0.87293900
C	-0.02037700	2.29343500	-0.92640000
C	1.31089900	0.75589300	-2.23991500
C	-0.07372100	1.41948800	-2.05091700
C	1.94991900	-1.19049000	-0.94965700
C	-1.20083400	2.09244800	-0.08172300
C	-0.72862400	1.86589500	1.27392800
C	-1.18894900	0.70340200	2.04664100
C	-2.04442500	1.14605600	-0.76494300
C	-2.46509900	-0.04625400	-0.04668000
C	-1.99829400	-0.27701000	1.31245100
C	-1.32182100	0.70781000	-1.98696700
C	0.00212800	-1.40269500	2.03260400
C	0.02769400	-0.00181500	2.55395700
C	1.23115900	-1.59941300	1.25081500
C	-1.25934600	-1.58362900	1.30372900
C	1.23914000	0.68695500	2.00799100
C	0.77374400	1.85235100	1.24357000
C	-1.30996300	-2.08880400	-0.06032300
C	-2.13743300	-1.20353800	-0.85096200
C	1.16707700	-0.77448400	-2.06556700
C	-0.08565800	-1.47798500	-2.00156600
C	-1.33731600	-0.74341600	-1.99230200
C	-0.07550700	-2.33540500	-0.78820100
C	1.17416300	-2.10706700	-0.10976100
V	0.01605700	0.00465500	0.58949300
C	2.06634300	1.19169800	-3.51880900
F	2.20532900	2.52674000	-3.53386900
F	3.28205000	0.62327700	-3.54655700
F	1.37571800	0.80831700	-4.60380500

PBE-D3(BJ)/def2-SVP

Singlet

$[V@C28]^-$ - $[CF_3]_2$

37

Isomer: 1

C	1.709287553	2.159468603	-1.178224617
C	-0.231606712	0.170252799	-1.875268833
C	-0.654226807	1.317312872	-1.157533496
C	0.328506237	2.269591579	-0.751106017
C	2.576935100	2.183741434	0.000924858
C	0.328489154	2.268981797	0.753133787
C	1.709295908	2.158498129	1.180097037
C	-1.571639882	0.874936536	0.000400006
C	3.441133026	1.026530043	0.000413649
C	3.167698442	0.278222525	-1.222040060
C	2.826737571	-1.138542939	-1.232905005
C	3.167713592	0.277193223	1.222256869
C	2.826777693	-1.139583544	1.231905559
C	2.630469518	-1.919786822	-0.000839524
C	2.104216153	1.010781463	1.955863587
C	0.535089445	-1.989423225	-1.242593944
C	1.574431477	-1.269854256	-1.995689953
C	-0.598493822	-1.060161972	-1.186028458
C	1.191380038	-2.482631180	-0.001092901
C	1.127357200	0.051812286	-2.372888100
C	2.104175348	1.012438698	-1.955032741
C	0.535129969	-1.990405510	1.240854555
C	1.574480225	-1.271497484	1.994577268
C	-0.654341189	1.316407995	1.158780714
C	-0.231604947	0.168742021	1.875496925
C	1.127407456	0.049828270	2.372967159
C	-0.598359014	-1.061050593	1.185085506
C	-1.526821585	-0.773651804	-0.000287345
V	1.193218998	-0.540260851	-0.000296873
C	-2.817123727	-1.622532308	0.000129648
F	-3.554346456	-1.401517631	-1.092979232
F	-2.426556002	-2.920991262	-0.002929117
F	-3.550280893	-1.405668026	1.096853111
C	-2.944376636	1.588307606	-0.000127688
F	-2.723023106	2.918044766	0.002919128
F	-3.648431789	1.276344361	-1.096554248
F	-3.652110376	1.271836904	1.092630076

$[V@C28]^-$ - $[CF_3]_2$

37

Isomer: 2

C	1.15846800	2.14427700	-0.04993900
C	2.02927000	-0.29842600	1.31858800
C	2.34982200	0.00988000	-0.06695600
C	2.15916200	1.31020700	-0.86176100
C	-0.01785700	2.37564100	-0.81015300
C	1.19693900	0.78494800	-2.03465900
C	-0.04300500	1.47550400	-1.97873700
C	1.85772900	-1.07369200	-0.84930700
C	-1.19366400	2.13913700	-0.00086800
C	-0.72457500	1.84868500	1.34731100
C	-1.16285800	0.66821400	2.07879500
C	-1.98426800	1.15058600	-0.70008400
C	-2.44963100	-0.02971200	-0.00617000
C	-1.96692600	-0.29681700	1.34204500
C	-1.30196200	0.75857700	-1.95471600
C	0.02595400	-1.43087500	2.09371200
C	0.04068900	-0.02998900	2.61442500
C	1.26615200	-1.61627200	1.31535400
C	-1.21647400	-1.58934100	1.30700300
C	1.24947500	0.68205800	2.09894000
C	0.77007500	1.84139200	1.31543600
C	-1.28303000	-2.07206000	-0.06021600
C	-2.06770400	-1.16426200	-0.81877900
C	1.13247800	-0.65087600	-2.02972300
C	-0.08071600	-1.42149800	-2.03999100
C	-1.29700400	-0.69009700	-1.98398600
C	-0.05974900	-2.52174100	-0.87106800
C	1.16125100	-2.04270100	-0.07195500
V	0.12768700	-0.07540500	0.65377300
C	-0.03760400	-3.99574100	-1.31372000
F	1.07226400	-4.24041700	-2.02894300
F	-0.04198500	-4.78982300	-0.22674800
F	-1.11539500	-4.26919300	-2.06236800
C	3.44944600	2.02641700	-1.29911400
F	3.15159000	3.10003800	-2.04442700
F	4.13371900	2.42152800	-0.20926800
F	4.21564800	1.18830200	-2.01584900

$[V@C28]^-$ - $[CF_3]_2$

37

Isomer: 3

C	1.20832700	2.19827300	-0.16214900
C	2.00953200	-0.21697900	1.24860900
C	2.40986700	0.04391500	-0.12210300

C	2.00339100	1.20964000	-0.85388900
C	0.00938700	2.40801200	-0.94932900
C	1.25300800	0.74869600	-2.06869100
C	0.00282000	1.45497600	-2.08009400
C	1.98138000	-1.12374800	-0.89205400
C	-1.14559600	2.18073000	-0.13566400
C	-0.70981400	1.90027700	1.22756000
C	-1.17937800	0.76167300	2.02673300
C	-1.91068900	1.12230600	-0.79139800
C	-2.36761600	-0.00824000	-0.06764000
C	-1.97832200	-0.25442400	1.31443700
C	-1.23100800	0.70889600	-2.03710700
C	0.03440800	-1.35139800	2.08125200
C	0.03438100	0.07549800	2.54655400
C	1.26420500	-1.52383800	1.28004500
C	-1.21552500	-1.56175300	1.31305600
C	1.22497300	0.77037800	1.97516900
C	0.78167800	1.92684500	1.21554500
C	-1.17766200	-2.01834500	-0.05244600
C	-2.17729700	-1.26199300	-0.92699200
C	1.22252300	-0.69880500	-2.05381900
C	-0.01182000	-1.44692900	-2.02252500
C	-1.22569300	-0.73609100	-2.02457000
C	0.02417500	-2.52131500	-0.84593200
C	1.25909400	-2.03204200	-0.08186400
V	-0.06204400	-0.07061300	0.58863200
C	-3.48579200	-1.95529600	-1.35690200
F	-4.30490000	-1.04270300	-1.91209600
F	-3.25372800	-2.92659500	-2.24586600
F	-4.08800200	-2.47958700	-0.27304800
C	0.06665800	-4.01199000	-1.23536800
F	1.17061300	-4.25540700	-1.96225000
F	0.10759100	-4.75690400	-0.11402500
F	-1.01250800	-4.35611600	-1.94865600

$[V@C28]^{-}$ - $[CF_3]_2$

37

Isomer: 4

C	1.20617700	2.07642000	-0.11280900
C	1.99313600	-0.28570100	1.19924500
C	2.47592100	-0.06046200	-0.15169400
C	2.00666900	1.13395600	-0.82312000
C	0.02620200	2.54201300	-0.97763800
C	1.26010600	0.71497900	-2.05014000
C	0.02671100	1.43043400	-2.05955900
C	2.06458500	-1.19970300	-0.94429200
C	-1.15674600	2.12710800	-0.07749000
C	-0.73132900	1.89685100	1.32222600
C	-1.20986800	0.70823200	2.09014700
C	-1.88151100	1.08873800	-0.73434000
C	-2.42072400	-0.05304600	-0.07066900
C	-2.00562300	-0.30122800	1.32907600
C	-1.19022500	0.68403300	-1.98902100
C	0.03495900	-1.39527900	1.96898200
C	0.03068200	-0.00969700	2.49987400
C	1.24177100	-1.58178000	1.20334100
C	-1.23226600	-1.58726100	1.26291800
C	1.23380300	0.67255200	1.96251800
C	0.76881900	1.86436600	1.25212900
C	-1.20275000	-2.07866300	-0.09976300
C	-2.19543500	-1.29002100	-0.96560700
C	1.25505900	-0.73390800	-2.07030600
C	0.00026100	-1.45809500	-2.04331700
C	-1.23347100	-0.74325000	-2.05271700
C	0.01095200	-2.30839300	-0.81229300
C	1.28246400	-2.11898700	-0.14521100
V	-0.22661300	0.13339900	0.52012700
C	-3.45273800	-2.04266700	-1.43066300
F	-4.23299800	-1.22422400	-2.15358200
F	-3.10644600	-3.10030200	-2.18032300
F	-4.14257500	-2.47134700	-0.35657200
C	0.05337600	4.00490600	-1.44961600
F	0.08556100	4.82156700	-0.37941000
F	1.14125400	4.22637100	-2.20322700
F	-1.04652600	4.27199400	-2.17085200