

Supporting Information

Low Temperature Non-Oxidative Coupling of Methane on Atomically Dispersed Titanium-Aluminum-Boron Nanopowder

Souvick Biswas¹, Avital Isakov², Nureshan Dias³, Matthew T. Finn⁴, Jack Cokas², Albert Epshteyn^{4*}, Anastassia N. Alexandrova^{2*}, Musahid Ahmed^{3*}, Ralf I. Kaiser^{1*}

¹ Department of Chemistry, University of Hawai'i at Manoa, Honolulu, Hawaii 96822, United States

² Department of Chemistry and Biochemistry, University of California, Los Angeles, Los Angeles, California 90095, United States

³ Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States

⁴ Chemistry Division, U.S. Naval Research Laboratory, Washington, D.C. 20375, United States

* Corresponding author. E-mail: albert.epshteyn@nrl.navy.mil

ana@chem.ucla.edu

mahmed@lbl.gov

ralfk@hawaii.edu

Contents	Pages
Experimental and computational methods	S3-S5
Figure S1. Schematic of catalytic microreactor-coupled molecular beam machine	S4
Figure S2. Mass spectra at 13 eV in the 300 K to 1500 K range with 100 K interval from the decomposition onset temperature of 800 K	S6
Figure S3. Comparison of mass spectra for the products with and without catalyst	S7
Figure S4. Photoionization efficiency curves for the major products at 1500 K	S8
Figure S5. Comparison of mass spectra ($m/z = 20 - 60$) at 800 K and 1500 K	S9
Figure S6. Mass spectra at 15.4 eV for representative temperatures	S10
Figure S7. Stack plot of branching ratios of major products at different temperatures	S11
Figure S8. Temperature-dependent individual branching ratios of closed-shell hydrocarbons and radicals at different temperatures	S12
Figure S9. Temperature-dependent individual branching ratios of C3 species	S13
Figure S10. Global and first local minima of the methane-TiAl ₂ B ₆ complexes	S13
Figure S11. Additional FES for the formation of ethylene (C ₂ H ₄) via the global minimum of the methane-TiAl ₂ B ₆ binding complex at 800 K	S14
Figure S12. Additional FES for the formation of ethylene (C ₂ H ₄), ethane (C ₂ H ₆) and acetylene (C ₂ H ₂) via the first local minimum at 800 K	S14
Figure S13. FES for the formation of acetylene (C ₂ H ₂) extended from Figure 4a	S15
Figure S14. FES for methyl desorption via the global minimum at 800 K	S15
Figure S15. FES for methyl desorption via the first local minimum at 800 K	S16
Table S1. Relative free energies for Figures 4a, S13, S14a	S17-S18
Table S2. Relative free energies for Figures 4b, 6a, S14b	S18-S19
Table S3. Relative free energies for Figure S11	S20
Table S4. Relative free energies for Figures 5a, S15a	S20-S21
Table S5. Relative free energies for Figures 5b, 6b, S15b	S21-S22
Table S6: Relative free energies for Figures S12, S15c	S23-S24
Data S1. Coordinates of the intermediates, transition states, reactants and products	S24-S46
References	S47

S1. Experimental methods:

S1.1. Synthesis of titanium aluminum boron nanopowder: The synthesis of titanium aluminum boron nanopowder has been reported previously.¹ First, in a dinitrogen (N₂) atmosphere glovebox, TiCl₄ (10 g, 52.7 mmol) was added to a standard 500 mL Schlenk flask and charged with 350 mL of Et₂O. Separately, in a custom 1 L pearshaped reactor with a built-in condenser and a side arm-equipped with a ChemGlass Teflon-valve (size 20), LiBH₄ (3.5 g, 160.6 mmol) and LiAlH₄ (2 g, 52.7 mmol) were dissolved in 250 mL of Et₂O. The reactor containing the LiBH₄/LiAlH₄ solution was connected to a Schlenk line and placed in a benchtop sonicator bath and the TiCl₄ solution was transferred by cannula into the sonicating solution of LiAlH₄ and LiBH₄. Immediately upon addition, a black precipitate was formed, releasing large amounts of heat and gas. This gas evolution acted to slow the rate of addition by cannula, ensuring that the reaction did not run away. The reaction was allowed to sonicate overnight (18h) with the solution reaching reflux temperatures, and the reactor was constantly purged with N₂. After stopping sonication and cooling to room temperature, the reaction vessel was brought into a N₂ glovebox and the reaction was gravity filtered through a fine porosity-fitted glass funnel. The raw products were processed by heating *in vacuo* at 100°C overnight. After cooling, the samples were washed with THF to remove leftover salts and dried at room temperature under a dynamic vacuum.²

S1.2. Details of the catalytic microreactor: The nascent gas phase products formed in the catalytic conversion of helium-seeded methane (2%) through the titanium-aluminum-boron nanopowder (Ti-Al-B NP) packing at distinct temperatures from 300 K to 1500 K through the chemical microreactor^{1, 3-6} are detected *in situ* by using single photon vacuum ultraviolet (VUV) photoionization (PI) mass spectrometry. The experiments were carried out at the Chemical Dynamics Beamline (9.0.2.) installed in Advanced Light Source (ALS).

Briefly, the microreactor was a resistively heated silicon carbide (SiC) tube of 20 mm length and 1 mm inner diameter, which was tightly packed with Ti-Al-B NP about a length of 10 mm inside the SiC tube. The packing was done in such a way that the interaction and residence time of the hydrocarbon with the nanoparticle surface is enough to trace the reactivity. A premixed gas with methane (CH₄, Matheson; Research Purity 99.9995%) in helium (He; Airgas; 99.999%) was prepared at 200 psi and the backing pressure was maintained at 300 Torr during experiments. The gas mixture was introduced into the silicon carbide tube where the temperature can reach up to

1,600 ± 50 K as monitored by type-C thermocouple. After exiting the reactor, the molecular beam containing the products, passed a skimmer and entered a detection chamber, which housed the Wiley-McLaren Reflectron Time-of-Flight Mass Spectrometer (Re-TOF-MS). The products were photoionized in the extraction region of the spectrometer by exploiting synchrotron quasi-continuous tunable vacuum ultraviolet (VUV) light from the Chemical Dynamics Beamline 9.0.2 and detected with a microchannel plate (MCP) detector. Compared to hard electron impact ionization, soft VUV-PI has the unique advantage of an ideally fragment-free ionization of the neutrals. Further, by tuning the VUV energy, structural isomers can be identified.

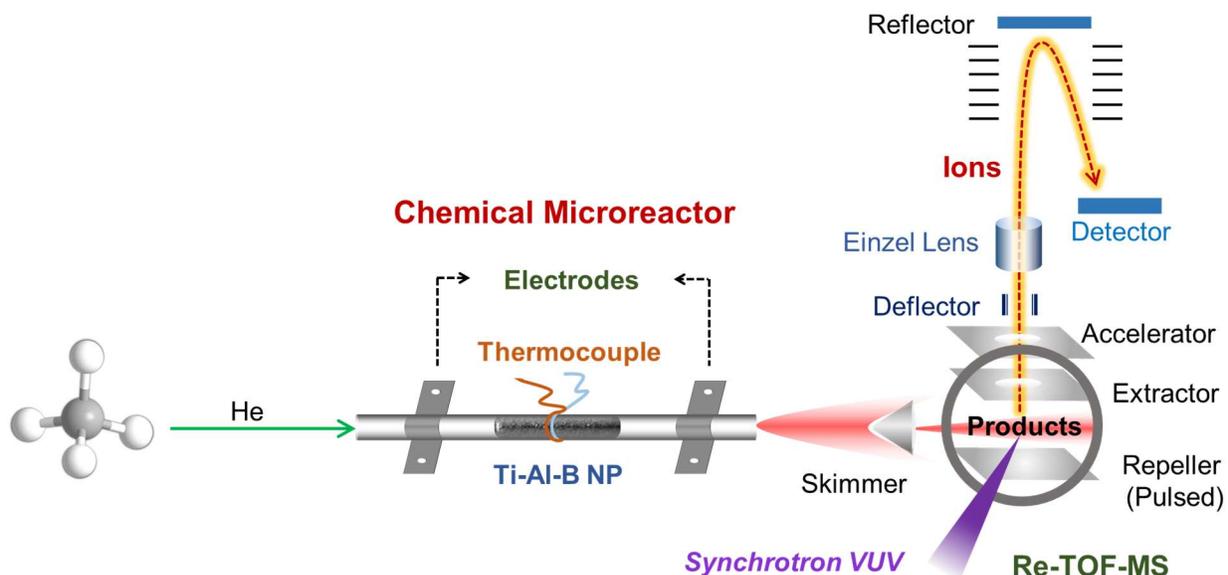


Figure S1: Schematic of the catalytic microreactor-coupled molecular beam machine.

Here, mass spectra were recorded at 13 eV and a set of additional mass spectra was also measured at 15.4 eV to determine hydrogen yields. The photoionization efficiency (PIE) curves, which report the intensity of a single mass-to-charge ratio (m/z) versus the photon energy, were extracted by integrating the signal collected at a specific m/z selected for the species of interest over the range of photon energies in 0.05 eV increments and normalized to the incident photon flux. The PIE curves were then fit with a linear combination of known PIE curves to isomer-selectively identify the products.

For each experimental run, the Ti-Al-B catalyst in the microreactor was warmed up to a well-defined temperature (the maximum being 1500 K) and upon equilibration of the temperature, mass spectra were recorded averaged over 5 million scans each which was equivalent to about 30 minutes of scan time. Upon completion of the data acquisition, it was cooled down to 293 K with pure helium flow through the reactor tube (without seeded methane). This process was repeated to acquire the next set of mass spectra, i.e. a total of five sets of heating – cooling cycles. The experimental approach mentioned via the repetitive heating-cooling-heating cycle of the catalyst packing not only ensures the reproducibility, but also carefully inspects the catalyst performance over time and a broad range of temperature.

S2. Computational methods: Calculations were carried out with Orca 5.4.0.⁷ Methane adsorption sites were randomly sampled on the lowest energy isomer of TiAl_2B_6 nanoparticle determined in previous work.¹ Boltzmann weighting was applied to these adsorbates at 800K. The two binding sites, 55% and 45% respectively, were then explored as starting points for mechanistic study. Geometry optimizations were carried out with a tight SCF convergence using the BLYP functional^{8, 9} with the def2-TZVP basis set¹⁰ and def2/J auxiliary basis set¹¹. Dispersion forces were corrected for using the D3BJ method.^{12, 13} All minima were confirmed by ensuring no negative vibrational frequencies were present. Potential Energy Surfaces (PES) for 0 K, 800 K, and 1500 K were constructed using the Nudged Elastic Band (NEB) method^{14, 15} and transition states were confirmed by checking that the single imaginary frequency vibrational mode aligned with mechanistic steps. As in previous work, only the vibrational entropy is considered when calculating the free energy of the TiAl_2B_6 particle and any adsorbed species to simulate the lack of translational and rotational entropy of the nanoparticle.¹ Vibrational entropy is calculated using the quasi-RRHO method as implemented in Orca 5.4.0.¹⁶ For gaseous species the entropy includes translational, rotational and vibrational terms. Translational entropy is calculated based upon the Sackur-Tetrode equation,¹⁷ rotational entropy, as computed by Herzberg,¹⁸ and vibrational entropy, as previously stated. When additional adsorption steps were required, random sampling of possible adsorption sites were performed and the mechanistic study continued from any found binding sites.

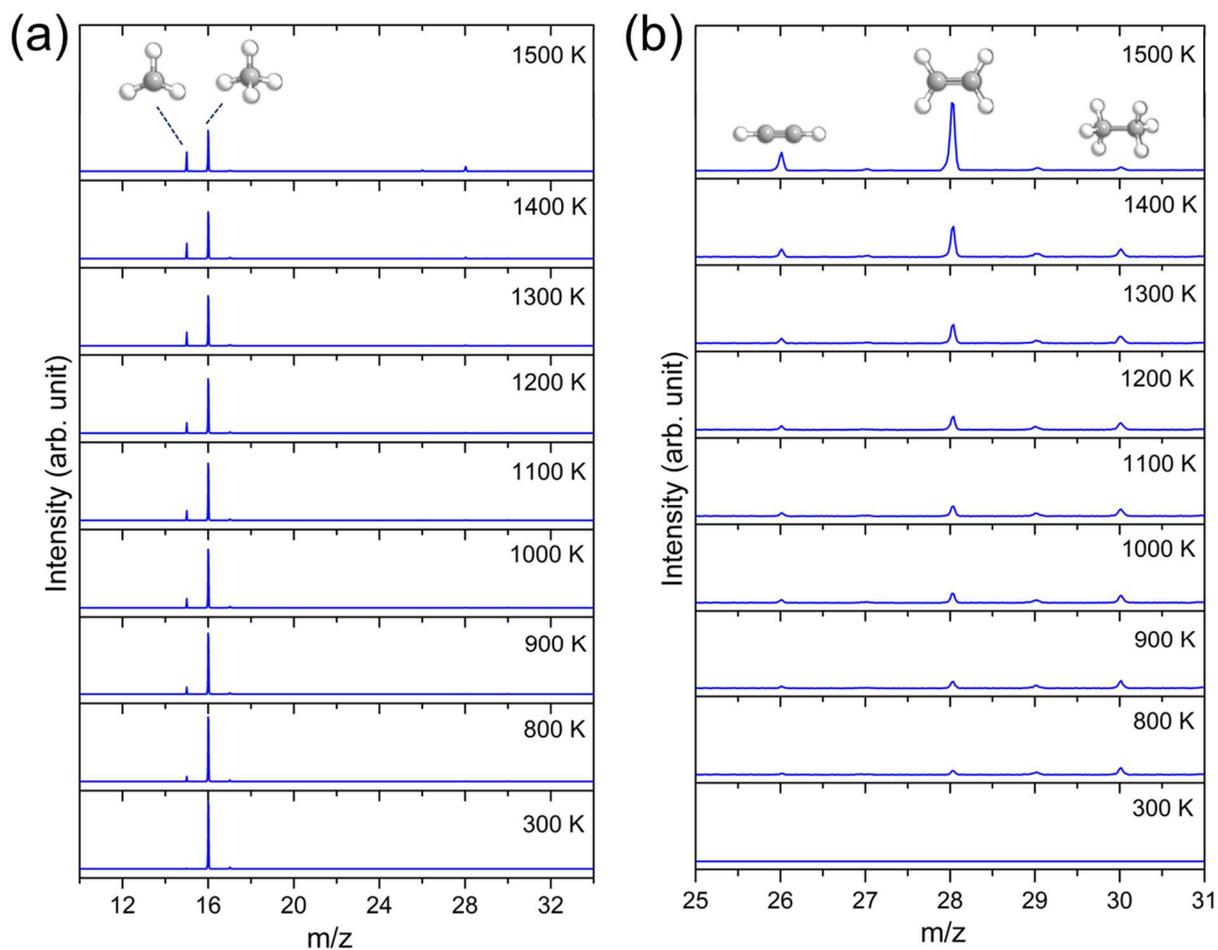


Figure S2: (a) Mass spectra recorded for the catalytic conversion of helium-seeded (2%) methane (CH₄) over titanium-aluminum-boron nanopowder (Ti-Al-B NP) in a high-temperature chemical microreactor at a photon energy of 13 eV in the 300 K to 1500 K range with 100 K interval from the decomposition onset temperature of 800 K. (b) The $m/z = 25$ to 31 segments in each spectrum are magnified forty times to locate two-carbon mass-growth products - further identified from the characteristic photoionization efficiency (PIE) curves (Figures 1b and S4).

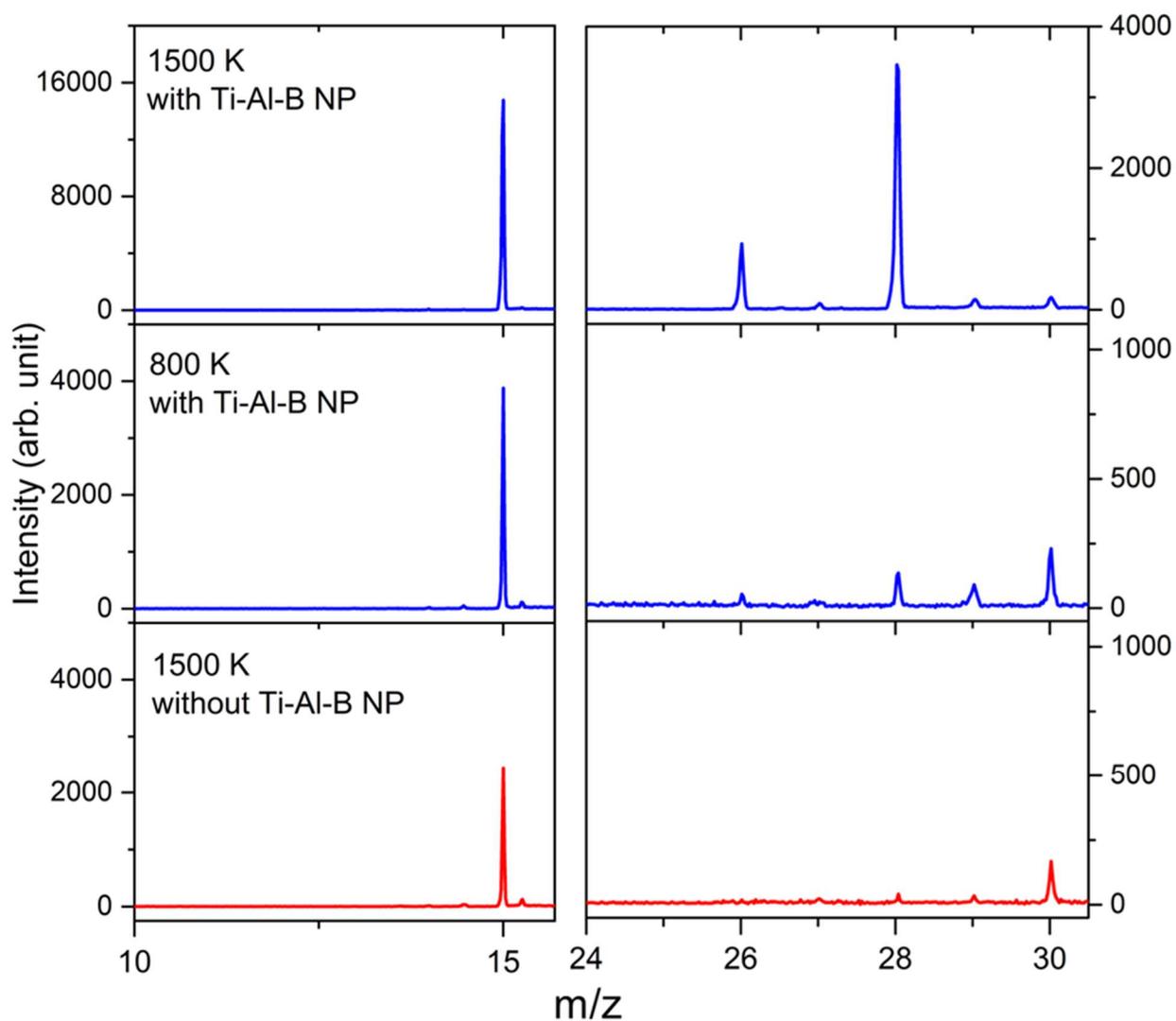


Figure S3: Comparison of mass spectra for the products formed upon decomposition of helium-seeded methane with titanium-aluminum-boron nanopowder (Ti-Al-B NP) [blue traces] and without any catalyst loading [red trace] in the microreactor recorded at a photon energy of 13 eV. The decomposition onset temperatures are 800 and 1500 K for Ti-Al-B NP loaded and blank microreactor, respectively, whereas the mass spectra at 1500 K with the packed catalyst is also displayed in the top most panel.

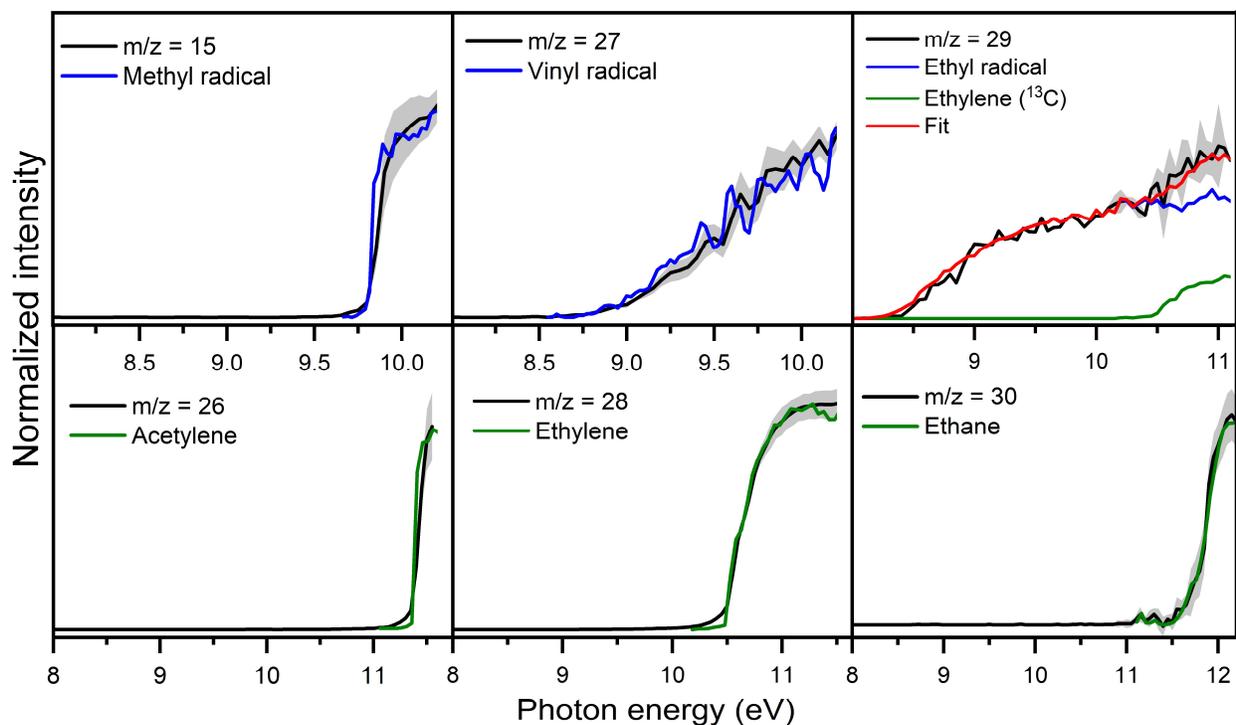


Figure S4: Experimental photoionization efficiency curves (PIE, black traces) for the major catalytically formed products (C1 and C2 species) at distinct mass-to-charge ratios at 1500 K. The experimental errors (gray shaded area) originate from the accuracy of the photocurrent measurement by the photodiode and a 1σ error of the PIE curves averaged over the individual scans. In case of multiple isomers, reference PIE curves are represented as blue and green traces; the overall fit is depicted in a red trace, whereas for a single species contributing to a mass peak, the reference trace is represented by the blue or green trace for radicals or closed-shell hydrocarbons, respectively.

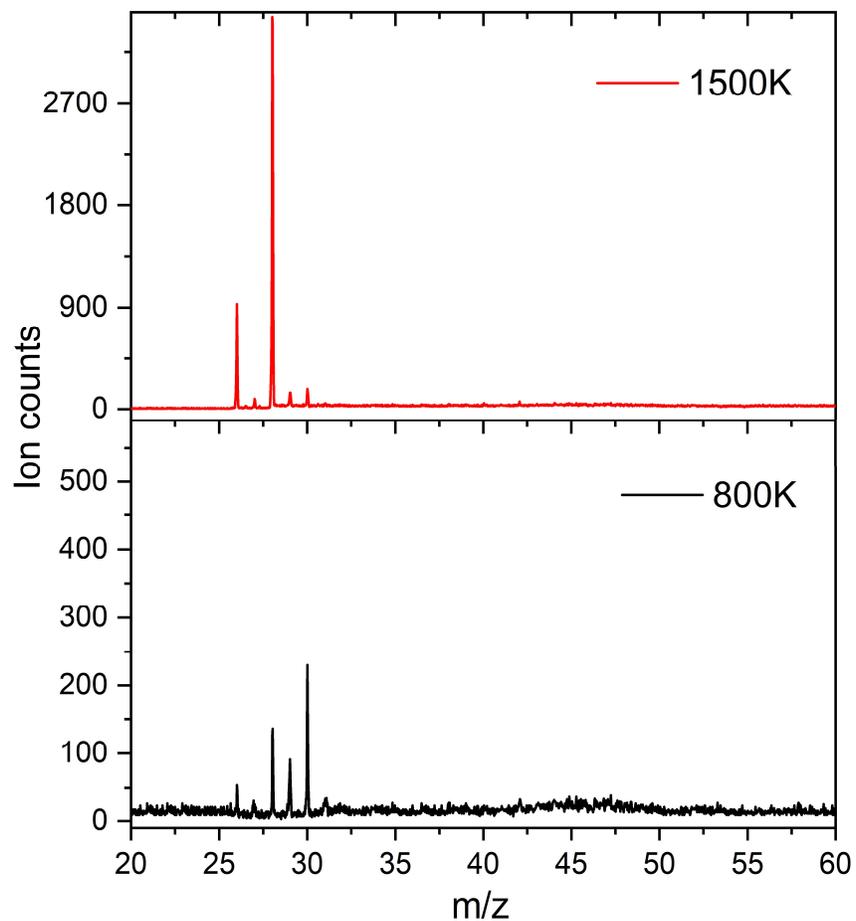


Figure S5: Comparison of mass spectra in the range $m/z = 20 - 60$ at 800 K (lower trace) and 1500 K (upper trace) for the catalytically formed products of helium-seeded methane over titanium-aluminum-boron nanopowder (Ti-Al-B NP) at a photon energy of 13 eV. Molecular mass growth beyond C2 species is negligible.

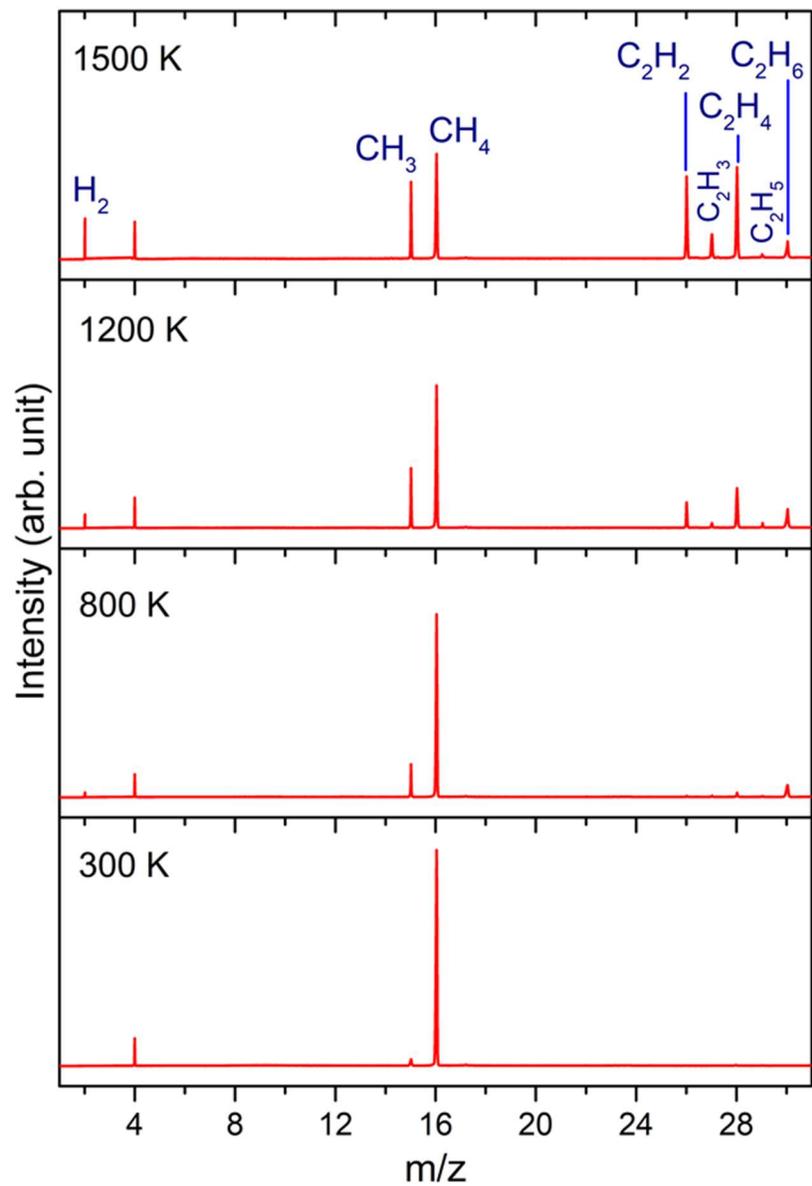


Figure S6: Mass spectra of the catalytically formed products of helium-seeded methane over titanium-aluminum-boron nanopowder (Ti-Al-B NP) recorded at a photon energy of 15.4 eV at selected temperatures.

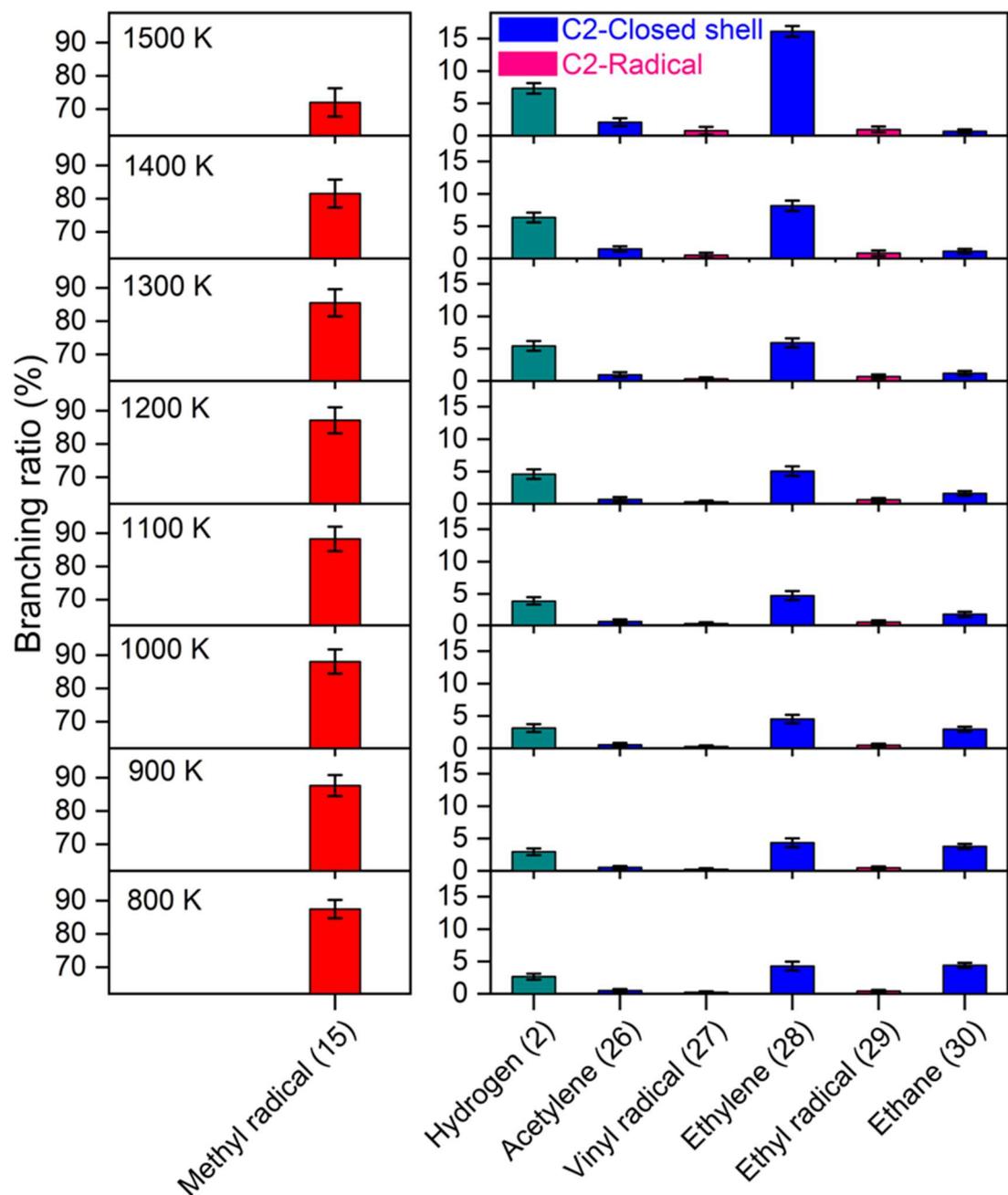


Figure S7: Stack plot of branching ratios of individual products up to C2 species at different temperatures including molecular hydrogen. The error bars are evolved due to the uncertainties determined by averaging the recorded photoionization efficiency curves and respective integral peak areas from mass spectra.

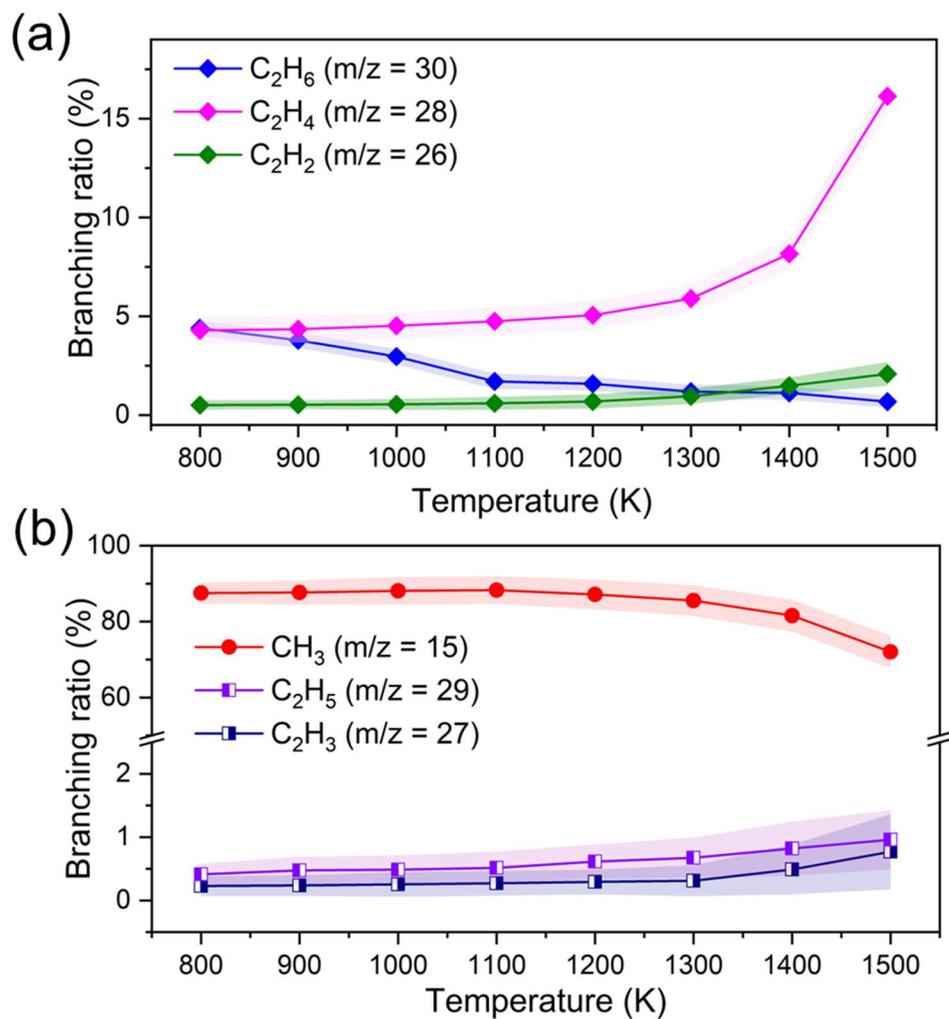


Figure S8: Temperature-dependent individual branching ratios of (a) closed-shell hydrocarbons and (b) radicals at different temperatures up to C2 species. The error bars are evolved due to the uncertainties determined by averaging the recorded photoionization efficiency curves and respective integral peak areas from mass spectra.

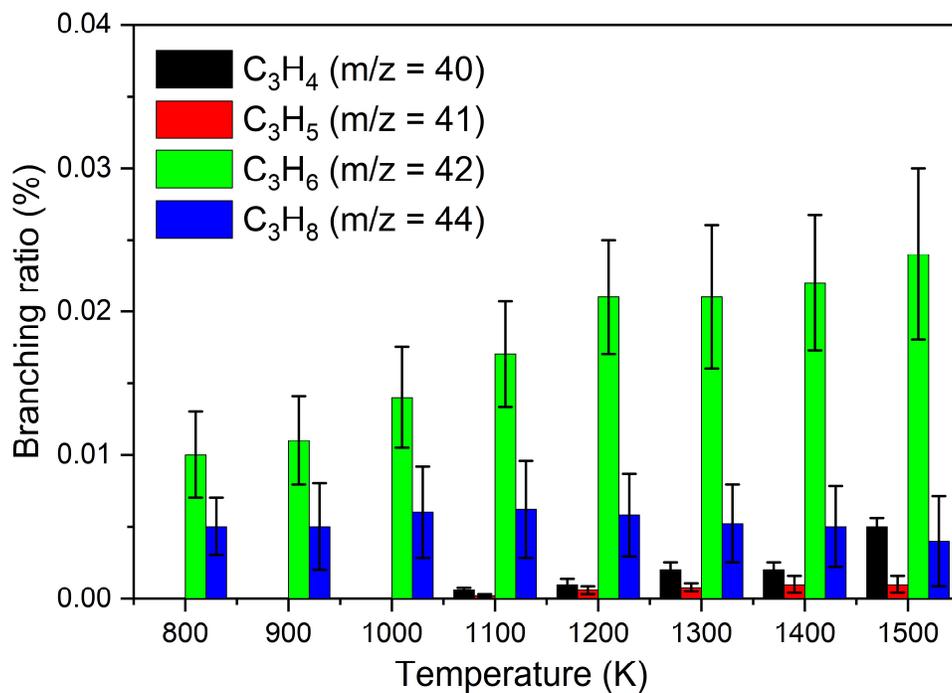


Figure S9: Temperature-dependent individual branching ratios of C₃ species. The error bars are evolved due to the uncertainties determined by averaging the photoionization efficiency curves (not shown) and respective integral peak areas from mass spectra.

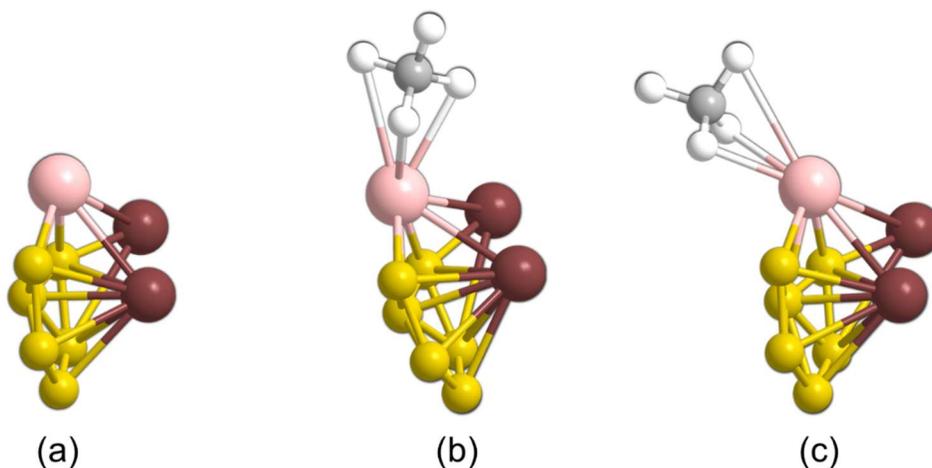


Figure S10: (a) Global minimum of the modeled TiAl₂B₆ cluster. (b) Global and (c) first local minima of the methane-TiAl₂B₆ binding complexes.

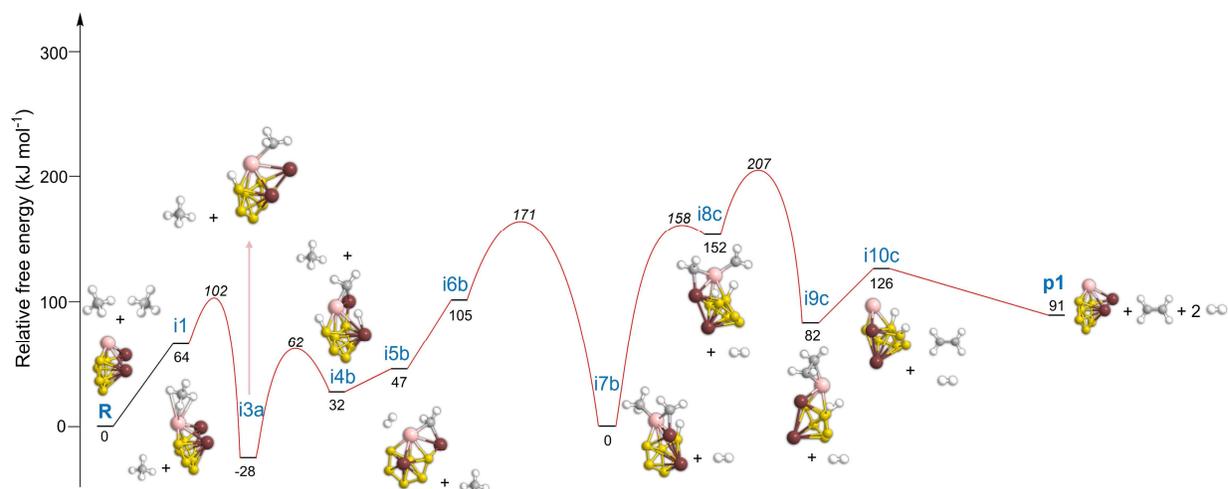


Figure S11: Additional free energy surface (FES) for the formation of ethylene (C_2H_4) via the global minimum (**i1**) of the methane- $TiAl_2B_6$ binding complex at 800 K. The second methane gets adsorbed while methylene (CH_2) group is attached on the Ti-center.

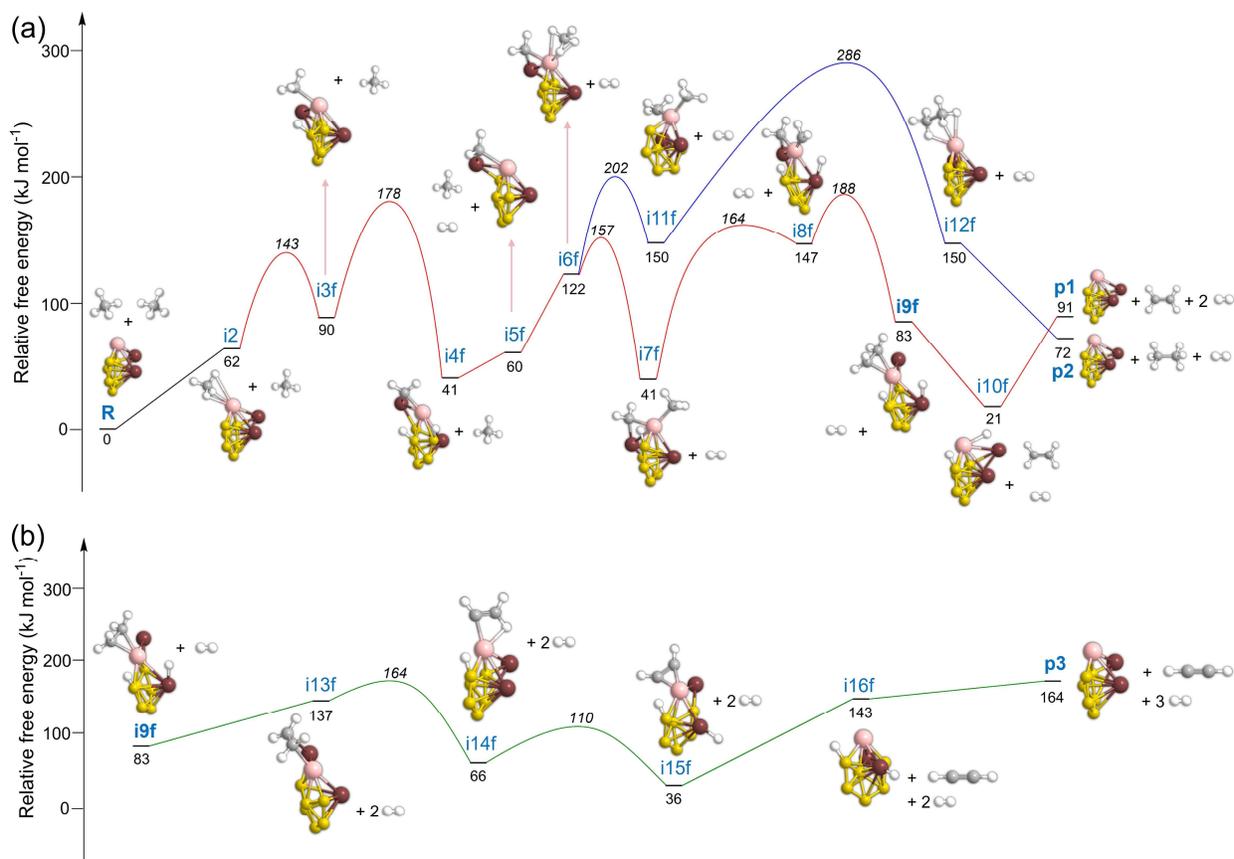


Figure S12: FES for the formation of (a) ethylene (C_2H_4) and ethane (C_2H_6); (b) acetylene (C_2H_2) via the first local minimum (**i2**) of the methane- $TiAl_2B_6$ binding complex at 800 K.

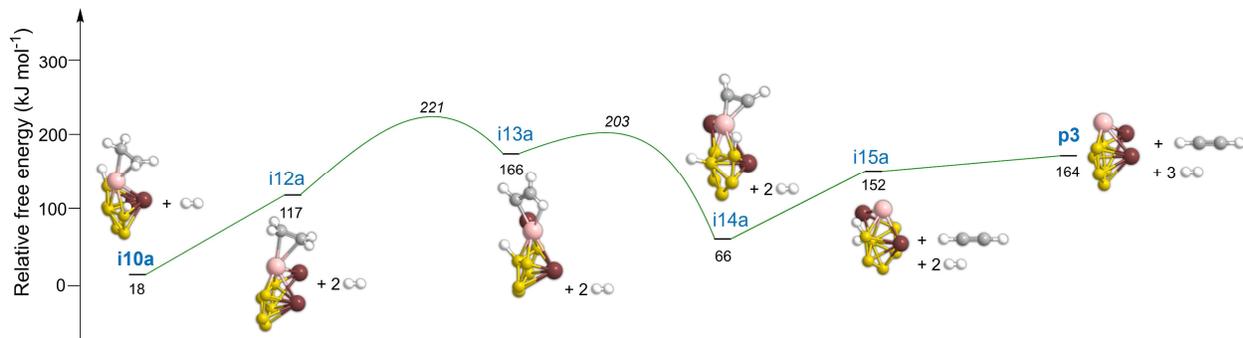


Figure S13: FES for the formation of acetylene (C_2H_2) via the global minimum (**i1**) of the methane- $TiAl_2B_6$ binding complex at 800 K, extended from the selected pathways in Figure 4a.

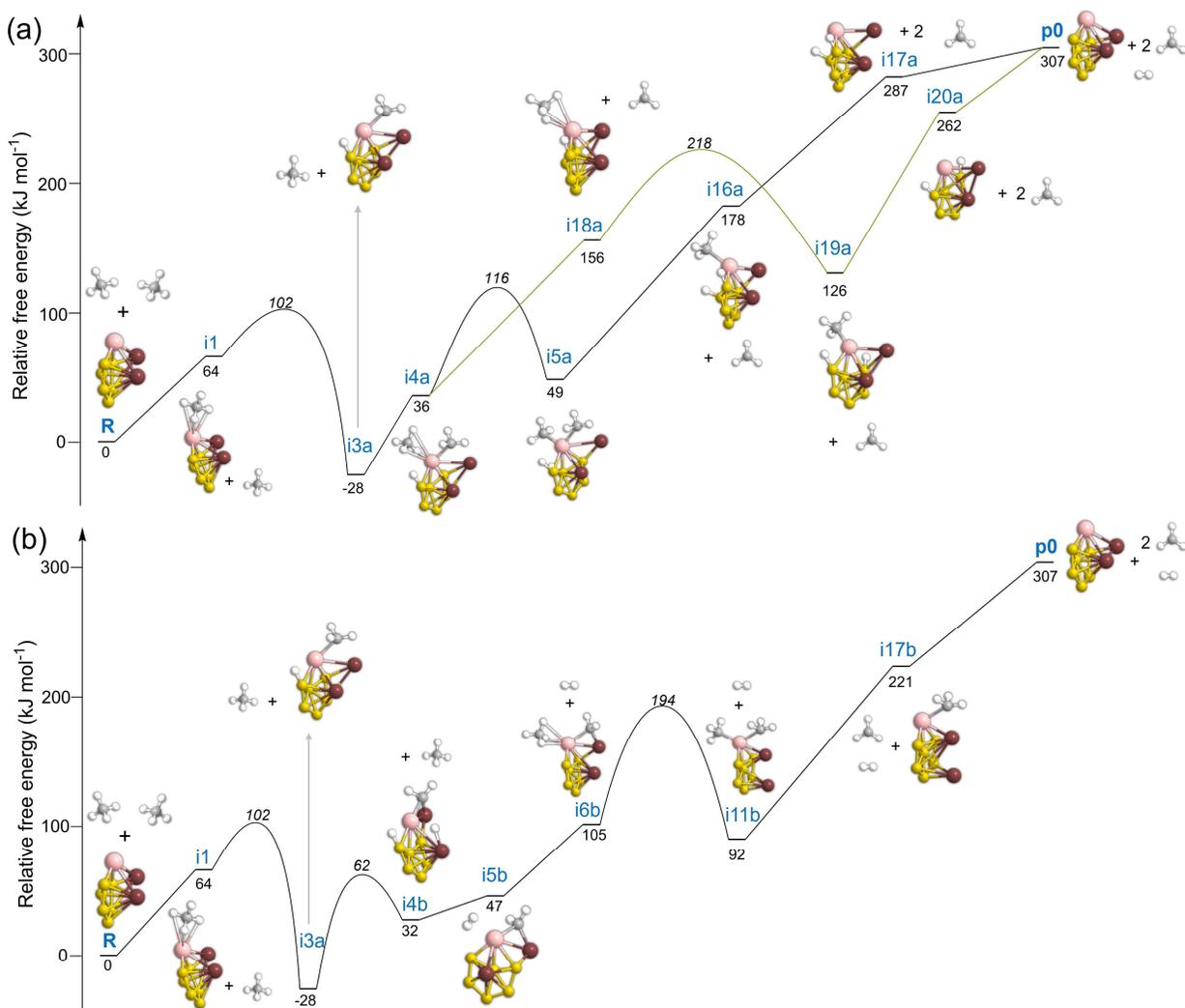


Figure S14: FES for methyl (**p0**) desorption pathways via the global minimum (**i1**) of the methane- $TiAl_2B_6$ binding complex at 800 K.

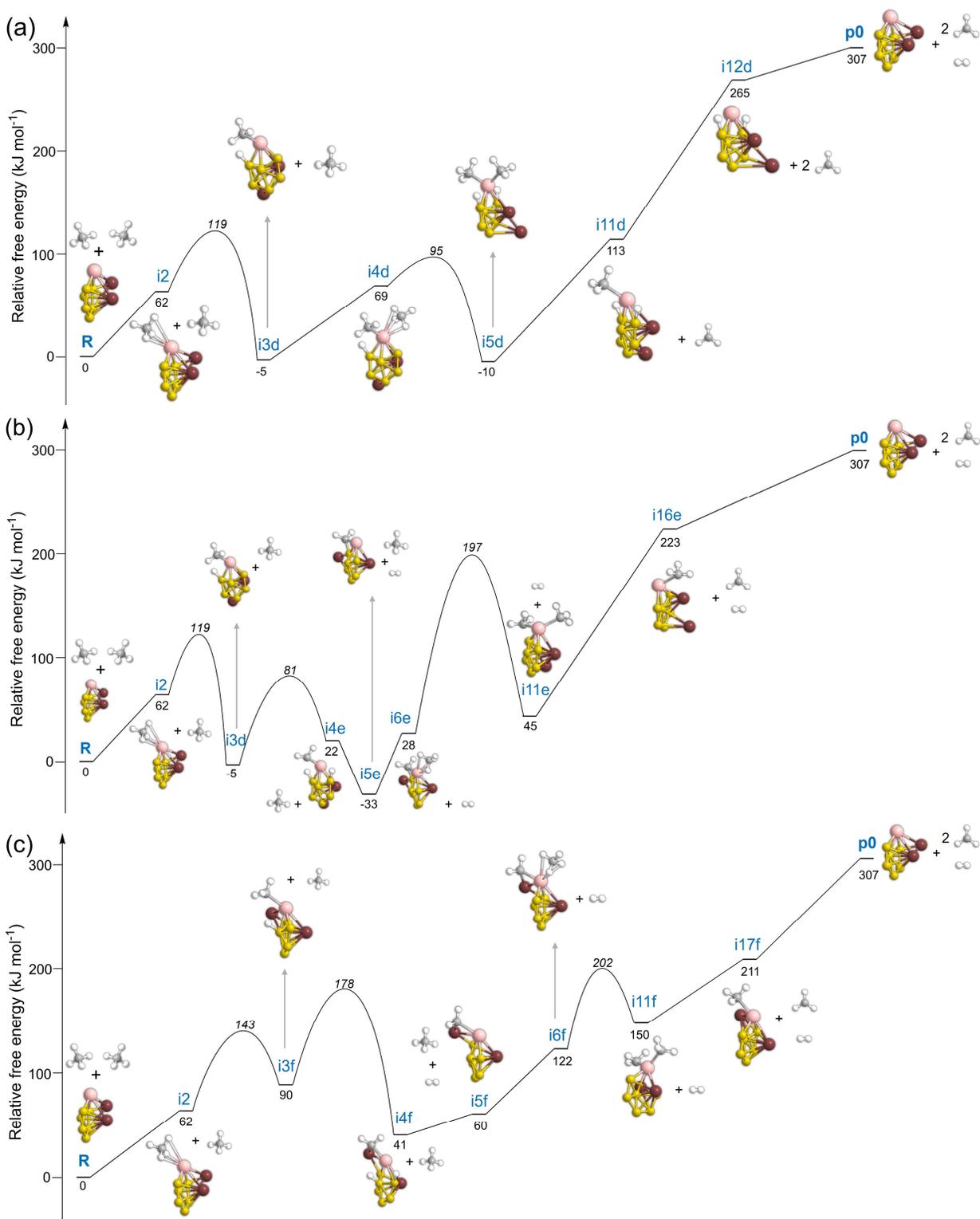


Figure S15: FES for methyl (p_0) desorption pathways via the first local minimum (i_2) of the methane-TiAl₂B₆ binding complex at 800 K.

Table S1: Relative free energies of the intermediates, transition states along with reactants and products for Figures 4a, S13, S14a.

Description	Label	Energy (kJmol ⁻¹)		
		0 K	800 K	1500 K
Cluster + 2 CH ₄	R	0	0	0
GM	i1	-38.1728	63.5999	142.319
Dehydrogenation TS	i1 to i3a	-8.08741	102.2788	189.8865
H-transfer to B	i3a	-132.835	-28.1771	46.04455
Second Methane	i4a	-168.977	36.39951	190.5334
Dehydrogenation TS	i4a to i5a	-102.822	115.645	277.3073
CH ₃ - CH ₃	i5a	-161.515	49.16732	200.6955
C-C coupling TS	i5a to i6a	25.07363	250.2334	422.521
Ethane Adsorbed	i6a	-86.6099	137.8488	313.9307
Ethane Desorption	i7a	-39.6	63.06826	133.3531
Hydrogen Desorption	p2	63.94313	71.71677	56.61815
Hydrogen Desorption	i8a	10.68006	142.546	234.4758
Dehydrogenation TS	i8a to i9a	33.52191	172.9872	273.1769
C ₂ H ₅ Adsorbed	i9a	-63.1332	67.76121	153.8913
Dehydrogenation TS	i9a to i10a	-30.3749	108.2404	200.4672
Ethylene Adsorbed	i10a	-114.585	18.48583	100.4177
Ethylene Desorption	i11a	54.40453	55.18	25.00711
Hydrogen Desorption	p1	177.1843	90.79672	-18.262
Ethylene Adsorbed	i10a	-114.585	18.48583	100.4177
Hydrogen Desorption	i12a	80.15841	117.1727	112.884
Dehydrogenation TS	i12a to i13a	182.276	221.4639	218.7903
C ₂ H ₃ Adsorbed	i13a	122.8238	165.5194	164.9206
Dehydrogenation TS	i13a to i14a	151.417	203.0516	205.7219
Acetylene Adsorbed	i14a	22.43256	65.72535	56.10079

Acetylene Desorption	i15a	229.2857	151.7172	35.04302
Hydrogen Desorption	p3	340.1001	164.3512	-39.9568
CH ₃ - CH ₃	i5a	-161.515	49.16732	200.6955
Methyl Desorption 1	i16a	23.2943	177.707	221.0229
Methyl Desorption 2	i17a	211.483	286.608	256.9878
Hydrogen Desorption	p0	319.3477	306.8796	179.4784
Second Methane	i4a	-168.977	36.39951	190.5334
Methyl Desorb	i18a	18.95776	156.2653	488.3862
Dehydrogenation TS	i18a to i19a	68.66229	217.6927	281.0309
Dehydrogenation	i19a	-12.6967	125.5242	176.4272
Methyl Desorb	i20a	186.0563	262.0684	214.7612
Hydrogen Desorption	p0	319.3477	306.8796	179.4784

Table S2: Relative free energies of the intermediates, transition states along with reactants and products for Figures 4b, 6a, S14b.

Description	Label	Energy (kJ mol ⁻¹)		
		0 K	800 K	1500 K
Cluster + 2 CH ₄	R	0	0	0
GM	i1	-38.1728	63.5999	142.319
Dehydrogenation TS	i1 to i3a	-8.08741	102.2788	189.8865
H-transfer to B	i3a	-132.835	-28.1771	46.04455
Dehydrogenation TS	i3a to i4b	-51.0091	62.14537	144.299
Above	i4b	-73.8903	32.32232	106.9929
Hydrogen Desorption	i5b	21.95299	46.58414	43.48786
Second Methane (A)	i6b	-23.1075	104.9042	183.4554
Dehydrogenation TS	i6b to i7b	19.81943	175.7795	267.5585088

Al-side	i7b	-122.3440467	0.1816320902	69.86828321
Dehydrogenation TS	i7b to i8b	-32.6906	97.01454	180.7221442
B	i8b	-85.2006	44.50454	102.9040833
C-C coupling TS	i8b to i9b	19.81943	149.5245	224.6889247
Ethylene Adsorbed	i9b	-111.456	18.24954	98.24865172
Ethylene Desorption	i10b	43.06461	44.27013	25.38142474
Hydrogen Desorption	p1	177.1843	90.79672	-18.262
Second Methane (A)	i6b	-23.1075	104.9042	183.4554
Hydrogen Transfer TS	i6b to i11b	55.65225	193.5831	281.7933
CH ₃ - CH ₃	i11b	-24.394	92.41203	158.8561
C-C coupling TS	i11b to i12b	150.656	279.7782	364.435
Ethane Adsorbed	i12b	35.37289	155.0617	237.0566
Ethane Desorption	p2	63.94313	71.71677	56.61815
Ethylene Adsorbed	i9b	-111.456	18.24954	98.24865172
Hydrogen Desorption	i13b	-5.50672	46.45801	51.5207116
Dehydrogenation TS	i13b to i14b	73.25828	125.223	142.8757192
C ₂ H ₃ Adsorbed	i14b	20.74828	72.71301	59.21108991
Dehydrogenation TS	i14b to i15b	99.51328	151.478	145.3945715
Acetylene Adsorbed	i15b	-58.0167	-32.307	-31.23436577
Acetylene Desorption	i16b	232.2354	144.0796	9.23320087
Hydrogen Desorption	p3	340.1001	164.3512	-39.9568
Methyl Desorption 1	i17b	166.5943	221.1404	191.1288
Methyl Desorption 2	p0	319.3477	306.8796	179.4784

Table S3: Relative free energies of the intermediates, transition states along with reactants and products for Figure S11.

Description	Label	Energy (kJ mol ⁻¹)		
		0 K	800 K	1500 K
Cluster + 2 CH ₄	R	0	0	0
GM	i1	-38.1728	63.5999	142.319
Dehydrogenation TS	i1 to i3a	-8.08741	102.2788	189.8865
H-transfer to B	i3a	-132.835	-28.1771	46.04455
Dehydrogenation TS	i3a to i4b	-51.0091	62.14537	144.299
Above	i4b	-73.8903	32.32232	106.9929
Hydrogen Desorption	i5b	21.95299	46.58414	43.48786
Second Methane (A)	i6b	-23.1075	104.9042	183.4554
Dehydrogenation TS	i6b to i7b	27.00805	171.1928	267.5588
Al-side	i7b	-122.344	0.18347	69.87004
Dehydrogenation TS	i7b to i8c	21.77542	158.3383	224.4565
Below	i8c	22.88601	151.7483	219.6154
C-C coupling TS	i8c to i9c	72.03275	207.3748	287.9307
Ethylene Adsorbed	i9c	-58.5071	81.95729	168.4208
Ethylene Desorption	i10c	122.0974	125.7368	97.68478
Hydrogen Desorption	p1	177.1843	90.79672	-18.262

Table S4: Relative free energies of the intermediates, transition states along with reactants and products for Figures 5a, S15a.

Description	Label	Energy (kJ mol ⁻¹)		
		0 K	800 K	1500 K
Cluster + 2 CH ₄	R	0	0	0
LM1	i2	-37.765	62.22677	144.1699
Dehydrogenation TS	i2 to i3d	8.001658	119.3498	144.1699
H-transfer to B	i3d	-105.572	-4.90727	207.5512

Second Methane	i4d	-138.639	68.80606	211.3127
Dehydrogenation TS	i4d to i5d	-138.924	95.06106	263.8227
CH ₃ - CH ₃	i5d	-217.404	-9.95894	132.5477
C-C coupling TS	i5d to i6d	-33.6194	200.0811	364.6734
Ethane Adsorbed	i6d	-112.384	95.06106	290.0777
Hydrogen Desorption	i7d	19.81943	175.7795	252.1713
Ethane Desorption	p2	63.94313	71.71677	56.61815
Dehydrogenation TS	i7d to i8d	46.07443	202.0345	304.6813
C ₂ H ₅ Adsorbed	i8d	-58.9456	70.75954	147.1513
Dehydrogenation TS	i8d to i9d	-32.6906	97.01454	199.6613
Ethylene Adsorbed	i9d	-111.456	18.24954	94.64132
Hydrogen Desorption	i10d	73.25828	125.223	109.2449
Ethylene Desorption	p1	177.1843	90.79672	-18.262
CH ₃ - CH ₃	i5d	-217.404	-9.95894	132.5477
Methyl Desorption 1	i11d	-26.659	112.5948	163.8712
Methyl Desorption 2	i12d	196.5344	264.6547	222.921
Hydrogen Desorption	p0	319.3477	306.8796	179.4784

Table S5: Relative free energies of the intermediates, transition states along with reactants and products for Figures 5b, 6b, S15b.

Description	Label	Energy (kJ mol ⁻¹)		
		0 K	800 K	1500 K
Cluster + 2 CH ₄	R	0	0	0
LM1	i2	-37.765	62.22677	142.319
Dehydrogenation TS	i2 to i3d	8.001658	119.3498	144.1699
H-transfer to B	i3d	-105.572	-4.90727	207.5512
Dehydrogenation TS	i3d to i4e	-29.711	80.72079	163.2608
H-transfer to opposite B	i4e	-80.3123	22.24828	92.93041

Hydrogen Desorption	i5e	-54.4911	-32.5406	-37.1468
Second Methane	i6e	-93.6337	28.22906	103.8984
Dehydrogenation TS	i6e to i7e	-73.0918	60.97167	145.9064
H-transfer from CH ₃ to B	i7e	-172.123	-51.1949	17.74042
Dehydrogenation TS	i7e to i8e	-76.9696	53.21857	130.4334
Above	i8e	-77.1797	44.92199	111.119
Hydrogen Desorption 2	i9e	114.5443	192.5356	118.7361
C-C Coupling barrierless Ethylene Adsorbed	i10e	6.132118	49.36969	56.71127
Ethylene Desorption	p1	177.1843	90.79672	-18.262
Second Methane	i6e	-93.6337	28.22906	103.8984
Hydrogen Transfer TS	i6e to i11e	72.32943	197.2777	288.0234
CH ₃ - CH ₃	i11e	-85.2006	44.50454	98.0515
C-C coupling TS	i11e to i12e	124.8394	249.0263	335.7377
Ethane Adsorbed	i12e	19.81943	149.5245	236.0731
Ethane Desorption	p2	63.94313	71.71677	56.61815
Ethylene Adsorbed	i10e	6.132118	49.36969	56.71127
Dehydrogenation TS	i10e to i13e	129.0767	164.494	156.7686
C ₂ H ₃ Adsorbed	i13e	-74.8813	-27.5805	-29.0164
Dehydrogenation TS	i13e to i14e	67.88448	121.0134	126.6939
Acetylene Adsorbed	i14e	17.51061	66.37852	62.16756
Acetylene Desorption	i15e	251.3732	170.972	55.66525
Hydrogen Desorption	p3	340.1001	164.3512	-39.9568
CH ₃ - CH ₃	i11e	-85.2006	44.50454	98.0515
Methyl Desorption 1	i16e	166.3791	222.825	193.544
Methyl Desorption 2	p0	319.3477	306.8796	179.4784

Table S6: Relative free energies of the intermediates, transition states along with reactants and products for Figures S12, S15c.

Description	Label	Energy (kJ mol ⁻¹)		
		0 K	800 K	1500 K
Cluster + 2 CH ₄	R	0	0	0
LM1	i2	-38.1728	63.5999	142.319
Dehydrogenation TS	i2 to i3f	34.4667	142.6511	225.9399
H-transfer to B below	i3f	-14.7299	90.02031	167.0141
Dehydrogenation TS	i3f to i4f	55.78051	178.0218	268.5972
H-transfer to B side	i4f	-70.2487	41.46694	118.3978
Hydrogen Desorption	i5f	40.92748	60.09234	50.92822
Second Methane	i6f	0.737293	121.7599	193.242
Dehydrogenation TS	i6f to i7f	24.98641	156.5898	237.0689
H-transfer from CH ₃ to B	i7f	-82.1576	40.93386	106.6372
Dehydrogenation TS	i7f to i8f	35.75621	163.6182	237.2758
H-transfer to Al above	i8f	22.45805	146.6181	210.9799
C-C Coupling TS	i8f to i9f	56.33488	187.6389	266.2111
Ethylene Adsorbed	i9f	-49.4544	82.8946	161.5548
Ethylene Desorption	i10f	16.48404	20.617	-8.79269
Hydrogen Desorption	p1	177.1843	90.79672	-18.262
Second Methane	i6f	0.737293	121.7599	193.242
Hydrogen Transfer TS	i6f to i11f	72.32943	202.0345	285.6769
CH ₃ - CH ₃	i11f	19.81943	149.5245	199.6613
C-C coupling TS	i11f to i12f	157.3641	286.162	374.4667
Ethane Adsorbed	i12f	19.81943	149.5245	252.1713
Ethane Desorption	p2	63.94313	71.71677	56.61815
Ethylene Adsorbed	i9f	-49.4544	82.8946	161.5548
Hydrogen Desorption	i13f	90.87139	136.9208	141.7906

Dehydrogenation TS	i13f to i14f	124.5443	163.9001	173.5019
C ₂ H ₃ Adsorbed	i14f	17.61091	65.60203	72.95427
Dehydrogenation TS	i14f to i15f	69.95122	110.1474	105.3373
Acetylene Adsorbed	i15f	-7.06703	35.77296	24.34469
Acetylene Desorption	i16f	230.2219	143.4491	19.08654
Hydrogen Desorption	p3	340.1001	164.3512	-39.9568
CH ₃ - CH ₃	i11f	19.81943	149.5245	199.6613
Methyl Desorption 1	i17f	151.84721	210.9214	183.7112
Methyl Desorption 2	p0	319.3477	306.8796	179.4784

Data S1: Coordinates of the intermediates, transition states along with reactants and products.

CH₄		C₂H₆
H -1.113 -0.000 -0.000		C 0.000 0.100 0.769
C 0.000 -0.000 -0.000		C 0.000 0.100 -0.769
H 0.372 1.049 -0.000		H 0.000 1.123 1.168
H 0.370 -0.524 0.909		H -0.886 -0.412 1.168
H 0.371 -0.525 -0.909		H 0.886 -0.412 1.168
		H 0.000 -0.923 -1.168
		H -0.886 0.612 -1.168
		H(8) 0.886 0.612 -1.168
H₂		C₂H₄
H -0.346 -0.000 0.000		C 0.000 -0.000 0.667
H 0.346 0.000 0.000		C 0.000 -0.000 -0.667
CH₃		H 0.000 0.927 1.240
C -2.58567319 -0.51212304 -0.26136102		H 0.000 -0.927 1.240
H -1.51818211 -0.50525504 -0.44359403		H 0.000 0.927 -1.240
H -3.14328323 -1.43672810 -0.34481802		H 0.000 -0.927 -1.240
H -3.09553222 0.40561403 0.00432500		
C₂H₂		TiAl₂B₆
C 0.00000000275546 -0.00000000297340 0.60314628958351		Ti 5.80883855549443 1.84415151014005 -0.79624864041208
C 0.00000000786840 -0.00000000788609 -0.60314629230685		Al 6.14973401840105 -0.18615295979409 -3.55820844043572
H -0.00000000616467 0.00000000624909 -1.67112162321035		Al 7.21253202386947 -0.32194303008861 -0.24050198111768
H -0.00000000445919 0.00000000461040 1.67112162593369		B 5.12078365372771 -1.44988232400490 -1.01509177730590
		B 5.63367423268675 1.00921715189560 1.08209307166144
		B 5.33011839765547 -1.69934325940942 0.51183133885710

	B 5.51134611940487	-0.51535265088059	1.52909566621362
	B 4.94802880209510	-0.01306008969222	-0.06511800903025
	B 5.12124334666515	0.01410166183418	-1.69098511843054
i1			
C 2.90564771026688	2.57036500721939	-5.06290167586163	
H 1.93744970718089	2.05189210753626	-5.12323590244081	
H 3.25993317898509	2.75313202515601	-6.08090198128308	
H 3.67396435960682	1.94768274558867	-4.56947602473311	
H 2.81172337107552	3.56698194657728	-4.58048140377080	
Ti 2.52237149137744	2.55616702670836	-2.58214592933252	
Al 3.95127565277731	-0.11186021547047	-0.94023529184394	
Al 4.76425210195312	3.22572335341897	-1.32803235342078	
B 3.49538073042189	2.40457682252023	0.65800347987131	
B 2.68823883835792	4.44884897968091	-1.76588379693595	
B 3.72009065016529	3.94624881243405	0.76859061420771	
B 3.27632920946575	4.93578857691381	-0.36689466247281	
B 2.61764306490537	3.30324915586009	-0.54043447752977	
B 2.84140395346042	1.68667194585620	-0.62730716445361	
i1 to i3a			
C -0.27619685851710	-0.14343580810914	-2.52263251453296	
H -1.2430491384026	-0.54130098737148	-2.88403427171453	
H 0.05576666620344	0.62904796653241	-3.22017473830294	
H 0.49083725973839	-0.94209395569553	-2.52194285315699	
H -0.40197415722404	0.79186047782092	-1.43505176761059	
Ti -0.6560507583899	-0.66071784669153	-0.37717587405171	
Al 0.82132535422680	-2.99413761218825	1.85913894561299	
Al 1.63060359138530	0.18182004663677	0.82260009160156	
B 0.26077571931294	-0.24960166536183	2.86566969135396	
B -0.41948224732927	1.34897200551894	0.10361411298934	
B 0.48556374983467	1.28965647751889	2.71054056040783	
B 0.14129684241858	2.06526895147895	1.3977793634312	
B -0.56425442550214	0.42331743498756	1.49437418273189	
B -0.32516159775492	-1.19865548507669	1.70729649832904	
i3a			
C 3.35051862294525	1.89270786472509	-4.37720536532358	
H 2.44084282381748	1.46622645331363	-4.84281741408472	
H 3.53131278266817	2.90433969054024	-4.82774350725902	
H 4.20169992133345	1.28223499812788	-4.69771581231096	
H 2.43980129648603	5.22866265842556	-2.59772746673869	
Ti 2.51866157145623	3.07050613041184	-2.81644654811639	
Al 4.11530597503154	0.51186747943206	-2.19101668584190	
Al 4.79609383905186	3.34219699316581	-1.28920984115953	
B 3.26226363712744	2.24947411264784	0.35299298453634	
B 2.92819890833692	4.85887809047234	-1.54535548381219	
B 3.58944590284898	3.68307642794751	0.84672691860685	
B 3.37418147654929	4.95242924569769	-0.03609811411138	
B 2.55618969671417	3.48548950727929	-0.66213676643622	
B 2.68712834563303	1.88786101781312	-1.09419508794851	
i4a			
C 3.24832780383118	2.82767345963865	-4.61646971031501	
H 2.36710263641829	2.83696049730482	-5.28053784828169	
H 3.84504664016859	3.75617381000165	-4.82446227890254	
H 3.89451306442992	1.99908887656026	-4.92805315387362	
H 3.65877986622826	5.76379795465756	-2.19770075394989	
Ti 2.70599734256780	3.94739283923528	-2.88155385337494	
Al 2.95065180584411	0.85017821448787	-2.77514360792020	
Al 4.68367175982759	2.76946998477863	-1.23961531926727	
B 2.57299590047457	2.30750160147617	0.05945776986742	
B 3.78649853887595	5.01391123388046	-1.24655184575373	
B 3.42164709122000	3.31411066611850	0.87765448897546	
B 3.97196460918151	4.64274691641182	0.27557744926410	
B 2.68723037303150	3.87573130251131	-0.68314552491929	
B 2.13951115460317	2.51371311636753	-1.46455594996049	
C 0.56850483850164	5.19594076009119	-3.59460279680074	
H 1.42946340134693	5.86957060163987	-3.43772645793464	
H -0.31984268454017	5.77956288633096	-3.33508471983367	
H 0.54738456802119	4.32738665480726	-2.89911537584288	
H 0.51063100996782	4.87265004370001	-4.63788347117626	
i4a to i5a			
C 0.77090849797902	-1.04798229155667	-2.19621459985807	
H -0.00373387658347	-0.50607201788179	-2.77895426546428	
H 1.67065461848402	-0.39177506286248	-2.10424497909618	
H 1.09056518053611	-1.88243159051943	-2.82890035220379	
H 1.21016643207555	1.96843191138349	0.23181254468907	
Ti 0.16869467416939	0.11335055014543	-0.47885420796908	
i5a			
C 3.30460661212413	2.94785803614212	-4.66270950381963	
H 2.53753131460576	3.03134208536116	-5.44742424783775	
H 3.91622533087007	3.88922391181103	-4.70660605582922	
H 4.00898657077704	2.15931770092775	-4.95587262765547	
H 3.83382480212465	5.84882122138322	-2.09323580026704	
Ti 2.57862167029401	3.99509747129481	-2.94018773683464	

Al 0.26778201727965	-2.91819728659340	-0.61438282594941	Al 2.67762507639718	0.92750427443729	-3.18524712032817
Al 1.98131815129378	-0.90083087933459	1.49451269710361	Al 4.42834376747761	2.88070999930804	-1.17497850161582
B -0.26512434044906	-1.34606567391840	2.54162239441367	B 2.50156402331791	2.28963333493520	0.06034312698267
B 1.22086354755555	1.22801943214584	1.19660925223942	B 3.89789993552232	4.97687696236100	-1.25773959790655
B 0.21201693342959	-0.13702097349689	3.37888300472220	B 3.21390620930327	3.36554001260438	0.90949154726360
B 0.96778894593669	1.05915057179004	2.74575998541487	B 3.90436079583967	4.60515219901948	0.28900585197398
B -0.11010660731369	0.15117664087524	1.62288818709459	B 2.46943296789745	3.93617565244736	-0.72267903686839
B -0.22918323123709	-1.45228507794155	0.96103056102565	B 2.30804418755989	2.33153831310841	-1.52071010416361
C -1.75436705918405	1.20408805873407	-0.77223020679748	C 0.89460373802362	5.10263635176949	-3.59510411036479
H -1.28086383859545	1.94881402283142	-1.43820982802847	H 1.10304884097867	5.37765017703590	-4.64374231640232
H -2.49642629113990	1.73123254433148	-0.16668220719280	H 0.65181688053975	6.00833109286223	-3.02679155672891
H -1.15025737780908	0.74727530122936	0.56595078913202	H 1.47807964642627	4.59953854812454	-0.98333769630315
H -2.27069637642755	0.43112182063884	-1.36039594327553	H 0.01976513992062	4.43287060506638	-3.57599950329464
i5a to i6a			i6a		
C 0.20203594852143	0.02719468882025	-2.27549814290797	C 2.24859109678206	4.62013646587092	-5.33001695986686
H -0.29381998188792	-0.42218329950692	-3.13868189273640	H 2.27130120760170	4.17453870087369	-6.33042136961024
H 0.85459164065094	0.84834973733685	-2.57992650905256	H 2.63317255891080	5.64356401726425	-5.38587452461305
H 0.87171473219542	-0.83971583638026	-1.83455009011177	H 2.98466328632059	4.01574636744876	-4.75316190901987
H 1.42503232627425	1.44204005578227	0.09036735344438	H 3.82967066416699	5.34505540228318	-2.60313432959783
Ti -0.23588167917471	-0.44142573427718	-0.27848605438599	Ti 2.03500569084644	3.75848922523170	-2.68924163678576
Al 0.44948905599559	-3.09289203665655	-0.13195159462006	Al 3.07306012063394	1.31604606667446	-3.13383247341566
Al 1.74953783183745	-1.36714382172180	1.62168417579072	Al 4.28488779952981	2.40562782358303	-1.11534646028841
B -0.21632667721972	-1.41555577972208	3.00787118198013	B 2.43173051474948	2.50968687928466	0.36537404857245
B 1.36590341326931	0.74148370833201	1.06178036532915	B 3.92627144203553	4.59872672399552	-1.65767347047976
B 0.57027487799129	-0.20487513308967	3.56738881066008	B 3.43550354802144	3.58508080575085	0.87751083339606
B 1.36113821072199	0.75374355568426	2.65001694955599	B 4.19009115274307	4.53820864923603	-0.09188017201349
B -0.11001227200017	-0.01394122348249	1.84157255555118	B 2.54169165744410	4.00637217100686	-0.68400858165431
B -0.44662408064043	-1.75832637471299	1.49025804813412	B 1.95189397115186	2.37310697357738	-1.13168029141147
C -1.41649045459096	1.11591354206405	-1.57055442720963	C 0.81971658344757	4.58238278357278	-4.76119332991898
H -1.50618193139563	1.43863523961913	-2.60813548652887	H 0.10297024192894	5.08043426189535	-5.42250504876869
H -1.21943003077710	1.97796851952284	-0.92758462130720	H 0.70939701051136	5.14181703430662	-3.80063636230905
H -1.05876067984702	0.61055510856150	1.29731704156199	H 1.57629010189819	4.79797530169182	-1.06778310909477
H -2.34619024992402	0.60017508382679	-1.28288766314730	H 0.45023907127596	3.54911570645186	-4.63189261312015
i7a			i8a		
H 3.81914622616571	5.27984475890645	-2.64984076921895	C 2.23291011469260	4.60943484377020	-5.50346331405724
Ti 2.02846328526872	3.75265607296325	-2.67065635700090	H 1.95299380287461	4.05726861845998	-6.40637142177185
Al 3.14643960669256	1.39852232593319	-3.16064438747044	H 2.51520299356234	5.63046916354689	-5.77833644153576
Al 4.27274507307248	2.39568781238247	-1.07915746540716	H 3.17138980806942	4.13346540511709	-5.14382223823621
B 2.41462899642810	2.51930357723929	0.37086766315905	Ti 2.65215232921310	3.58000531352835	-2.96974814817657
B 3.92432133220502	4.56908927878802	-1.67385661287419	Al 2.48275916603669	0.81032838235658	-2.81026546539821
B 3.43921708478690	3.58398511759318	0.86738230409819	Al 4.49599905026368	2.80703103242869	-1.18071210341615
B 4.20108869545841	4.52753742849355	-0.11128888393531	B 2.47656350428804	2.35771460227653	0.20344994480841
B 2.52350640317719	4.01423240819602	-0.67890029667084	B 3.44518334425946	4.90318805789168	-1.60094381381693
B 1.93527546649355	2.37187729855589	-1.12972258798880	B 3.20770958515911	3.58080774979839	0.82973318895241
H 1.57126448025134	4.82163994094868	-1.01587824669064	B 3.63384315813204	4.83079410408211	-0.01908635176439

	B	2.45591336649817	3.77281790704086	-0.80954126861240
	B	2.04858005626513	2.27449382581332	-1.33720136097584
	C	1.07812143204628	4.61867429716457	-4.48365862662332
	H	0.20243381334396	5.13963614165881	-4.88444485301559
	H	1.32692190676325	5.19138659610120	-3.55476742554550
	H	0.71150951853197	3.60156461896452	-4.22730061081468
i8a to i9a				
C	-0.19299240160671	0.65368427875089	-2.61519105524598	C 2.21080101410886
H	-0.73127414466875	0.45257382041292	-3.54985873681515	H 2.03394902697345
H	0.47439353477927	1.50858750083011	-2.77340659144304	H 2.45965859326256
H	0.47549932425069	-0.24099937451832	-2.50538957988077	H 3.22172414068121
Ti	0.22441157910720	-0.37765131539591	-0.23925852639307	Ti 2.53706095569331
Al	0.73402374186862	-3.69175770674978	0.80184845812475	Al 3.01507660377418
Al	2.15580244594293	-0.62906954338346	1.59617186471888	Al 4.48590247306669
B	0.25902085653958	-1.63237207330209	2.92554786388228	B 2.46684107014898
B	0.52946992508576	1.09504648205588	1.17433863654970	B 3.18521175568973
B	0.67611406020577	-0.26363239695969	3.56805685489396	B 3.09265160383648
B	0.72074342306353	1.06944496254080	2.75231194879316	B 3.36923495107213
B	-0.07242968927051	-0.27822081490391	1.93808888970980	B 2.28116377899022
B	-0.10997658044211	-1.81186921613889	1.36982770701129	B 1.98314261424993
C	-1.13314247579763	0.88864282578351	-1.42210422054333	C 1.09620250160625
H	-1.62888633725404	1.86068793142713	-1.48238651204396	H 0.64161762791177
H	-0.46067019469225	1.28193094008924	-0.20476191240960	H 2.92400475804985
H	-1.92010706711133	0.11497369946159	-1.33383508890890	H 0.32506314088429
i9a to i10a				
C	-0.63951119726782	-0.00429768928604	-2.25886301359452	C 1.58581464142140
H	-1.53831352444477	-0.36733570676230	-2.77315192532142	H 0.53829672974986
H	0.26765989810903	-0.41630277867569	-2.70475431298105	H 2.07885414423906
H	-0.52050500687077	-1.00543681497775	-1.15442953516982	H 1.54959883304716
Ti	-1.05876943822540	0.27310417826619	-0.05218372776052	Ti 1.77474657776531
Al	2.90761127804910	-2.24531782206735	0.95764946985740	Al 4.69195379960847
Al	1.63614944673862	0.25456390269735	0.74902304679747	Al 4.21829892480892
B	0.69183236686792	-2.02686267774141	1.65732243721045	B 2.65173229224776
B	-0.26895270890679	1.08196384591684	1.91985422067518	B 2.47371584559677
B	1.09437805082146	-1.08167900576732	2.85859734436270	B 3.15629916067158
B	0.62548413586371	0.39405570939526	3.01969725850839	B 3.06174472199734
B	-0.23627834128510	-0.61344419670722	1.85287459205467	B 2.07755620998212
B	-0.18664155693433	-1.53304708383239	0.43471784403963	B 2.13429261428891
C	-0.61814925520582	1.40302770932232	-1.85744408241047	C 2.35966489998714
H	0.31321184941144	1.95832356985394	-1.94049841841014	H 3.43274839941908
H	-0.97084163487069	1.91826908594719	1.38476552919506	H 2.18416600332053
H	-1.49836436184980	2.01041577441840	-2.09317672705300	H 1.89719448184836
i10a				
C	1.58581464142140	4.04691333806329	-5.00131337507634	C 1.58581464142140
H	0.53829672974986	4.15190943710922	-5.30586045925160	H 0.53829672974986
H	2.07885414423906	3.16497205232391	-5.41345181804406	H 2.07885414423906
H	1.54959883304716	2.06352457842113	-2.83434972039536	H 1.54959883304716
Ti	1.77474657776531	4.19127793173644	-2.83703307784878	Ti 1.77474657776531
Al	4.69195379960847	1.05786842977025	-0.63089427983153	Al 4.69195379960847
Al	4.21829892480892	3.61956884757588	-1.65635385347744	Al 4.21829892480892
B	2.65173229224776	1.94541172365370	-0.32271199812527	B 2.65173229224776
B	2.47371584559677	5.19081014257956	-0.96466374942579	B 2.47371584559677
B	3.15629916067158	3.09373264208355	0.61856899285150	B 3.15629916067158
B	3.06174472199734	4.62414363806108	0.36918694904665	B 3.06174472199734
B	2.07755620998212	3.54852074232201	-0.67006448583652	B 2.07755620998212
B	2.13429261428891	2.31148451990470	-1.79707645694759	B 2.13429261428891
C	2.35966489998714	5.21801787765209	-4.69920522233494	C 2.35966489998714
H	3.43274839941908	5.22846904933135	-4.88635796505338	H 3.43274839941908
H	2.18416600332053	5.98641500694231	-1.84608582247123	H 2.18416600332053
H	1.89719448184836	6.20653439246918	-4.74936321777806	H 1.89719448184836
i11a				
H	1.59413905571551	2.04393401652520	-2.84739986167878	H 1.59413905571551
Ti	1.79797759522028	4.20659430776100	-2.72766795810602	Ti 1.79797759522028
i12a				
C	1.48713686031912	4.26786353096639	-4.98486356722581	C 1.48713686031912
H	0.64805194283847	4.96242362691167	-4.89494486188547	H 0.64805194283847

Al 4.68077529894509	1.01670681782229	-0.68831876980375	H 1.25100567880465	3.26292321001118	-5.34234321120462
Al 4.18730436286439	3.59819165689026	-1.67350399615205	Ti 2.05290485319874	3.92962426239124	-2.74006006800179
B 2.73964227601419	1.91760840080302	-0.31721401597068	Al 4.57133973076956	1.48669346689542	-2.65081030855098
B 2.50576785407937	5.17911684873161	-1.02175533223176	Al 3.95883292137710	4.49426939259559	-0.99736486446401
B 3.09413451219194	3.12067081439660	0.65834942309757	B 3.27500138371310	2.22548285592622	-0.02491627150704
B 3.02506207172625	4.63520064912310	0.37489402018260	B 1.62096133666721	4.91488933943031	-0.91670232083465
B 2.05734017812577	3.55370963595709	-0.65430335906720	B 2.84157586771107	3.32757930408344	0.99983810031918
B 2.11476875019420	2.34670111758325	-1.78564911094723	B 2.03091056689499	4.60649784149442	0.58358035243171
H 2.17719301492296	6.01432393440655	-1.88890854932268	B 2.05270859785088	3.28776585128161	-0.57085961502510
			B 2.89681108383946	2.28419268152237	-1.57792880959005
			C 2.79121935594690	4.71363704054146	-4.91520818768802
			H 3.63118279657716	4.07292934385265	-5.18072933286555
			H 3.02327045349146	5.76286301209581	-4.73328107390762
i12a to i13a			i13a		
C -0.81981284277168	0.66131110340243	-1.97493804117961	C 1.89450337902268	3.95874038211913	-4.45178367642837
H -1.82766222391583	0.64696387344775	-2.38713888798507	H 1.27684490593934	3.36329910495827	-5.12345076099515
H -0.76070564096428	-0.61087501388211	-0.69324609476851	H 1.36141097593920	3.22389531417501	-1.79169657642429
Ti 0.04209744321058	0.88997495954518	-0.11986654475602	Ti 2.81625976844417	4.27955433981433	-2.61920181725611
Al 0.54796731275114	-2.39135194129888	-0.70390812733969	Al 3.45028647150240	0.96486989001837	-3.09194212735475
Al 1.46510922292211	0.97821071346871	2.14811839215550	Al 4.12966051477031	4.19556782920802	-0.27258774844417
B 0.86329757709551	-1.62796869661695	2.13091699714287	B 3.15251161794348	2.02238919773740	-0.05148050760228
B -0.96099067953580	1.10197825327063	1.78299569821285	B 2.18816835288573	5.13348402274127	-0.72244099992694
B -0.25840403245996	-1.22106395262327	3.15759122037241	B 2.31641920053663	2.88138473654855	0.94038390905531
B -1.10936391780007	0.10703435150245	3.00755120431491	B 1.91100814070300	4.36181983557667	0.64436924403010
B -0.24614840747385	-0.44172773358545	1.65238572422921	B 2.17769045364264	3.30551768827017	-0.81920932888999
B 1.20699231038307	-0.83052761299251	0.79998333303911	B 3.60387228820462	2.48726769476020	-1.51223625765824
C 0.28434633780689	0.86576465326484	-2.72114501875782	C 2.43566262899020	5.11701571649129	-4.85657574045138
H 1.29757415299215	0.76484657340034	-2.29275509210665	H 3.03228529742493	5.77105960629480	-4.16479429989958
H 0.27570338776003	1.10743046969683	-3.78654476257349	H 2.37513353405042	5.58940073128620	-5.84116512175398
i13a to i14a			i14a		
C 0.09256850510940	-0.10600337305498	-2.42454379937999	C 2.12429285098821	3.71461101850766	-4.70336985529395
H 0.51409561431771	-0.46801609517583	-3.36427941940745	H 1.97241715009826	3.40356836183189	-5.74211254891862
H -1.82701929605503	-0.38549682110603	1.38959009380144	H 0.78394451563798	3.10053212570421	-0.33255025875708
Ti -0.86289754859230	-0.02052995903629	-0.52902362326437	Ti 1.89256475532857	4.17980701636419	-2.64571521196970
Al 0.95083551035318	-2.31799481193133	-1.28311614081173	Al 2.85847878438740	1.56007545728946	-3.82601526938816
Al 1.50191962226357	-0.03780644196651	0.93446996228945	Al 4.01079697205978	4.06046780216552	-1.08457085069450
B 0.45516439787454	-1.63322330976193	2.23275995977258	B 3.25862590261075	2.07734209201678	-0.25781359251454
B -0.17091674390896	1.34791745253463	0.94545477569444	B 2.23495625697179	5.18113326163653	-0.53620143063661
B 0.44967387037297	-0.32149845787974	3.08456166553367	B 3.24723205911318	3.06571611965475	0.93663264343446
B 0.20695379649664	1.09871781855917	2.46585137110774	B 2.79171355862967	4.54738705156804	0.80670357936773
B -0.60271622263638	-0.32509178913998	1.61889200045049	B 1.95404596445827	3.39577425572047	-0.44922011802905
B 0.09442849458718	-1.70477422921566	0.67664988593269	B 2.77483010256144	2.38577828788852	-1.74515507094498
C -0.25570662410616	1.15524341467439	-2.17254214788995	C 2.80283435846151	4.81621417658281	-4.31813704888964
H -0.36997377878790	1.66049155086049	-0.79818108748731	H 1.60992342998477	5.99206949869030	-1.18728216235019
H -0.17640959356116	2.05806505163959	-2.77654349634170	H 3.35156018870821	5.54727120437859	-4.91462455441500

i15a			i16a				
H	1.30494762095275	2.23923093162869	-0.57496887585836	H	3.88049490824480	5.88053570864601	-1.97373686356518
Ti	2.38729695366147	4.42684440506354	-2.72189275959478	Ti	2.55090752601598	4.03110192994760	-2.86623272660421
Al	1.10483884035244	2.17296197420945	-2.40687707342664	Al	2.74981949027381	1.43594777914608	-3.45686617594007
Al	4.16594668635318	4.66550407898092	-0.93317970868468	Al	4.40922743688952	2.86917459148073	-1.17100767219665
B	3.89793188394436	2.36912906889776	-0.56942723244652	B	2.52602948093689	2.23382743838319	0.08631229301612
B	1.88644008675313	4.87196707866171	-0.62165267145690	B	3.90207678973338	4.97402260124776	-1.17813606908711
B	3.46178637254593	3.06465096888607	0.75100088275011	B	3.25115068311682	3.28745569341099	0.95081647071009
B	2.48119262644715	4.27495981851664	0.72683703329722	B	3.93326367682505	4.54523799894607	0.35486517495683
B	2.23841233517318	3.14125203191678	-0.69286663841548	B	2.46226875369819	3.90568141213869	-0.65782158809407
B	3.39885090372750	2.77724483976762	-2.02764333710193	B	2.27967080770264	2.30458392637653	-1.47795435757568
H	1.08946799008873	5.54233778347055	-1.25051735906199	C	0.85749495992703	5.02517225652835	-3.66897707303722
				H	0.88497985533675	4.84179169194320	-4.75892512206906
				H	0.89336221003425	6.11044157190198	-3.48965053634298
				H	1.47427579014057	4.59460325426825	-0.87388353368317
				H	-0.09408466887573	4.63849834563448	-3.27971478048761
i17a			i18a				
H	3.80034577625569	5.64412080227609	-2.17679283201427	H	3.79265761140782	5.72893026975564	-2.18901759849116
Ti	2.13379236823644	4.04947614249606	-2.62515593447901	Ti	2.45974676491842	4.07334629035351	-2.78391505123466
Al	3.48619078013892	1.92378346232631	-3.45352561727951	Al	3.30938338743303	1.49427763224652	-3.29219706631824
Al	4.36612948666912	2.55064206307543	-1.12211652203695	Al	4.45347247841826	2.53118717502194	-1.11873533173795
B	2.39801950869123	2.28138643932443	0.15161429526450	B	2.43936780877766	2.38988434618849	0.24343500640839
B	3.89048967216234	4.77155194461942	-1.34029526783259	B	3.85312696904872	4.95251493770559	-1.26029815822194
B	3.29552734999182	3.29521554559646	0.92501066240446	B	3.50522658225678	3.27687110639944	0.92615406629884
B	4.05167396783077	4.45413350106173	0.20651713911580	B	4.13851844860097	4.52014523023012	0.22966427538644
B	2.47033335077958	3.95391849811181	-0.58830132887667	B	2.68077139098494	3.97321079651499	-0.60378240621602
B	2.04480918835776	2.39241566489314	-1.38663584836098	B	1.85880753235985	2.64394990363747	-1.21958281690340
H	1.48187390088626	4.74552826621904	-0.85396380590476	C	0.87257119219266	5.16825342944293	-3.67201848458340
				H	1.26229349833896	6.13542823662837	-4.03593684138198
				H	0.02314243224262	5.37561502090240	-3.00816244795348
				H	0.92545870744936	2.67393773974149	-1.99395515331504
				H	0.50069186556986	4.59838362523091	-4.54277235173635
i18a to i19a			i19a				
H	1.84459770151735	1.64690976875037	-0.23490995360793	H	3.74919867713462	5.77898963948045	-2.08289535583057
Ti	0.32789198056541	0.17956096163586	-0.95167814022531	Ti	2.56228505282969	4.02345272786861	-2.69984628069466
Al	0.53666322265893	-2.52028682943043	-1.34802263085094	Al	2.67476315033330	1.38178006000451	-3.12266086578617
Al	1.97653389787564	-1.54425007323178	0.75230179915508	Al	4.59697409357629	2.69592889161424	-1.28660702900363
B	-0.20200266157698	-1.46765294063001	1.93046476024168	B	2.65283219232985	2.28131383122080	0.17272685970329
B	1.72771637716265	0.90142730170491	0.71617951551542	B	3.88189787642107	4.97515776461881	-1.18157186207948
B	0.89215185414630	-0.74696828148575	2.76226053599916	B	3.62745488597053	3.22306471396298	0.92794438939698
B	1.78839049774556	0.42446581212209	2.21318934359683	B	4.19580229491916	4.53471107593061	0.30415098204686
B	0.39358674837717	0.04086475293824	1.23182376713247	B	2.75850875299910	3.89421871328540	-0.53217110216841
B	-0.54811603980027	-1.10184192727005	0.42475729739248	B	2.06224501615499	2.56927085117179	-1.27906671157396
C	-1.68117509862010	0.90987533622235	-1.57189202038285	C	0.53677323038000	5.12776702605467	-3.68167445381692
H	-1.29483690532891	1.94348227497656	-1.47972650121414	H	1.23994565214262	5.94376474397894	-3.44492015143052

H -2.72638096098873	0.92543368406832	-1.25308572651782	H -0.43515676827005	5.59388869782728	-3.86647987830893
H -1.39445475514971	-0.16427671785179	-0.57012630526320	H 0.38031965652386	4.44323405366311	-2.81952913290174
H -1.64056585858431	0.57325687748111	-2.62153574097094	H 0.83124581655489	4.57712196931771	-4.58738937755210
i18a to i20a			i3a to i4b		
H 3.78877126207042	5.63178539968919	-2.25888911985889	C 0.12590858370089	-1.22960733702127	-2.00265362545264
Ti 2.44896248216461	4.00939593196226	-2.71129749154126	H -0.56788121589496	-0.83732137519591	-2.79866053867703
Al 3.58134118089253	1.63921444571682	-3.53040979171568	H 0.99098087721001	-0.08748784544865	-1.13039311652748
Al 4.28246065619828	2.43084708909187	-1.14403323593434	H 0.98194936024634	-1.68309852338907	-2.50955875938687
B 2.38605854034481	2.47761554310740	0.34942303301101	H -1.43588183660890	2.17623169370316	-0.44022765331866
B 3.83547266378870	4.91128442473314	-1.28322362774422	Ti -0.80606712259026	0.03022704850900	-0.76856271112310
B 3.54410936500490	3.30264097209993	0.95418789246324	Al -0.37254798685120	-2.76073786970109	-0.51021204345551
B 4.20458180783567	4.47902457523572	0.18993628739335	Al 1.58075334620944	0.75458390438822	0.49656532523830
B 2.62181162931429	4.03887820423280	-0.55761382114440	B 0.52762638554921	-0.60194637325874	2.22260000621688
B 1.77663513585746	2.70868025898375	-1.09448294068388	B -0.77290902560623	1.91164871416954	0.53936764456899
H 0.94633295652830	2.62888859514708	-1.97582741424492	B 0.65194598977584	0.88514378238800	2.67646117928435
			B -0.01502061624864	2.07209577926859	1.89132523825512
			B -0.59339889808384	0.48255033486387	1.37222721762678
			B -0.29545784080771	-1.11228193327566	0.96172183675086
i4b			i5b		
C 3.27900361505661	1.24954153511266	-4.04741320350888	C 2.95903140009610	1.48007459912746	-3.96483505347782
H 2.48446066642539	1.74384767846436	-4.68155163705928	H 1.98334024456304	1.80010797367578	-4.35736987737023
H 4.64293225467878	3.32394280192732	-2.63850001167510	H 4.65262854395771	4.73042934651809	-3.98709309231695
H 3.83741125905964	0.58940345649115	-4.71843341461817	H 3.58056908318465	1.09137193232134	-4.78659298006423
H 2.05150851173888	4.89588728860466	-2.75156969401715	H 4.16634869678045	5.03266164696768	-3.52918053091129
Ti 2.78425544722276	2.75528401468500	-2.86226200244076	Ti 3.94534879225900	3.16582385002504	-2.76265910765763
Al 3.01393060690663	0.05189224137463	-2.35354081871611	Al 3.08027489132706	0.64848382751013	-2.26435691064096
Al 5.07951425668753	3.47041775946087	-1.04032860956566	Al 4.90947787389002	3.85038786897243	-0.30075585718750
B 3.64188891732875	2.36177710077035	0.38344551628149	B 3.47987911984949	2.10655037979008	0.56769374864212
B 2.48636058855620	4.75622961627591	-1.62946098924180	B 2.89341908082504	4.50643242725858	-1.59171607145107
B 3.62064299189987	3.89962794909905	0.74226080334668	B 2.72055935667416	3.39338554264420	0.96396806280520
B 3.08076127045708	5.01787082632960	-0.22247305245908	B 2.46910096474982	4.52859440519291	-0.06264284690901
B 2.72448630125789	3.37549518650853	-0.74123804698807	B 2.82889216747356	2.99768965901616	-0.87176986641901
B 3.13924558272380	1.74840354489578	-0.98911882933802	B 4.04228255436955	1.75973562097987	-0.89039611704144
i6b			i6b to i7b		
C 2.64886110415549	1.96198101404414	-3.92576495667583	C 0.46390379902331	-1.16093683852686	-2.15368912037957
H 1.74695939863296	1.54251654853328	-4.40075544386799	H -0.42781047165251	-1.64323220143566	-2.57945143226356
H 3.32833340110083	2.37990303134795	-4.68054620320765	H 1.15507835423208	-0.82626711643556	-2.94118022599785
Ti 1.92162291929366	3.29508975738011	-2.32667655191143	Ti -0.15739736875720	0.43363498096057	-0.79249325797091
Al 3.51158580467960	1.19249432575918	-2.40060333812212	Al 1.24754496236686	-1.79893717172633	-0.53123094432962
Al 4.90750827314708	2.95070273238953	-1.22732623201042	Al 2.81035816875814	-0.84398846284287	1.16311203760975
B 3.32375405032618	2.10230543707773	0.65774224670251	B 0.49368072915504	-0.78747017875543	2.41193550092706
B 3.22896930603381	4.67352713658712	-1.43476947482847	B 1.50891494491298	1.45420982848016	0.13038835707634
B 4.09093790548770	3.44572507294855	0.92418407345121	B 1.67555639436076	0.22418160708165	2.68980877352909
B 3.98916433482932	4.70879714692695	-0.02150429777696	B 2.09173980621816	1.35586067431117	1.61693012745264
B 2.86735524915189	3.39768169078781	-0.36164062861629	B 0.80082010553248	0.35946226231762	1.16606649073553

B	2.45326329064860	1.81880939823268	-0.64985276096866	B	-0.24057885963400	-0.92211678921748	1.00229507297289
C	-0.29656315355591	4.28928712164404	-2.21625183156105	C	-2.26848708972171	0.90621263886653	-0.32059424128825
H	-1.16936258999989	4.83682416980727	-1.84969223953541	H	-3.06583926651407	0.79329019649005	0.41726726537985
H	-0.24262192340833	3.36011618073289	-1.61254627913741	H	-1.49979520381643	-0.18493006635219	0.30520336674937
H	0.57027734176220	4.96992239139892	-2.03305707367232	H	-1.91172387423301	1.95626415759292	-0.26298077521274
H	-0.44076734228539	4.07180244440155	-3.28380331826152	H	-2.67596513023086	0.68476247919170	-1.32138699499003
i7b				i7b to i8b			
C	2.59768049188989	2.25787095514414	-3.91016144348148	C	0.16324604509276	-0.91968803959781	-2.20044026996563
H	2.35706755685309	1.19862270058394	-4.06793840480248	H	-0.59042614880115	-1.71151978328545	-2.29588123153862
H	2.40936535179270	2.83906987432078	-4.82707026539624	H	0.66784173338371	-0.76212458287750	-3.16855307735225
Ti	1.72006019901463	3.32640918284127	-2.29504045585552	Ti	-0.26457387163351	0.92305183582259	-1.27378422152065
Al	4.17982788410131	2.56562052555289	-2.82572123105882	Al	1.38525229661729	-1.08421361203886	-0.65922892000884
Al	5.14187401496360	2.06991352701410	-0.53815761946066	Al	2.56600895367017	-0.48465445556709	1.51605754966708
B	2.98934423268003	2.17944591216046	0.83054089813638	B	0.35949053363234	-0.71125385224540	2.52610174304307
B	3.63463481151627	4.35692241844480	-1.63248108064371	B	1.54973409866528	1.06094152260816	-0.10281866574983
B	4.08817099410352	3.32499486472107	0.93741029839691	B	0.81047776341382	0.76347806573292	2.60590343899731
B	4.27473111050454	4.41553396172193	-0.19088992297487	B	1.39328664060552	1.52675354092135	1.38543649098712
B	3.01610987710314	3.24266907523308	-0.52585913771868	B	0.24930296486074	0.14689756451160	0.90816567422960
B	2.06977634032114	1.92348991801113	-0.41965044268999	B	0.23777685179088	-1.60801287537960	1.23129859858221
C	-0.12964971440710	4.30207409604611	-2.48010262713445	C	-2.01398158621918	1.58788664874807	-0.70761304440950
H	-0.68177237307941	4.43889791344068	-1.54045961940607	H	-0.98125749104784	0.57721785192928	0.41730617798968
H	1.15005252711881	1.54746991097810	-1.11034597882559	H	-0.34238333968925	-2.54352345912724	0.77258991300031
H	0.09597365443944	5.29741376705132	-2.90399395545012	H	-2.34606221852533	2.32647158068850	0.03127658882127
H	-0.76058626891583	3.74995432673388	-3.19667960163445	H	-2.84373322581623	0.91229204915650	-0.98581674477232
i8b				i8b to i9b			
C	2.40328107670700	2.20605100079133	-3.91554144757972	C	-0.69677064545073	-0.43953557695394	-1.75995203819337
H	1.66084052956427	1.39869396991303	-3.95665250797659	H	-1.50540665704466	-1.17728783997917	-1.64461816935511
H	2.81760803085980	2.38219220000963	-4.92170784435128	H	-0.59024706865644	-0.17423427590002	-2.81218986382552
Ti	2.01944126405746	4.04072447909491	-2.91709286676453	Ti	-0.87724855949384	1.08674009042043	-0.14599697646985
Al	3.72920646010297	2.03808645963572	-2.47572642608596	Al	0.98197277428120	-0.76975647165597	-0.81012512702086
Al	4.95555359619333	2.60745231574866	-0.35370985862989	Al	2.80274291854028	-0.27363030387335	1.06885749042774
B	2.96104605904868	2.23360665401333	0.83755240137276	B	1.29161105722378	-1.21029225818322	2.62051048399411
B	3.91560718794433	4.13253889038631	-1.80835558163668	B	1.23812769218565	1.13065202764693	0.14561047457689
B	3.29457367718338	3.73820184915150	0.92737853475194	B	1.25417172713053	0.31190287373786	2.87397658717355
B	3.77512463438942	4.55764667927906	-0.30357022866374	B	1.20972713420052	1.32552326416035	1.71000822393562
B	2.65701504455535	3.13603001695969	-0.75921552394744	B	0.33931607586958	-0.28177481490594	1.38702159965068
B	2.86744843275690	1.35352354259786	-0.48220286332731	B	1.03028359399251	-1.95374435581995	1.24776944002430
C	0.31450004981757	4.87988972252794	-2.56711757074423	C	-1.96644067117621	1.69974307887529	-1.64058163517626
H	1.47782702518552	3.48496786609300	-1.12677311958588	H	-0.92417536202597	-0.16489247780081	1.34313410966551
H	2.35607701774359	0.36379528413594	-0.90919115064667	H	0.73469087790400	-3.00722206325911	0.78032090870927
H	0.01221105215024	5.72868128219702	-1.94051325335727	H	-1.46048403180045	2.52268988666311	-2.18406843361960
H	-0.56550845825997	4.31006570746490	-2.91684761282740	H	-2.86187085567976	1.37511921682751	-2.17967707449711
i9b				i10b			
C	1.85979967064666	2.45830639028670	-4.06051717287063	Ti	1.60264213403033	4.10425039195594	-2.48744297868729
H	1.37698082120280	1.48645744038610	-3.90047285731873	Al	3.33359905652416	2.28992483088253	-2.65668656915748

H 2.65769479276190	2.35645481177543	-4.81518358928014	Al 5.39944723611031	2.58658612320551	-0.78712655707246
Ti 1.52832707318988	4.06687686156905	-2.48038913803799	B 3.16792052648680	2.08037650310216	0.58380668743755
Al 3.44653594197144	2.35318133306329	-2.57108272316612	B 3.48486275200740	4.44215067044770	-1.85550716907046
Al 5.48683163432125	2.57424540341780	-0.67250545933592	B 3.58355949804774	3.54398366461166	0.83788767701948
B 3.21644800753790	2.05825448876329	0.53051067816321	B 3.79431047809789	4.54476283420365	-0.32094609645211
B 3.47443248831256	4.44205546168342	-1.91940748691428	B 2.52725877067909	3.21769476250802	-0.64950844341265
B 3.62568692638166	3.52649317389431	0.77507836210456	B 2.68954051615337	1.35910111256444	-0.71959565802279
B 3.77253659639205	4.53731137219485	-0.38748729295789	H 1.27066124335996	3.61757570063560	-0.74689643267284
B 2.49788032243155	3.21228755926623	-0.62712535068441	H 1.97019716850293	0.49390158588278	-1.11657866990894
B 2.65070910288819	1.36042323193631	-0.75211359495642			
C 0.88818021255541	3.56602179036801	-4.40126960875261			
H 1.23959977890632	3.61862799072456	-0.67713678583413			
H 1.88501150734617	0.53055131774602	-1.13693542117675			
H 1.23889626620836	4.27170533712760	-5.16472126158145			
H -0.14470179305420	3.25126334579691	-4.58048836740023			
i6b to i11b			i11b		
C -0.23577598356245	-0.81357899986716	-1.91482556639306	C -0.03487582933460	-0.94161441959902	-2.17726435139246
H -1.00592293035602	-1.46268526662927	-2.35301077256937	H -0.93326621465684	-1.56844873949923	-2.01945360230635
H 0.27205749294754	-0.26053764590505	-2.71761505923140	H 0.56791798445746	-1.49743860951589	-2.91016674587385
Ti -0.38387227595912	0.33411137095473	0.16284346217369	Ti -0.62475852258192	0.13913344754280	-0.26374166260514
Al 1.03236859716674	-1.72225735113213	-0.72299957773278	Al 1.55840857212779	-0.94369581739131	-0.71654962360737
Al 2.60745240973608	-0.03296901479836	0.29159995145884	Al 3.23828811892016	-0.78616946552031	1.15582085013380
B 1.71667806479373	-1.41760123878464	2.36626321781947	B 1.09223945111563	-0.97475864790545	2.49284257786486
B 1.10542197450204	1.56756184809673	1.03819698633905	B 1.23675736427641	1.32465638865002	0.07112630050093
B 2.54185184092353	-0.13248598976142	2.71808438558748	B 2.00136716943993	0.35013058451486	2.61135113483409
B 2.22660575323457	1.30901324002579	2.14806141216037	B 2.06240588276484	1.44271483547170	1.42889996929137
B 1.00908893932646	0.05882882152686	1.87250037000598	B 0.94453594959038	0.18616469376984	1.27566055536323
B 0.52011492729638	-1.43086209550083	1.31232747901380	B 0.17912673329122	-1.31302248620921	1.23140630081429
C -2.30167081405663	0.85073659797931	-0.75344271282235	C -2.49700097810771	1.02934612638665	0.08168877450826
H -3.01008376109393	0.85673050646242	-1.58416683044903	H -2.60693370378960	1.92129886039592	-0.55570594616145
H -2.78785487862448	0.35261406696963	0.11139667152586	H -3.29861494884349	0.30727807589309	-0.14492889973840
H -2.04196185002861	1.90042559151113	-0.49999829416191	H -2.57385121337200	1.32913112712681	1.13707780212781
H -1.26449750624580	0.04295555885226	-1.47521512272463	H -0.31174381529765	-0.00470595411128	-2.69806443375362
i11b to i12b			i12b		
C -1.22629132104126	-0.63870135215515	-2.19240482688260	C -0.71300001289308	-1.73694880288211	-2.84980363728098
H -1.02379848066536	-1.67663433283614	-1.86958645465433	H -1.21143195319787	-2.71157058609074	-2.85566213672125
H -2.10071332936909	-0.59779212079074	-2.83434233337259	H -0.28583625615799	-1.54462004044265	-3.83927962485638
Ti -0.30358708936242	-0.02244841992032	-0.29202264115456	Ti -0.11333655062621	-0.25582246841351	-0.55040961920838
Al 2.26470583306611	-0.92200490695809	0.12869069062631	Al 2.18289504402998	-1.15751617147624	0.46655070694790
Al 4.07405528233816	-0.65875300441259	2.15390055986053	Al 4.00830198150224	-0.56216640794345	2.89394101500684
B 1.25580769404118	-0.85909239384440	2.61858349430539	B 0.92103790565602	-0.58973933943434	2.57867723778635
B 1.34729934561485	1.33946024142853	0.10883969385106	B 1.40768703636747	1.13368134540207	-0.20683913501869
B 2.20070648030493	0.44757145100702	2.63670615994944	B 2.10835328027577	0.47575785241029	2.42086285856013
B 2.27496043542913	1.45211001369465	1.37732034928931	B 2.33156071574053	1.29369434961885	1.06001572908463
B 0.99089152185223	0.36981751155246	1.49939106293992	B 0.8283559099740	0.51552486851266	1.28037062792808

B	0.23321204236719	-1.18788297160169	1.46606841431923	B	-0.11875968072114	-0.90162301434066	1.43561829259978
C	-2.25416688846008	0.64066883685145	-0.66182954707144	C	-1.70532776948340	-0.62211957473901	-2.46168173272708
H	-1.77131979370567	1.63701417968710	-0.53218692746535	H	-1.24620706580601	0.38875469195948	-2.48865725651624
H	-3.17346011779160	0.72221792439005	-1.23204260988883	H	-2.53343646356520	-0.57144877056336	-3.17624684043590
H	-2.43237053249646	0.12068040437567	0.30920826047431	H	-2.18952956066556	-0.80398277186114	-1.47905261852060
H	-0.35593108212186	-0.16623106046782	-2.68429334512581	H	0.15820075854704	-1.85478815971611	-2.16859886662820
i13b				i13b to i14b			
C	1.34060590978660	2.23715439537761	-3.89800752793827	C	-1.71229648279539	-0.25797131415206	-1.70577587057349
H	0.37989300227009	2.55877777104776	-3.49297564205532	H	-2.41369368529176	-0.18901340110811	-0.87227805510038
H	1.21183241325353	1.71077487038973	-4.85558633934710	H	-2.13854036767468	-0.55874564678237	-2.66477221116431
Ti	2.81565252745168	1.38200875316897	-2.70988702168434	Ti	-0.07858155850645	-1.43494764107356	-0.65190281661932
Al	4.99214302358636	2.18292910160238	-1.28760782082108	Al	2.08123733707368	-0.18063019930592	0.58548702926339
Al	5.70511793557318	3.94087265705112	0.81229644571295	Al	2.65702468862876	1.21915076468299	2.92864117602556
B	3.21380692199349	2.19346199221406	0.46951498946874	B	0.64546902657567	-0.83246512113222	2.54955058158665
B	3.26809431831047	3.53804954248765	-2.54295523421323	B	-0.01335088918228	0.84237072628451	-0.21570253707528
B	3.57025090573856	3.73405295473580	0.20805567698567	B	0.47899285699376	0.73251070155615	2.52528949333856
B	3.63048410509599	4.33745331171793	-1.23907256476991	B	0.34192759304494	1.49517128503527	1.15309692688917
B	2.76640821962451	2.84747908251307	-1.04447694650004	B	-0.18899121487798	-0.19029117683797	1.18278918981277
B	2.75451221325614	1.17446444585880	-0.62778344909530	B	0.43844055314142	-1.83706668768423	1.36077389739075
C	2.40191382819145	3.37633817987098	-3.93082984546873	C	-0.53561106243713	0.55294458741778	-1.65607541990193
H	1.87912396037283	4.34092784665086	-3.95174075086481	H	-0.19258867849500	1.13699968090514	-2.51023869608675
H	3.04194680549485	3.34156588531303	-4.82355439940900	H	0.63056188380244	-0.49801655780540	-2.00888268778539
i14b				i14b to i15b			
C	1.14004723302532	2.42343832214189	-3.87014414844823	C	-1.25417860398589	-0.37154609586468	-2.09536466611552
H	0.42861398529597	2.21184313345544	-3.07133790325545	H	-1.68148968755459	-1.27320499349551	-0.76862669914589
H	0.82236304601881	2.09142491517477	-4.86207014285796	H	-1.94042438070965	-0.55288202626136	-2.91715528845373
Ti	3.03131040979882	1.61400609648641	-2.94192767849259	Ti	0.08404925551513	-0.99003886774900	-0.81708412181342
Al	5.25032383318611	2.01028600895858	-0.98779469234606	Al	2.10473176764595	-1.34158545732041	0.77600934861299
Al	5.62409168936653	4.13756278147947	0.90332117636626	Al	2.40173749926457	1.04048857462353	1.87656044266714
B	3.28276959923531	2.11479891779541	0.29893200460835	B	0.19503111818097	-0.33825683060029	2.76216216700715
B	2.71184996434207	3.91457729864937	-2.49585418684862	B	-0.17537062329520	1.17130021520876	-0.28339617736015
B	3.55513428043681	3.69741129775766	0.17589527969924	B	0.04710908732714	1.19869728626405	2.51801764942470
B	3.36868863640733	4.48615135573533	-1.17933913709250	B	-0.12973306097285	1.89614645000033	1.11372628275445
B	2.77593441252078	2.87931019335432	-1.10752301659725	B	0.03216315770214	0.15696887127080	1.05193603026183
B	2.90024539183123	1.16390986333395	-0.90768766372699	B	0.25724390329495	-1.46475897978817	1.67110938348312
C	2.01822605421640	3.54651581053889	-3.76458508653119	C	-0.78494323463062	0.87127691243517	-1.69451255473524
H	2.35709173912695	3.99488090797042	-4.70632488509436	H	-1.01303332709569	1.76291410323926	-2.28291294926793
H	4.83127240519141	2.02396258716792	-2.69224324938252	H	1.85710712931364	-1.76551916196250	-0.91046884731950
i15b				i16b			
C	1.79504160107719	2.42389895822479	-4.45395981333882	H	2.33232	0.44726	-0.87376
H	2.32322848308108	0.42683096895212	-0.87620051388810	Ti	2.46672	1.73821	-2.63564
H	1.43726943320351	2.44678231976380	-5.48190739171974	Al	4.82435	2.37872	-1.70378
Ti	2.43860269710631	1.73419555875080	-2.71025531352602	Al	5.81988	3.93005	0.42416
Al	4.84810972391979	2.27958231807454	-1.59883498699533	B	3.11268	2.53864	0.69042
Al	5.82782664211843	4.01387567259286	0.38806309549800	B	2.89146	3.75197	-2.40358

B 3.12722786710276	2.50997651826943	0.66894451300401	B 3.27246	4.05921	0.35610
B 2.83397685747169	3.83853637880992	-2.39660511851899	B 3.22428	4.62017	-1.11404
B 3.29753553434098	4.0389666324416	0.33624034496823	B 2.64685	3.02280	-0.89375
B 3.24756965442041	4.63619826127189	-1.09439115953572	B 2.87422	1.44062	-0.42724
B 2.65728966679161	3.01808282473840	-0.91867183790353	H 4.11503	1.26933	-3.12618
B 2.86733801988494	1.41519419627826	-0.42195827632613			
C 2.20266743549509	3.58836710389027	-3.83172983343140			
H 2.17493210393304	4.53554354579071	-4.38090630212075			
H 4.11153663005304	1.28555630134791	-3.08363389616560			
i17b			i7b to i8c		
C -0.06067774871713	-0.92906397754654	-2.17392823383998	C 0.16324604509276	-0.91968803959781	-2.20044026996563
H -0.95424571010067	-1.56990497982989	-2.03574980388050	H -0.59042614880115	-1.71151978328545	-2.29588123153862
H 0.58812725752814	-1.48621941852338	-2.86485786766370	H 0.66784173338371	-0.76212458287750	-3.16855307735225
Ti -0.59057666958432	0.11164558242886	-0.29406180572464	Ti -0.26457387163351	0.92305183582259	-1.27378422152065
Al 1.59648969901303	-0.94246268743894	-0.68569366069966	Al 1.38525229661729	-1.08421361203886	-0.65922892000884
Al 3.38428905052386	-0.82888580282615	1.19446852140525	Al 2.56600895367017	-0.48465445556709	1.51605754966708
B 1.09090775546774	-0.98125897863372	2.46604801909583	B 0.35949053363234	-0.71125385224540	2.52610174304307
B 1.16519324829126	1.34862542382650	0.08352730547841	B 1.54973409866528	1.06094152260816	-0.10281866574983
B 2.01582568685316	0.32632929861382	2.57109949231484	B 0.81047776341382	0.76347806573292	2.60590343899731
B 2.05793701805057	1.42876384860559	1.40530237903996	B 1.39328664060552	1.52675354092135	1.38543649098712
B 0.90362040134737	0.21158435398863	1.29633600785298	B 0.24930296486074	0.14689756451160	0.90816567422960
B 0.11273285757325	-1.27330589476647	1.23789739299656	B 0.23777685179088	-1.60801287537960	1.23129859858221
H -0.33322001624628	-0.00290096789829	-2.71852046637537	C -2.01398158621918	1.58788664874807	-0.70761304440950
			H -0.98125749104784	0.57721785192928	0.41730617798968
			H -0.34238333968925	-2.54352345912724	0.77258991300031
			H -2.34606221852533	2.32647158068850	0.03127658882127
			H -2.84373322581623	0.91229204915650	-0.98581674477232
i8c			i8c to i9c		
C 2.40328107670700	2.20605100079133	-3.91554144757972	C -0.69677064545073	-0.43953557695394	-1.75995203819337
H 1.66084052956427	1.39869396991303	-3.95665250797659	H -1.50540665704466	-1.17728783997917	-1.64461816935511
H 2.81760803085980	2.38219220000963	-4.92170784435128	H -0.59024706865644	-0.17423427590002	-2.81218986382552
Ti 2.01944126405746	4.04072447909491	-2.91709286676453	Ti -0.87724855949384	1.08674009042043	-0.14599697646985
Al 3.72920646010297	2.03808645963572	-2.47572642608596	Al 0.98197277428120	-0.76975647165597	-0.81012512702086
Al 4.95555359619333	2.60745231574866	-0.35370985862989	Al 2.80274291854028	-0.27363030387335	1.06885749042774
B 2.96104605904868	2.23360665401333	0.83755240137276	B 1.29161105722378	-1.21029225818322	2.62051048399411
B 3.91560718794433	4.13253889038631	-1.80835558163668	B 1.23812769218565	1.13065202764693	0.14561047457689
B 3.29457367718338	3.73820184915150	0.92737853475194	B 1.25417172713053	0.31190287373786	2.87397658717355
B 3.77512463438942	4.55764667927906	-0.30357022866374	B 1.20972713420052	1.32552326416035	1.71000822393562
B 2.65701504455535	3.13603001695969	-0.75921552394744	B 0.33931607586958	-0.28177481490594	1.38702159965068
B 2.86744843275690	1.35352354259786	-0.48220286332731	B 1.03028359399251	-1.95374435581995	1.24776944002430
C 0.31450004981757	4.87988972252794	-2.56711757074423	C -1.96644067117621	1.69974307887529	-1.64058163517626
H 1.47782702518552	3.48496786609300	-1.12677311958588	H -0.92417536202597	-0.16489247780081	1.34313410966551
H 2.35607701774359	0.36379528413594	-0.90919115064667	H 0.73469087790400	-3.00722206325911	0.78032090870927
H 0.01221105215024	5.72868128219702	-1.94051325335727	H -1.46048403180045	2.52268988666311	-2.18406843361960
H -0.56550845825997	4.31006570746490	-2.91684761282740	H -2.86187085567976	1.37511921682751	-2.17967707449711

i9c			i10c				
C	1.85979967064666	2.45830639028670	-4.06051717287063	Ti	1.60264213403033	4.10425039195594	-2.48744297868729
H	1.37698082120280	1.48645744038610	-3.90047285731873	Al	3.33359905652416	2.28992483088253	-2.65668656915748
H	2.65769479276190	2.35645481177543	-4.81518358928014	Al	5.39944723611031	2.58658612320551	-0.78712655707246
Ti	1.52832707318988	4.06687686156905	-2.48038913803799	B	3.16792052648680	2.08037650310216	0.58380668743755
Al	3.44653594197144	2.35318133306329	-2.57108272316612	B	3.48486275200740	4.44215067044770	-1.85550716907046
Al	5.48683163432125	2.57424540341780	-0.67250545933592	B	3.58355949804774	3.54398366461166	0.83788767701948
B	3.21644800753790	2.05825448876329	0.53051067816321	B	3.79431047809789	4.54476283420365	-0.32094609645211
B	3.47443248831256	4.44205546168342	-1.91940748691428	B	2.52725877067909	3.21769476250802	-0.64950844341265
B	3.62568692638166	3.52649317389431	0.77507836210456	B	2.68954051615337	1.35910111256444	-0.71959565802279
B	3.77253659639205	4.53731137219485	-0.38748729295789	H	1.27066124335996	3.61757570063560	-0.74689643267284
B	2.49788032243155	3.21228755926623	-0.62712535068441	H	1.97019716850293	0.49390158588278	-1.11657866990894
B	2.65070910288819	1.36042323193631	-0.75211359495642				
C	0.88818021255541	3.56602179036801	-4.40126960875261				
H	1.23959977890632	3.61862799072456	-0.67713678583413				
H	1.88501150734617	0.53055131774602	-1.13693542117675				
H	1.23889626620836	4.27170533712760	-5.16472126158145				
H	-0.14470179305420	3.25126334579691	-4.58048836740023				
i2			i2 to i3d				
C	0.95915884295571	-0.12790495980499	0.25428850613157	C	-2.40243226215977	0.70295000401141	-0.50699011833882
H	1.69282081224708	0.62985079843722	0.62012538256515	H	-2.20877464090345	1.67932924118563	-0.01840237931590
H	1.22755846487577	-1.15918578854878	0.55598608172410	H	-1.47237995538775	-0.37256567466836	0.33483719066835
H	0.78393582810214	-0.05093404730169	-0.82781641597417	H	-2.81309329980501	0.86040786495765	-1.52119950830308
H	0.02414011303288	0.10717690722544	0.77193996826581	H	-3.15993377309896	0.18569169821948	0.08792757969084
Ti	3.37734745755074	-0.57112252315060	-0.06988403022298	Ti	-0.26014052585877	0.73446004270725	-1.08938674917886
Al	4.39827509700194	-3.84175188477870	-0.13395074710165	Al	2.27026176837803	-3.15272869344470	0.13520625649334
Al	6.03110312890568	-0.77602453125288	0.07464414005078	Al	2.23548556473132	-0.32576960629320	-1.06484103249008
B	5.45961313630213	-2.08195356402023	2.13648790831381	B	1.06708453565048	-1.50406863861438	1.05984633299533
B	4.46357019698944	0.81553204396142	1.00467285263144	B	1.28414459879513	1.64312367086905	0.07297642880020
B	6.14933244522602	-0.75113370002726	2.56408791508515	B	2.25057739440125	-0.52458795627160	1.47372683912068
B	5.63768296422252	0.64810910594437	2.07109907830813	B	2.31103997399800	1.00354980589782	1.09318520732276
B	4.51762260570286	-0.67844713776116	1.78299062571491	B	0.85053687164613	0.13278034053787	0.72545311447733
B	4.19038421688479	-2.14810586892211	1.14420957450788	B	0.04762374961336	-1.06257209909392	-0.11266478060540
i3d			i4d				
C	1.42379798369867	-0.03917946340034	0.21197409270581	C	1.65599250177189	-0.21871536804623	-0.22017495500687
H	1.32757009419644	1.04060068303548	0.41482071552458	H	1.70970965832713	0.79877134718887	-0.64442351327709
H	3.22091964103673	-2.48537037283089	0.34719395737866	H	3.03093800001493	-2.64335394506635	0.87806974527471
H	0.85023059816359	-0.27910107113620	-0.70646589845243	H	0.92677424541241	-0.80901558431382	-0.80893485101410
H	0.98924044398629	-0.59778355715875	1.04735293854872	H	1.29606554700666	-0.15051811352088	0.81112916891757
Ti	3.45038850899570	-0.35652425610978	-0.27627710551783	Ti	3.55453445853814	-1.07205150358229	-0.58449986916269
Al	6.97840489679268	-3.13225275427580	1.61661252539826	Al	6.68761007200327	-3.34108217082762	2.39008026701537
Al	6.18381227965800	-0.94714283155462	0.06514753822702	Al	6.21088266596744	-1.90966527748810	0.05678807113049
B	5.09750837497474	-2.08413393473530	2.25899007380146	B	5.04182740140779	-1.80352924397179	2.48857816151553
B	4.74981362698014	0.88103373170342	0.79263712896453	B	5.08751639808796	0.27184519611688	-0.10150263909765

B 5.92935164948045	-0.80065647452611	2.62372713351547	B 6.09052357759595	-0.64653401614012	2.28703885006126
B 5.72964718413705	0.61483766480453	1.99671211520416	B 6.08778566393934	0.37872248068927	1.11004851079810
B 4.49524275602026	-0.60350696554337	1.63624413590236	B 4.66674611309389	-0.65153296700509	1.27817216138487
B 4.20871119187914	-2.08303747827224	0.92016827879920	B 4.10293861954059	-2.22120444205346	1.25628800350554
			C 3.73192799761748	-1.25816398294987	-3.05116726557233
			H 2.67987981128830	-0.95039334471292	-3.09977560680632
			H 3.83202988321041	-2.29063063213040	-2.67532662711733
			H 4.35728912351795	-0.52218090928678	-2.48345519927923
			H 4.15312773165823	-1.24987929289924	-4.06010319326980
i4d to i5d			i5d		
C -2.37624250321358	0.79630665785940	0.03574249834333	C 1.53906083810313	-0.19853604916990	-0.24888486769391
H -2.37176804563487	1.74709136612400	-0.52253444144061	H 1.49433415064605	0.78551853643691	-0.74801618124468
H -1.00570973520976	-1.55320234229752	1.30051106444352	H 2.98178857378310	-2.51914560672349	0.77961135712303
H -3.16145512917814	0.14492664370214	-0.39522020397504	H 0.82265030772823	-0.86980077920409	-0.75612640264563
H -2.62727908412974	1.00199989295671	1.08120105367068	H 1.23805264900330	-0.08115782543386	0.79746420653625
Ti -0.53491349912455	-0.16329474608772	-0.36670069910243	Ti 3.46593261301180	-0.95700657494075	-0.64286949491525
Al 2.78546178336093	-2.15648628700615	2.74698317802101	Al 6.73080847668102	-3.37906121337297	2.05533076737433
Al 2.14234893390953	-1.12516232039210	0.25351955710721	Al 6.17447874098789	-1.83608548674099	-0.12378731575658
B 1.12325181004081	-0.61476769020690	2.67705940911539	B 5.06378897896003	-1.84668171713965	2.34466124451248
B 1.11300735196823	1.13106622896417	-0.12724365343100	B 5.16916192127288	0.40406489732836	-0.06063310010309
B 2.19634631529051	0.46930718689252	2.29524670160345	B 6.13549622891395	-0.71886808936780	2.23533953944072
B 2.20436081041872	1.31075570769057	0.98265699555627	B 6.18507880273046	0.36616544101111	1.13258489342958
B 0.73041428458942	0.40204190023898	1.36038175128848	B 4.68922252311321	-0.57253165039016	1.22655012585342
B 0.10789373210969	-1.14671318385331	1.55887108142083	B 4.09166766821798	-2.15190244585964	1.11212644039110
C -0.14341411988486	-0.11816585706913	-2.56836804732516	C 3.71335726170360	-1.46387082589812	-2.67628007776141
H -1.14114676575738	0.26274808796787	-2.83569152932285	H 2.85320234960293	-0.97282408769230	-3.16742537070292
H -0.14403451017526	-1.22403465550448	-2.55322409380488	H 3.55493467628648	-2.55730835189308	-2.71589351590254
H 0.53273207073698	0.64166768190238	-1.58797549124986	H 4.62565009994392	0.80094263005672	-1.06449871958468
H 0.57014629988333	0.19391572811859	-3.33521513091832	H 4.62541585930996	-1.22781666100627	-3.23316706835022
i5d to i6d			i6d		
C -2.23604994737033	0.57772721495593	-0.72118315236001	C 1.29367633510225	-0.60829785316830	-1.71377035100660
H -2.15929489756442	1.66749928892690	-0.79442728740740	H 1.07999558278073	0.40352645392211	-2.07479593914305
H -0.52879146827052	-1.67975177178747	0.55892267631821	H 3.08687377141361	-2.56621972356714	0.24706664102641
H -3.13581756279971	0.23645646149325	-1.23449581321844	H 0.34451734267115	-1.13653800473668	-1.57745182396745
H -2.27272409551618	0.24891963565763	0.31997649842395	H 1.66789468163674	-0.48754095777502	-0.65999833805863
Ti 0.14623483444547	0.19896721139948	-0.64289148581203	Ti 3.77057654007502	-0.73467248268244	-0.83683267341155
Al 2.81565924518353	-2.37397018332223	2.35551581692239	Al 6.50089626072526	-3.52806684551365	1.90502578269414
Al 2.60708903250964	-0.59342379862798	0.31412437307191	Al 6.20459082756430	-1.67938082567504	-0.13848090831280
B 1.15117986327300	-0.92561671254405	2.53422619859045	B 4.98234200015952	-1.99682369445879	2.16716991902686
B 1.49616408420132	1.58047791190861	0.40484131172499	B 5.25900739490691	0.51286929226534	-0.00652396376119
B 2.06354010206578	0.31968940908522	2.73839124845993	B 5.91371567659243	-0.73107418305434	2.31646173543386
B 2.24545439470999	1.51610068835647	1.77671656467815	B 6.09139752385510	0.44776743778442	1.33387421749319
B 0.82383624281041	0.44989456852942	1.49221874658919	B 4.61067519968413	-0.54116520223533	1.19107880299648
B 0.38550431555246	-1.12197969354390	1.10834144881604	B 4.01931785295237	-2.05163288649394	0.83029739133804
C -1.20930935115945	-0.39028609982662	-2.10657583810942	C 2.20064012860087	-1.38367639704577	-2.68475892644126

H -1.71949260398130	0.07547533539500	-2.95123148628547	H 1.80737906740367	-1.32261080824128	-3.70648628085514
H -1.52216416688350	-1.43850568540427	-2.01960394583248	H 2.28115907296305	-2.44715468023816	-2.42644939725749
H 1.10714975869691	2.03523030841476	-0.66470911355285	H 4.84221822392568	0.95543114115056	-1.09314912319915
H -0.05816777990308	-0.38290408906616	-2.46815676101712	H 3.23721132698698	-0.94565228023650	-2.83299403459464
i7d			i8d		
C 1.67983790780033	-0.80365964296559	-1.51944684097632	C -1.74382964592187	0.26815853828580	-0.90220022165721
H 2.24338768667127	0.12061284827221	-1.24107538035741	H -1.66167606413783	1.37140230004374	-0.82148049793525
H 0.62642435547145	-0.52793007672356	-1.40558234096318	H -2.70422819949960	-0.02380944398024	-0.47066613402246
H 1.84046149405672	-1.59278245037017	-0.74162982198188	H -1.03350599361226	-0.48817787353325	0.08963546814768
Ti 3.96957997157058	-1.21993227395789	-1.00323105679186	Ti 0.43663340504083	0.20465287334343	-0.68722919547031
Al 6.51873976022627	-3.33512338739123	2.46873127228543	Al 2.27134119105543	-2.36651592289911	2.80056380535632
Al 6.42902321207610	-1.37327574672199	0.07975511164649	Al 2.71512329594843	-0.51853795150298	0.60119439431956
B 4.91559220176278	-1.82763833627032	2.17651065528992	B 0.86124692363508	-0.64503690946339	2.55597242093818
B 4.89755248275159	0.47844757011512	-0.15347684787794	B 1.63617223148885	1.66134782681143	0.32047985205242
B 5.66191646543050	-0.42624021629354	2.32309452907611	B 1.93886184025096	0.49891575871219	2.80324023307901
B 5.59323684661515	0.71384990338454	1.25259563615552	B 2.24538539871305	1.66194835149714	1.78338094368216
B 4.49831064867531	-0.64637649917287	1.06296818028433	B 0.90040702760753	0.61588935820580	1.44139228602002
B 4.23633851092099	-2.26343199153903	0.76237917870345	B 0.29832142054186	-0.89465810410874	1.06561533421002
C 1.97534852815343	-1.28394567401219	-2.95351902030312	C -1.58300448576123	-0.23838359751470	-2.34356683076899
H 1.79355822970347	-0.48575698366853	-3.68062909034016	H -2.23350325291365	0.29000639613626	-3.05232511693053
H 1.35955907617713	-2.15139956623802	-3.21297994123682	H -1.78570628658266	-1.31304849186386	-2.41678605292350
H 3.02612543193655	-1.60554139644683	-3.12909900261249	H -0.55803880585293	-0.08415310816951	-2.76722068809714
i8d to i9d			i9d		
C 1.88751699124742	-0.57252162905657	-1.41638766258697	C -2.22283184030157	-0.29665072708261	-1.24777149706899
H 1.82691905355847	0.52028008129419	-1.43817070694763	H -3.18365995786086	0.22107097483833	-1.18578461572402
H 1.09200623736461	-0.99845193611362	-0.80280323149000	H -2.29988601982753	-1.37714773563859	-1.11913973734420
H 3.14301504475086	-2.71099808060871	0.34037827990135	H -1.17034541566119	-0.34147645475460	1.96832613139701
Ti 3.87602179492998	-1.16568355588203	-1.07579260901819	Ti -0.68007669063126	0.59825901206386	0.01248114934596
Al 6.42379867856767	-2.96135300948836	2.66356949573347	Al 2.08131529434066	-2.40966090604249	2.88708635720105
Al 6.32305721357599	-1.69027455273605	0.17427203248207	Al 1.45089527286957	-1.15144837713620	0.19800841557275
B 4.67100570720277	-1.60757013935072	2.29363750123115	B 1.51542369977160	-0.25681458751438	2.59224961205433
B 5.11222800374248	0.35743898042700	-0.34909677621439	B 1.27707777625121	1.24896177250979	-0.34639984571932
B 5.62954572332003	-0.36212196969514	2.25460545556421	B 2.72417474263188	0.34563200773910	1.78407579904532
B 5.79269232751629	0.61505230902834	1.04702885097014	B 2.63197300207321	1.08047524873267	0.40741865274588
B 4.44973612382295	-0.53494424752972	0.96928026807377	B 1.13200377516109	0.88140367383117	1.35915446636016
B 4.05516769706174	-2.15496549267647	0.91191683559995	B 0.03604204122999	-0.22453056123559	1.92638289756870
C 2.03222077758253	-1.21079065569354	-2.79809546418462	C -1.22074908602143	0.21853804100109	-2.16759224280112
H 1.94215307322137	-0.50321511449805	-3.63039452243776	H -1.47916072464086	1.11171664272481	-2.74514744008477
H 1.35553759972473	-2.05568074360517	-2.96634190621275	H -0.64302442058021	-0.49433585925914	-2.75819524612810
H 3.06106359280992	-1.67845601381532	-2.98535772046382	H 0.05082855119570	0.84600783522279	-1.56515285642065
i10d			i11d		
C	1.532	-1.384	-1.633	C 1.47324554118669	-0.16108055117568
H	0.555	-0.932	-1.427	H 1.54546848209171	0.91153775068413
H	1.533	-2.475	-1.591	H 2.97449993125580	-2.54777132807939
Ti	3.078	-0.492	-0.383	H 1.00253964288246	-0.25337574893005

Al	6.269	-3.450	1.693	H	0.80908513620350	-0.62988597723346	0.44825694110764
B	5.042	-1.656	2.248	Ti	3.41454368444886	-0.99912454278582	-0.49102100622679
B	4.938	0.703	-0.074	Al	6.91990885354344	-3.27872279658929	2.16835246684694
B	6.178	-0.619	1.944	Al	6.06837980212255	-1.93938273292086	-0.11282079772429
B	6.155	0.522	0.890	B	5.20021651784083	-1.82467625176299	2.36809173077286
B	4.600	-0.267	1.300	B	5.16522805164193	0.30394422836714	-0.16553529121584
B	3.755	-1.711	1.290	B	6.22077855881869	-0.65485215532462	2.15690440144722
C	2.462	-0.708	-2.491	B	6.23445065210913	0.35076529861985	0.98156919740420
H	2.205	0.266	-2.916	B	4.72809994534918	-0.56212475746350	1.25083699262947
H	3.161	-1.280	-3.100	B	4.07866918738004	-2.12127397895937	1.25680365677344
Al	5.600	-1.638	-0.338	H	4.57205858312511	0.63193760355392	-1.17805894853673
i12d				i3d to i4e			
H	3.06398847135850	-2.61494768080377	0.93771334412726	C	-2.52261106246980	0.68412762582845	-0.62740693667636
Ti	3.54026527541830	-1.02435863799388	-0.46713202578402	H	-1.25242045452443	1.57096856365622	-0.39135910620557
Al	6.73668817017839	-3.46290258039097	2.13764300223523	H	-0.49078767701928	-2.12657399042895	-0.54318077186773
Al	6.05346355218452	-1.90060909630369	-0.09632463592902	H	-2.82297356341978	0.68664516211522	-1.71229457244587
B	5.31097087444221	-1.84172836133846	2.38160799002981	H	-3.26739593854337	1.17785902704404	-0.00413021646293
B	5.12278682313279	0.30203805715354	-0.17662518276470	Ti	-0.80059826723267	-0.00505902210363	-1.08237643837396
B	6.23058304953722	-0.56439421887847	2.15359997058508	Al	3.33735602102041	-1.99806515075836	0.45082748382988
B	6.20143710184741	0.43416425951116	0.97837673254653	Al	2.04135922612123	0.06408943121284	-0.91683826354112
B	4.73377482354429	-0.51902924425599	1.29650991715633	B	1.36515525403086	-1.37760607883483	1.31597921228451
B	4.07673699437180	-2.03811662143360	1.30076622728769	B	0.26808576431138	1.45867795059913	-0.01879201096276
H	4.50613862398453	0.58860270473414	-1.22372042949020	B	1.93175057381827	0.07136359354390	1.63437035853389
				B	1.35185917492068	1.41809079883554	1.11378228321368
				B	0.44009447163033	-0.06682176846222	0.75022837398971
				B	0.42112647735615	-1.55769614224736	0.03119060468462
i4e				i5e			
C	1.48836000813108	-0.37746241498518	0.26623240080691	C	2.46665219791114	-1.52903370855805	0.48163416025798
H	3.89052723172278	1.47009273995533	0.13244206821937	H	1.57283234440405	-1.25567170294621	1.05487181899054
H	3.19900639754805	-2.51876899797490	0.49214769548876	H	2.24370599769272	-2.14961323307700	-0.39174209267095
H	1.27917748293559	-0.01065627400987	-0.78298712890311	Ti	3.44104632158170	0.47327938140361	-0.27486968063921
H	0.58788365257487	-0.43181048359226	0.87760955666997	Al	3.46031051166433	-3.18134139969724	2.10498985463514
Ti	3.27773428275204	-0.52259822365023	-0.21119350147101	Al	5.85964347129340	-0.61700738331066	-0.23344881488001
Al	6.97107074035345	-3.12426092420048	1.42683479303380	B	5.10515661744039	-1.56897003458283	1.99462766921897
Al	6.13726161398593	-0.91083677631277	0.04795832283115	B	4.98860954217356	1.50940768007723	0.66247043256706
B	5.18833047761154	-2.04358029759202	2.27760308086053	B	6.19270408602193	-0.45858644671212	2.21553663369871
B	4.68761995147032	0.89961310049036	0.85231659323754	B	6.13113212047313	0.98908689586718	1.62535110284632
B	6.01887989855504	-0.74464276143308	2.55786143673750	B	4.61904351237047	0.12071230616465	1.55339761244449
B	5.75824332097198	0.66183342209469	1.96086391124499	B	3.87924491697280	-1.23703326462851	0.96178399353086
B	4.49144070988298	-0.58424334071882	1.65221182150319				
B	4.22788693150429	-2.10112392807077	0.99717215974040				
i6e				i6e to i7e			
C	2.83862118316713	-2.03271803642965	0.23904132067369	C	-1.53589002311761	-1.44992509903618	0.71885834940939
H	1.81824339113644	-1.64198872206653	0.33666613119692	H	-2.55619477993039	-1.04699355279942	0.78994536859247
H	2.87910929457211	-2.98801409510694	-0.29277308054946	H	-1.51380511306235	-2.47505637736376	0.34039908343491

Ti 4.06386001432865	-0.43204007650497	-0.95441076158754	Ti -0.48561894946785	0.08654819812015	-0.67488480373898
Al 3.15735073287718	-2.71209962899729	2.66250879523706	Al -1.29013673127976	-1.61828566342096	3.22167048187456
Al 6.31279143545515	-1.14164285314683	0.30505882395891	Al 1.90831995992378	-0.54127206891970	0.52856085243472
B 4.83596953531390	-1.16546011584073	2.36616510488514	B 0.50606367416328	-0.28173163845542	2.64270332961941
B 5.24841045735830	1.06555752730991	-0.09800754229302	B 0.81369354346200	1.62461140324392	-0.06261584950292
B 5.83852197160721	0.04349472279373	2.41393819964757	B 1.51958856862656	0.91102961561665	2.50435654240102
B 6.01533297367705	1.11007203602608	1.28390306371241	B 1.67237094482547	1.81265285285460	1.24157495488008
B 4.58053309786407	0.12067719781031	1.12293201473001	B 0.19868625225512	0.82910203674230	1.28004862396441
B 4.02727468555050	-1.43219988116903	0.97269210239668	B -0.31410790175112	-0.77071380658119	1.32872043730406
C 4.47343343998195	-0.33276886085545	-3.40675144758666	C 0.15920501657894	0.50151999151851	-2.77827286205165
H 3.37285622730961	-0.28720819529527	-3.42168993127229	H -0.86979985075398	0.73614541059481	-3.11110758229891
H 4.91999613063878	0.46586933732679	-2.76867397583968	H 0.57022553620835	1.22024690372294	-1.64181827165709
H 4.83017397529557	-0.13496851328790	-4.42089302554552	H 0.85361503204130	1.04013843505553	-3.42769970397380
H 4.83375540386602	-1.33416482256616	-3.12049977176416	H 0.36378482127826	-0.57801664089281	-2.90043895069168
i7e			i7e to i8e		
C 2.90098275341453	-2.07237776914473	0.18512122739862	C -1.60089880189249	-1.21636893576878	0.33059683915614
H 1.85534913010300	-1.74531784703837	0.26462774314805	H -2.64999693976131	-1.02496397892450	0.58619721757432
H 3.00973222797563	-3.03310951159001	-0.32768278181634	H -1.47887761987658	-2.12531457834892	-0.26609624774858
Ti 3.91193845308990	-0.43566131162272	-1.02829861461251	Ti -0.68764356130923	0.52362626471238	-0.83822303200027
Al 3.19224016527445	-2.69817297158925	2.59560592142178	Al -0.54030059370499	-2.48915906714555	2.41851300779352
Al 6.33463450266368	-1.02060501945493	0.12839488763664	Al 2.21349306317134	-0.21399944206090	0.10104033704909
B 4.92628775443402	-1.11860933421466	2.24580792971652	B 0.72946205156345	-0.53537880269662	2.16774425561906
B 5.19575094191940	1.15207444070688	-0.11627829402729	B 0.61074039883547	2.13870384770420	0.20476156919292
B 5.90221247128340	0.09051455464622	2.32018389357456	B 1.67613729830081	0.70720970328535	2.29803043684204
B 6.03102503483837	1.16610524631632	1.21561942113178	B 1.63188982988032	1.95152608973365	1.35854057875588
B 4.53871236041885	0.18144106604376	1.07003341921135	B 0.24321863894723	0.88292180787939	1.23842188249786
B 4.05230584619270	-1.41444418962363	0.93626984143653	B -0.47530157748851	-0.60967626600416	1.13924888796918
C 4.32924203826708	-0.56962285818224	-3.10562616185143	C -0.18487710862534	0.17878005309401	-2.61764511718370
H 3.65337401857686	0.09874828255049	-3.66978973067367	H 0.48502228831549	0.06192525897275	-3.46885832070943
H 4.81885895160630	1.51478625920694	-1.20455164893630	H 0.06797481770478	2.58411961412566	-0.77872721705614
H 5.35334542590972	-0.39463472091637	-3.45344936667003	H 0.97539549094701	-0.22970427111782	-1.24313599006827
H 4.05715613403198	-1.6155595609369	-3.34799179608825	H -1.01543767500744	-0.58424729744015	-2.63040908768362
i8e			i9e		
C 2.77790428373584	-1.94261982627421	0.09643341078445	C 3.21933622551180	-2.24877557083305	0.16698206370099
H 1.72508085802746	-1.67981409405778	0.25887617241816	H 2.20682011403841	-1.81576527420068	0.09909913795908
H 2.88779117918552	-2.90544144644052	-0.41139237705893	H 3.26020330145553	-3.25266915655045	-0.25718274114058
Ti 3.80445161217254	-0.31145082331017	-1.12221745222482	Ti 4.17578411915008	-0.63683741383551	-1.15715882244141
Al 3.64633282721177	-3.11552243820485	2.37332115103611	Al 2.90930786664684	-2.43340550984342	2.68271455814941
Al 6.70168504559462	-1.05884348695562	0.11629606383851	Al 6.52893414073810	-1.14153964354711	-0.01321470906591
B 5.00873912151213	-1.23185787129000	2.04028270374250	B 4.65543459670415	-0.96607105635435	2.48371918182890
B 5.06800858616420	1.35684179546980	-0.05337010541870	B 5.57557592710939	0.87415874763782	-0.22577802368569
B 5.97770452383841	-0.00087320995706	2.16074612706681	B 5.52283169991283	0.37519914684500	2.53606597375011
B 6.01657993504437	1.20000521693199	1.15932537939392	B 5.94693308463170	1.22623270911208	1.26011964593147
B 4.63549272488505	0.13865775623941	1.00624697676095	B 4.87193732362047	-0.05182106365669	1.05392211783265
B 3.86565353455957	-1.34080560137390	0.95670108532113	B 4.31238483672264	-1.61751529199484	1.02804561515659

C 4.17430380108224	-0.61189741333926	-2.92564731857228	C 3.48488567555630	-0.62318773728254	-2.98382298805764
H 4.74318865423575	-0.68703764372991	-3.85289185517103	H 3.60251939838228	0.09739805808700	-3.80533063075435
H 4.59369023550747	1.74997366589253	-1.09314522232171	H 2.78899081981925	-1.42221487358320	-3.29523312916362
H 5.54747375333857	-1.07001999338945	-1.18091049136094			
H 3.35611539390423	-1.39053291621095	-2.86922132823410			
i10e			i6e to i11e		
C 3.18914098302309	-2.53447065477684	-0.07110552086720	C -1.31293301200448	-1.20191338757096	0.30688681027602
H 2.30164203535103	-2.47198096937619	0.57053301546905	H -2.39380111008820	-1.02971437297192	0.37233717398858
H 3.45712267253496	-3.59433583160792	-0.16907635380641	H -1.06281475542367	-2.04053721243025	-0.34470359975467
Ti 4.76604877371300	-1.11768999219809	-1.16450073429892	Ti -0.21827314193489	0.61830942095086	-0.70985022655524
Al 5.90308188676603	-2.22322239387143	3.49888934995625	Al -1.00603071292978	-2.22544557053751	2.72872399298155
Al 6.71442065114058	-1.09918003992499	0.71745305111494	Al 1.90765595311289	-0.39905603147990	0.70431800962432
B 4.57701096400778	-0.97262199206832	2.25684417677923	B 0.03382117369605	-0.16842841458026	2.82844505491467
B 5.42152374444417	0.77437847690496	-0.45978201116800	B 1.28609462895022	1.82604296741693	0.39203598138084
B 5.42514787908465	0.35758103111757	2.26642884430729	B 0.97100502502645	1.09876186874387	3.06807506698601
B 5.74712809237759	1.23660375185739	1.00518307743503	B 1.56919218756971	2.01816260479831	1.92406128787272
B 4.60388833265838	-0.08132966241432	0.79354231488986	B 0.42239293789987	0.85390286575573	1.50328606416130
B 4.29168804786802	-1.72546242009248	0.84767571506945	B -0.36257212675589	-0.59077024665805	1.31133294850363
C 2.84879926987605	-1.88302154386753	-1.44718652127830	C 0.10321241731271	0.17024498894592	-2.76902264127100
H 1.98985982369225	-1.20842617089646	-1.40031404611962	H -1.14223571626048	1.19845361121506	-2.06978543926161
H 2.73484233346225	-2.60702281878529	-2.26431760748266	H 1.03291201224609	0.76169604785535	-2.83470454723427
			H -0.43413874004821	0.19061763531020	-3.71527020092395
			H 0.33179460963160	-0.87955737476338	-2.48693290568891
i11e			i11e to i12e		
C 2.63539409513695	-1.97827402512635	0.20552881536829	C -1.63617297405422	-1.60755303757642	-0.49057224025103
H 1.80134932266349	-1.95025572952580	0.91860576177119	H -2.66143106138604	-1.67655856696789	-0.13275082336923
H 2.77241317000574	-3.01381855304617	-0.13034055441904	H -0.94806660578546	-2.01046577203112	0.28318099369969
Ti 3.96325869731613	-0.12849009464606	-0.99511098999273	Ti -0.09640002366369	0.06155441525025	-0.29058881375105
Al 6.28934510465853	-2.86252385074950	2.14223584807406	Al -0.03457919544207	-0.37967003199773	3.26402599092291
Al 6.33532516283593	-0.94191675058355	0.11633815639460	Al 2.22541830465645	-1.03359731803564	0.67395763242708
B 4.77254585653937	-1.16738033191463	2.25269173455701	B 2.15306997047406	1.23514181735588	2.04469608033151
B 5.13052962960059	1.26570403346773	0.02834607674062	B 1.81785149753313	0.49401667094877	-1.13406842122528
B 5.80432842011471	0.00799213267490	2.39075323751152	B 3.32498624489936	1.39202041272646	1.00781550063897
B 5.93621066214356	1.19182408089271	1.38017366396873	B 3.15955926378867	1.05797926852714	-0.52279835970909
B 4.53173677964525	0.15670655697253	1.20546967367158	B 1.70246079179502	1.23386736610336	0.40960179631183
B 3.95429378721864	-1.37722479601628	0.87990305726557	B 0.66895882259627	0.81880007187049	1.62995981279828
C 4.79661553448368	-0.65200410510074	-2.85856945947057	C -1.93937457363425	0.42728203363640	-1.21702271235582
H 2.22361297542385	-1.45883816112433	-0.70374746096949	H -1.49351499782809	-2.13327952022558	-1.43816614454360
H 5.64426164865900	-0.06325287544544	-3.22751797249866	H -2.12456477663806	1.16626115762154	-0.40793207287615
H 3.90470869397023	-0.39313516870899	-3.47853128997872	H -2.87484384765922	0.12529687019084	-1.67959252823923
H 5.00861145958424	-1.72036441202000	-2.99960852799394	H -1.24335683965185	0.82890416260327	-1.99974569080982
i12e			i10e to i13e		
C 1.87647192492031	-2.73329398276129	0.13919497230865	C -0.93052062908507	-1.31060576524375	-0.66270656041723
H 0.79775187558410	-2.79090782810988	0.31978233447103	H -1.59083013006180	-0.86986529096609	0.70244784723036
H 2.28197480781263	-2.14866345726856	0.99709827870824	H -0.88319877018062	-2.39680401599134	-0.56180811997839

Ti 3.59305507810529	-0.58245140423572	0.07539042177278	Ti 0.63028105270758	-0.00031862703145	-1.39724849233812
Al 4.25768536597860	-1.44989996538180	3.41819351344641	Al 1.68511439723429	-1.06822725717528	3.06754938169802
Al 5.96145589880738	-1.74085986937358	0.45910689697501	Al 2.55623148700843	0.48227105238952	0.37522704265605
B 6.26510379778209	0.19753323904253	2.01065803990307	B 0.31088343273212	0.19865148514295	1.91884191334956
B 5.21304849522141	-0.00174488729173	-1.08277473270862	B 1.07383645944277	2.00060448298805	-0.76515259276798
B 7.23804995477545	0.33402245462188	0.79545334747250	B 1.11314367754987	1.57611022884285	1.91688421998759
B 6.72684718131231	0.29076524490880	-0.68773298592347	B 1.26313112663052	2.55504789260372	0.69984108071259
B 5.43855208274483	0.48331891626288	0.51272504057959	B 0.26581927785347	1.10134507017399	0.46846097973211
B 4.67723176528146	-0.03526662291575	1.86528080800370	B -0.39853606505671	-0.43698198780279	0.57850460189548
C 2.16651598328755	-2.14590149145137	-1.25430117092831	C -1.42284797874731	-0.75698553996513	-1.87145432657246
H 2.31340080443302	-3.73086670513944	0.24117019134480	H -1.71727888897980	0.30317178880277	-1.88129705670583
H 1.67133297313904	-1.17205313977752	-1.42439703952336	H -1.95522844904773	-1.37741351676802	-2.58808991848173
H 1.79266153042566	-2.80972912056115	-2.04052685598883			
H 3.25357247038831	-2.05117172056810	-1.49571662991319			
i13e			i13e to i14e		
C 3.39146446093876	-2.59919448988081	-0.53040006490244	C -0.86303901558382	-1.53985148558456	-0.90952160821751
H 3.22095439822239	-1.61263308164010	2.8792942420332	H -0.45832863589928	-0.76498711319782	2.33066227340986
H 3.61153492601381	-3.65086683379974	-0.75583067360942	H -1.08181672674383	-2.60970923244698	-0.98618876084758
Ti 4.91873220970796	-1.15381810848781	-1.33113478485923	Ti 0.30434051547548	0.22825008312260	-1.94941359040517
Al 6.84264964839809	-0.66208419506687	3.56126405759138	Al 0.08297220431949	0.85837340034796	3.62014640309678
Al 6.48525266939701	-1.54265862458175	0.84822316388960	Al 2.37309938830712	-0.14892267941512	-0.08257655433858
B 4.11287750405266	-1.29689727198282	2.15086181130806	B 0.26818601272078	-0.27887990452297	1.46283017290759
B 5.66642445726930	0.50777220521000	-0.31809982445161	B 1.28058399431336	1.85677803880745	-1.05858956928853
B 5.13274147812496	-0.02264034461553	2.36168758986385	B 1.05839619927673	1.15724984593627	1.67816530879691
B 5.77604400768824	0.81580694167958	1.20561211830814	B 1.61546825189649	1.97976273534660	0.48440249749637
B 4.48921456680526	-0.24625144282847	0.74126588024014	B 0.26227738330136	0.85979673436795	0.09834709401424
B 4.12590669069326	-1.91520388898581	0.59122480653416	B 0.30054293916784	-0.93273003686828	-0.08237532681873
C 2.74626114615842	-1.86212913108477	-1.55704743213529	C -1.56630338547066	-0.61636104153453	-1.65743200706021
H 2.21644257357192	-0.93628488113284	-1.31691825345064	H -1.04525943800779	0.68577628902158	-0.79653668439378
H 2.39413880295774	-2.36872566280223	-2.45852297853004	H -2.53111968707327	-0.73454563338015	-2.15191964835166
i14e			i15e		
C 3.39447922389992	-2.76272602120258	-0.52734122828930	H 4.10673869500893	-2.16702885521729	2.64962823016021
H 4.07285476099259	-2.00602185005843	2.95252399178136	Ti 5.51045297130646	-1.86908035310511	-1.59898377542482
H 3.08005023418124	-3.81568677487432	-0.50986143391629	Al 5.15101774503287	-0.32640620990790	4.23450114282033
Ti 4.90043978876819	-1.26939942437356	-1.57856894146076	Al 6.66362016366317	-1.56955323615006	0.73371869712661
Al 4.83993042076910	-0.11884778217644	4.16179747723774	B 4.66132453794973	-1.47631709080199	1.83045186082602
Al 6.49179532003536	-1.49960483011878	0.51368504737313	B 5.30527426339821	-0.09054581192932	-0.59315897388077
B 4.73654312045466	-1.60345199952181	2.01053683495099	B 5.61094123492428	-0.07897559304186	2.14940529042362
B 5.68563772093422	0.45312073464437	-0.62466861028890	B 5.89395716269713	0.55811066174270	0.74046482486110
B 5.68311282206422	-0.21690568861458	2.15028932562454	B 4.22198182201629	0.01761866208444	0.94253421195730
B 6.08063111896781	0.62568664839711	0.89502319114406	B 4.48783945095817	-1.50371669175385	0.11801280879813
B 4.51610002599413	-0.30645682566133	0.69331194886175	H 3.23414321304465	0.67465329808027	1.06662925233224
B 4.39355360928336	-2.11432813980237	0.43828986889114			
C 2.97513306340500	-1.86795044048282	-1.49557845760323			
H 3.44669255060643	0.22496794288422	0.66098343238586			

H	2.08095842964356	-1.98600578903861	-2.11547266669212			
	i16e			i2 to i3f		
Ti	3.80244079663299	0.05598201270770	-0.89044175610949	C	-2.12961977719627	0.46800657075274 -0.59552717314430
Al	7.15818799095853	-1.36267868920853	1.66962458222952	H	-2.35976180531196	1.52572227344206 -0.81953522425612
Al	6.00784674863915	-1.01014250456583	-0.66628807405918	H	-0.83959486887543	0.18106715986058 0.29349479286499
B	4.46354215549114	-1.43103964625633	2.10299785947490	H	-2.38701740948310	-0.18214403023119 -1.45667330136853
B	5.33792654271812	1.16304795694690	0.19391628398359	H	-2.74217738936493	0.15593969995025 0.25352110613726
B	5.34462104436934	-0.20899351041728	2.65734332841123	Ti	-0.04699960376554	0.60066568582546 -1.20976479397657
B	5.76027493404428	1.03213931201939	1.72888276099087	Al	-0.36202308691526	-2.92759592304920 -0.38946058561337
B	4.69623552767772	-0.10583950218172	1.09759639369912	Al	2.63418027500714	0.33745065957805 -0.69963905567965
B	3.93673698216044	-1.52168114430345	0.59734063697319	B	1.70737841879482	-1.46228402076962 0.84338288785546
C	4.91928933314809	-0.78634219384984	-2.60672419350780	B	1.00776062314197	1.69682528307995 0.26563738560949
H	5.76952546327616	-1.28810857967678	-3.09138914004759	B	1.99781497858516	-0.34227718412513 1.88498711332013
H	4.83661294113875	0.19548809374661	-3.11409126582284	B	1.71601382476336	1.16585164834626 1.58121927588360
H	4.03853096974505	-1.41589719496083	-2.84219420621552	B	0.79799793310270	0.00430394785019 0.62717397436739
				B	1.00604788751732	-1.22153177051041 -0.57881640199976
	i3f			i3f to i4f		
C	1.34669992290912	-0.24297105907062	0.09942684385944	C	-1.95458045026354	0.04558696810293 -0.79013799134790
H	1.05246286398464	0.76969397619297	0.43086724692125	H	-1.15461650798735	1.25874650753442 -0.32436918803197
H	3.24228699721869	-0.53434314171956	1.84153417100605	H	-0.38917859859351	-0.40434043241555 1.43774406996942
H	0.99371885003512	-0.38940367068282	-0.94141202610938	H	-2.45229851437773	0.29531550081127 -1.76188822463221
H	0.83681350015738	-0.97175519043242	0.73854297153208	H	-2.69527797002018	0.01679624241640 0.01009638219053
Ti	3.45772388919806	-0.13196993845104	-0.10287600639136	Ti	-0.15606225794145	0.35956783710808 -1.50879085166529
Al	3.14023110849992	-3.57068918518602	0.49537966205668	Al	-1.07865770932517	-2.26384870201361 -0.42263238573817
Al	6.14537507599375	-0.42411312843888	0.21846602875654	Al	2.27265140567081	0.46332328849719 -0.58798084017320
B	5.52255825401729	-2.09483353465436	1.80521697662363	B	1.97304133014072	-1.27317891287972 0.71658323018919
B	4.78626533681407	1.06572024854794	1.11765974427109	B	0.45875936317591	1.59064966620145 0.10150096617272
B	5.98278056346856	-0.90947220011630	2.70121435289026	B	2.20627251062370	0.01019295381598 1.60258617701520
B	5.68340947381284	0.58247611576088	2.34212780019487	B	1.45139014914548	1.36683257008248 1.34036773804231
B	4.49249548215770	-0.64115849316220	1.69621181659691	B	0.53920493683159	-0.12102036725786 0.72632867144275
B	4.62040180173273	-1.95187572858753	0.48799140779192	B	0.97935231292071	-1.34462312000345 -0.53940775343340
	i4f			i5f		
C	1.49139423142403	-1.09729579882837	0.02668660686851	C	1.52606080548736	-1.11671011035721 -0.06422017582372
H	4.19473948117467	1.98859042798011	0.65432233708118	H	1.00689803837841	-1.30004765878103 -1.01810664883678
H	3.34577112911483	-0.30590051570191	2.10895847755536	H	0.86109164802805	-0.56970603205440 0.61930553700697
H	1.38811387926188	-0.51449418662621	-0.93279797199760	Ti	3.55696087730271	-0.08665396656839 -0.27192943003022
H	0.47531643868461	-1.35319834120250	0.34294164098611	Al	2.67369669081115	-2.47329972021901 0.61546731998930
Ti	3.27482076300460	-0.24060681766797	0.08267851030351	Al	6.23829676380324	-0.34720993086434 0.09620057741868
Al	2.50000548087136	-2.95861440339568	0.17196017394076	B	5.67124616625480	-2.07270130389491 1.70013604628611
Al	5.96231366934019	-0.53357590748114	0.08177517421701	B	4.47213770564741	0.93922925563899 1.25578492033460
B	5.52454416268334	-2.00204904053506	1.88417604352642	B	6.08491951111563	-0.90278636958832 2.61900152874663
B	4.98171625220711	1.16626522646531	1.05922446556048	B	5.52611759310239	0.52789833087481 2.37757992940889
B	6.19952507553055	-0.81232831820293	2.59263543575403	B	4.52250966302116	-0.70069983080341 1.61981279288352
B	5.98610665568798	0.66457824668858	2.17425651696691	B	4.62516836704758	-1.99185501338278 0.48208039261599
B	4.56381442020781	-0.44397932067947	1.80059031672821			

B	4.41743280080692	-1.96924369081272	0.74698587250908			
i6f				i6f to i7f		
C	1.82568600615161	-0.93184890480816	-0.55946283147094	C	-2.44745741876489	-0.63069143881309 -0.06507290274743
H	1.33884482521503	-1.30388598248729	-1.47317184870305	H	-2.98433384374734	-1.12841833772824 -0.88596292072557
H	1.28733194756131	-0.05420294604392	-0.17400930846162	H	-2.96031118563675	0.30228515584280 0.20818930071714
Ti	4.04124084850908	-0.42774971417060	-0.79883806722498	Ti	-0.25243746629417	-0.19792453939280 -0.49086731642436
Al	2.59001547426595	-2.15604715502919	0.67449557706717	Al	-1.64426079670512	-1.66589518766890 1.30920002624818
Al	6.54418757858449	-0.97393148373308	0.18986795909042	Al	2.32394664112199	-0.75809758047137 0.46737373202586
B	5.43605132817302	-2.06303472113872	2.01326355124910	B	1.26322929943613	-1.43520625708825 2.50310933658920
B	4.87209443404545	0.84562888007016	0.58733106960450	B	0.71984247519713	1.22809994583464 0.65034978393784
B	5.94534711880762	-0.73690923407548	2.62513687140052	B	1.84666922330943	-0.04318571019101 2.84322659306937
B	5.67741671492313	0.63358552070446	1.93943618060831	B	1.60674059816742	1.20556117577208 1.95263801601883
B	4.58029509474575	-0.61288897841083	1.35917604351145	B	0.43025809277834	-0.08432362942205 1.63500908014067
B	4.60046709940204	-2.19721471178401	0.64968820878483	B	0.36105962591616	-1.78083333178673 1.22739199121546
C	4.37930076343636	0.51067325321881	-3.03763130847486	C	0.31054394247181	0.91695814294598 -2.31013050995114
H	4.71764914882424	1.13689248909957	-2.17974230876907	H	0.54653561395487	1.34259160319633 -0.98170355637936
H	4.87087703577778	-0.47902434714032	-3.04607481813365	H	0.67260580043300	-0.05563516627664 -2.70066377193779
H	4.70987019112586	1.03570148307800	-3.93720552796343	H	0.94344016348301	1.69537598601668 -2.74113007284620
H	3.28302419045102	0.41644254265063	-3.06886908211465	H	-0.73607076512105	1.08933916923059 -2.62095680895069
i7f				i7f to i8f		
C	1.80250776284876	-0.83964456566016	-0.49378786808394	C	-2.30966917420361	-0.58302559131620 -0.47751507046512
H	1.26233581200454	-1.28182339594212	-1.34179752386690	H	-2.77032192468535	-1.05754954919087 -1.35124533712308
H	1.27108910526124	0.04837215071762	-0.12225376843427	H	-2.99651624925149	0.19720930066410 -0.09724978102806
Ti	3.93280474978622	-0.38914567265035	-0.97438022485324	Ti	-0.43675288849702	0.48742527771952 -0.64476011452367
Al	2.68423527812241	-1.89352828296956	0.83674545116922	Al	-1.63545258367588	-1.73234879987392 0.90753730971027
Al	6.46125728028354	-0.65421365612271	0.05844981464796	Al	1.78845368789244	-0.82314338864191 0.12939016044331
B	5.59537586800163	-2.07227463079023	1.67273232951251	B	1.53497418880725	-1.54160827380998 2.31005041225549
B	4.76149673498385	0.88629008038355	0.65446530420242	B	0.59413892469738	1.38382870837104 1.13515378046776
B	6.00245890959936	-0.79680210127478	2.45305604089495	B	2.58730224888558	-0.41894803279388 2.10843892186839
B	5.59539767856042	0.62025223165031	1.97486249218570	B	1.96889967234176	0.96499381715697 1.73870320631034
B	4.51887907860450	-0.64139509546248	1.33876184751271	B	0.27221805285095	-0.12505714080446 1.68296518182999
B	4.69228413036953	-2.11343689041424	0.34872352468764	B	0.06167470303384	-1.76365822856797 1.86891921404361
C	4.44333691859344	0.07190214176214	-2.95305687275873	C	0.14255854429071	1.06129822096685 -2.34450114033711
H	4.07318842544248	1.55044397264160	-0.10010823145251	H	0.00634151532465	2.18083317544004 0.41269179804011
H	4.79015310715435	-0.83852905063899	-3.46931390618272	H	0.87106663322468	1.39856078944165 -3.08145293364077
H	5.14482030714656	0.88614631493305	-3.16744852602619	H	1.06936883397805	-0.19866449844705 -1.47812227181041
H	3.44390543323707	0.34264333983737	-3.35359779315458	H	-0.74828418501392	0.56985421368607 -2.81900333604107
i8f				i8f to i9f		
C	1.94515490343032	-1.12237798907190	-0.82829990843231	C	-2.25066288694930	-0.19050328144257 -0.57050601059726
H	1.49284806185300	-1.73564962209229	-1.61714570292134	H	-2.78297462362191	-0.70792955993388 -1.37670616833381
H	1.28628876056431	-0.25603427025918	-0.64182244100347	H	-2.71470143474692	0.79021657796486 -0.42139247043511
Ti	3.90227281576725	-0.21901382780317	-1.16523581253243	Ti	-0.00164202237289	-0.08039094320238 -0.69407159953906
Al	2.52430981688826	-2.03387359293412	0.75746433825555	Al	-1.92920680263585	-1.29376396741265 0.99199448643618
Al	6.06439166785123	-1.31009974907933	0.20597793808209	Al	2.48081339770191	-0.53705840731091 0.59713574911690
B	5.60315302671794	-1.76984901367240	2.35487788697609	B	1.22865107353589	-1.46827709901307 2.41577434355303

B 4.88219601522005	0.86984080210595	0.56152652669050	B 0.94164477791663	1.36250743981846	0.75155754634497
B 6.68592103790615	-0.66699610303256	2.15631648277003	B 2.11476117479922	-0.20844681942227	2.72174569437157
B 6.16037658019371	0.61686026765135	1.43669361792597	B 1.89232899450449	1.17266544625217	1.98500486944970
B 4.39893818220544	-0.48320007291864	1.35053141167855	B 0.53814164684819	-0.03541107501370	1.54616618077257
B 4.21145133031874	-2.09291769367301	1.73966194677215	B 0.03339766895614	-1.64268107426801	1.42764757721576
C 4.19182742235239	0.49812968368447	-2.84499913634268	C -0.51097000291813	0.66749852410792	-2.36652259561413
H 4.41978997441767	1.54684002218500	-0.35301341417685	H 0.42130643298893	1.90839017488924	-0.20480076284135
H 4.68191465205297	1.06056059105029	-3.64048478027292	H -0.89689797117785	1.48228343252180	-2.98225995042407
H 5.59106968253196	-1.42576539911025	-1.35467538831092	H 1.94396004779144	-0.92220467107718	-0.88319567471812
H 3.19709409972835	0.07349989696986	-3.15580339515800	H -0.50794947061997	-0.29689469745785	-2.93757121475777
i9f			i10f		
C 1.78808644041309	-1.35352439356427	-1.39951594582235	Ti 4.12848540483782	-0.78042252619602	-0.88463242487661
H 1.63249474930852	-2.03449979140946	-2.24420313649371	Al 4.27112932511269	-3.46080537684138	0.19225659335672
H 0.88784358084422	-1.38167535751273	-0.76136136450109	Al 6.31538309677138	-1.56590670374765	0.61134329384822
Ti 3.94311145981281	-0.90209388941623	-0.89880206648006	B 4.68786757987621	-1.02256089243393	2.41992510267717
Al 2.24926449742827	-2.80799045123608	0.53113329473900	B 5.68869954967279	0.62835660628490	-0.19939023476812
Al 6.27598295331324	-1.58474486719759	0.66224714454232	B 5.84892437660999	0.00723533346506	2.47331119625554
B 4.89924361591408	-1.17084584055342	2.39015725714109	B 6.30358881531634	0.84712514193268	1.24010396514957
B 5.43672461008533	0.76220981057651	-0.26321774996136	B 4.71066345334715	0.04767228228176	1.03249985641799
B 6.06520661635469	-0.09947405693108	2.31231860453393	B 3.85736308852229	-1.38281768643184	1.10755645178832
B 6.28270858208663	0.81383274747748	1.04726969626333	H 5.35781956900726	0.94903883905531	-1.32406033638663
B 4.71428428905780	-0.06315682994971	0.95684631980073	H 4.21316614092597	-2.53445748736887	-1.38617927346218
B 3.88534803890190	-1.49160070422988	1.21669175467580			
C 2.26179633521964	0.01516226987805	-1.73485330705982			
H 5.05156310754727	0.93692297308551	-1.39614436988666			
H 1.82569776225302	0.84784329362693	-1.18165176092055			
H 5.90325008948514	-2.02256345760004	-0.85697306163278			
H 2.41320666197406	0.25289999495603	-2.79541050893781			
i6f to i11f			i11f		
C -1.97176963643643	-0.24982627392135	-0.59574899211201	C 1.76034104939531	-0.71156284503357	-0.60159972257996
H -2.52036897785281	-0.78156032238168	-1.38619180950536	H 1.60763795331951	-1.03888459168964	-1.64425883413732
H -2.54900152607721	0.62684908199587	-0.27437244432121	H 0.79586646508424	-0.86713872007707	-0.09772558965777
Ti 0.44319595368310	-0.02090287344443	-0.44353496778553	Ti 3.98750737332042	-0.34739168585629	-0.86019420398916
Al -1.45917375314047	-1.39615961054608	0.89912949829771	Al 2.79285326598534	-1.94643842480541	0.84955751144570
Al 2.57830627841314	-0.63860893857547	1.08694249306229	Al 6.46643352078445	-0.63881593478188	0.14985030682577
B 1.09367900565074	-1.66569808127842	2.63676133788675	B 5.62460523064447	-2.11318373251903	1.81389798381005
B 0.99350358770510	1.24236417074745	1.08550134917103	B 4.68505685464288	0.86488230786886	0.70973211020892
B 1.55702804963867	-0.34948213489693	3.30236113785924	B 5.95849020176689	-0.79380910616597	2.55654431424990
B 1.48685710451800	1.03438839725192	2.57558307184814	B 5.51536704290292	0.62145041467874	2.03656857727483
B 0.45222566012570	-0.17559485596828	1.84133240613303	B 4.55769171135996	-0.69567292224388	1.47732702425927
B 0.50509411234526	-1.80250861645003	1.15286854882673	B 4.80675579998397	-2.19594065724430	0.45055933371908
C -0.02590947368503	0.85717429620960	-2.38826900041288	C 4.68133001979686	0.20982209753713	-2.76821461811093
H 0.63545340504689	1.66011142493624	-2.00166946750684	H 5.31978525057258	1.09752810195445	-2.83594052370856
H 0.56519679815785	0.02586142335214	-2.82812052358222	H 5.14522331232440	-0.61676067797716	-3.32542166495044
H -0.67395159438860	1.27260513412851	-3.16041668707398	H 3.70177675175316	0.44488175411045	-3.23906528510877

H -1.11036499370390	0.36098777884094	-1.50215595078487	H 1.87540916636247	0.40086757224460	-0.56981286955060
i11f to i12f			i12f		
C -1.72436978504433	0.39562613304348	-0.60048930260438	C 1.54496269544867	-0.10862486783641	-1.58501608503959
H -2.25474210827202	-0.45634977854404	-1.02969561128064	H 0.82529495393137	-0.89141938677464	-1.84495856953700
H -1.69267087552926	0.35855602413507	0.48519531177057	H 1.95017667398117	-0.39151093664217	-0.58421338738836
Ti 0.81151795836342	0.01507929713661	-0.64566374083994	Ti 4.10949131306195	-0.61334450268518	-0.88854123797004
Al -0.83841801823872	-2.93539762180841	0.29559782691092	Al 2.92753509431274	-3.45901681946898	1.20481162149458
Al 2.81155836967104	-0.52367936963183	1.08062476321905	Al 6.50704032939172	-1.07263216888423	0.14360000263726
B 0.81648722131146	-1.47455253989782	2.46869987019550	B 5.17881675459224	-1.78848036069573	2.12829610392305
B 1.32407670557534	1.36624195846590	0.91336965606151	B 5.02639536524917	0.86604891174800	0.22256952447629
B 1.09594651888137	-0.13243329682166	3.22842633904233	B 5.83585419092215	-0.43936430464570	2.54140944193162
B 1.34163307961317	1.23197943064328	2.48798842435333	B 5.74233359621054	0.84387966622947	1.64286302430464
B 0.61645791885697	-0.03821982484546	1.57328456624441	B 4.61379824439708	-0.41902094067124	1.22330834440550
B 0.71941605870158	-1.57705548074397	0.88314132088495	B 4.40851397298431	-1.99520487660751	0.72493344319455
C -0.31144776255228	0.54984867748404	-2.29719704177788	C 2.58883920167033	0.07526834071244	-2.70669811770112
H 0.31095566316615	1.47463198240986	-2.25415808855696	H 3.34061678449651	0.85870664251869	-2.46141065240281
H 0.27092851768088	-0.31969265814262	-2.71205954118653	H 3.09573616750086	-0.87220360187929	-2.99209935213807
H -1.17621753773139	0.71626590752893	-2.93304982995443	H 2.11282784069527	0.41884960579157	-3.63189929682755
H -2.12111192445338	1.34915115958865	-0.94401492248183	H 1.00930282115385	0.82879859979094	-1.40653880736295
i13f			i13f to i14f		
C 1.39584653905126	-1.18772626293261	-1.53170715016676	C -2.38385864103166	0.30235868410575	-1.34493309381629
H 1.30451013759046	-2.06201943486499	-2.17070326277788	H -3.30013567195443	0.23192342487960	-1.93395708996694
H 0.80691170428961	-1.18535577620737	-0.61798527786758	H -2.50857238567026	0.41519380988954	-0.26752715850696
Ti 3.94102314424287	-0.63550368556400	-0.75007294161621	Ti 0.45051428775767	-0.69124584094384	-0.81385997999154
Al 3.10413842633293	-3.09114176627481	0.32203247436815	Al 0.88616642212001	-3.36561031626204	1.45510057659460
Al 6.16069272149376	-1.66192202411279	0.42608534105504	Al 2.71307719306503	-0.49683637647491	0.65502875246415
B 4.83203867194270	-1.12588469591618	2.49090214241893	B 1.03449000036788	-0.58830236582286	2.53162663312050
B 5.58259693935168	0.55656991819300	-0.19371688864380	B 1.18904609240551	1.15404209692668	-0.20202518232619
B 6.00021461328707	-0.09116583444603	2.45406516139802	B 1.66027097279725	0.84935022321082	2.48654256889660
B 6.33371260653647	0.76923527750685	1.17723670505278	B 1.65736346737295	1.72915009765701	1.19667952488649
B 4.73129412516487	0.03075686951016	1.19250725267719	B 0.60947098489039	0.30819538312118	1.14195888449967
B 3.78329915834104	-1.32352932676789	1.31384300424612	B 0.34818746370205	-1.30776988672744	1.27362791326745
C 2.08347576333672	-0.06753487950667	-1.94014229596135	C -1.15590712113246	0.24897503054451	-1.90684866860610
H 1.99810716796755	0.87636560342338	-1.38591519767066	H -0.13167672725834	0.97496878011630	-1.26843706540192
H 2.50313848107087	0.00119794795997	-2.94878085651200	H -1.06843633743158	0.23560725577971	-3.00297661511351
i14f			i14f to i15f		
C 1.88480629548988	-1.26071364745987	-1.92874111648975	C -1.53158942003154	-0.47818380057580	-1.63774966430682
H 1.11208261469271	-1.79607445488919	-2.48673818887124	H -1.64269066222009	-1.46403953565068	-2.08572094234289
H 2.47021841702034	-2.00741873355313	-1.31282739853146	H -0.16220803454015	-0.83741213663588	-0.82092365350202
Ti 3.71681600776460	-0.47967289348283	-0.60746085716605	Ti -0.66711057647415	0.80672329752712	-0.22573693456309
Al 2.58828312481739	-3.00515001633604	1.49402671277678	Al -1.57130165895112	-2.03712617519786	1.46081017952710
Al 5.94300050002633	-1.66428620175987	0.33826933083592	Al 1.46273923163946	-1.39678455253872	0.07840660813614
B 4.88667457205056	-1.14600947261118	2.50440877156962	B 0.83905196818253	-0.63255284365691	2.48060719072984
B 5.52935322737839	0.65012519278820	-0.10274077493580	B 1.56028680800449	1.26540745064514	-0.06347851714778
B 6.19244444279092	-0.31431840803749	2.39183730786734	B 2.30263828051113	-0.19681621026962	2.13794432641340

B	6.47571684001298	0.60627982703425	1.17035843981747	B	2.64450833054155	0.71680319445172	0.92006614535296
B	4.75509764401895	0.07118983366825	1.26131370185285	B	0.93418980088744	0.67443748239248	1.35990794254537
B	3.70499901462659	-1.18792389375883	1.41850260959675	B	-0.46729894578778	-0.14563437307227	1.72168994240867
C	2.16285987784455	0.04798028397765	-1.89746585469762	C	-2.00193389268055	0.74231812339639	-1.81438426881422
H	4.98681161506078	1.14527164459380	-1.07750885922057	H	1.03022089484040	1.88051593327389	-0.96699376130700
H	1.59447194640483	0.76149928982632	-2.49327907440424	H	-2.72950212392163	1.10234414591099	-2.54444459312965
i15f				i16f			
C	1.82400361306891	-1.14486389368391	-1.57299945220712	H	7.54475300485012	-2.31215165356472	0.90618782435079
H	0.90456891185919	-1.44732191669158	-2.08296108180048	Ti	4.03612459065515	-1.27153160266044	-1.05314008803756
H	7.24750301170412	-2.60240513517449	0.92515868173493	Al	1.86548992713079	-1.15294132749937	0.73103529066658
Ti	3.88649678023030	-1.01921054672101	-1.06435487737976	Al	6.15764103113163	-1.68378177317234	0.48401944498329
Al	1.66233038116477	-2.28476516685617	0.57393167713306	B	4.49398559075603	-1.44725055050122	2.24210292538169
Al	6.01691589192751	-1.69836316952752	0.55728055096293	B	5.42206051461453	0.29409844656814	-0.34248837170336
B	4.46870613867672	-1.10677214085027	2.31585829052957	B	5.25672493868717	-0.11223332908462	2.38469545376661
B	5.58227440406618	0.33526707649123	-0.38423079749037	B	5.72479861853422	0.71695851693998	1.15867856374238
B	5.52482514042928	0.03889139279313	2.34027246881194	B	4.33904385183718	-0.33005966647603	0.82248965592261
B	6.06052573112194	0.74526871808464	1.06010249063671	B	3.97694102895614	-2.06686084802586	0.86566262089235
B	4.52661245684855	-0.11461381724235	0.90324500209962	H	5.13243503284696	0.58398418747650	-1.48571204996538
B	3.76720339509951	-1.66086628924305	1.00448809553656				
C	2.21263511896674	0.10262304773591	-1.25716670186692				
H	5.20660479588432	0.58579948868672	-1.51822030745458				
H	1.71568418895166	1.07229414219879	-1.30833234924611				
i17f							
C	1.73631280384415	-0.74231709960252	-0.60700339783017				
H	1.66122018540968	-0.92519804755461	-1.69741369077909				
H	0.71927554538013	-0.88418488947660	-0.22011179673733				
Ti	3.95466683249841	-0.38939601362224	-0.66275278415924				
Al	2.60907909895812	-2.27512421139044	0.69201576445681				
Al	6.50466159835712	-0.68808677287197	0.04291791627816				
B	5.58991191651731	-2.04860667929228	1.87532368238310				
B	4.73672570542265	0.92118781527844	0.71894108927929				
B	6.03965843503137	-0.72868837969447	2.55307545487644				
B	5.62627000231443	0.68647691273782	2.01278646961269				
B	4.65605954355365	-0.61814322125045	1.41675965649971				
B	4.68030181459625	-2.11931215762547	0.56703484282259				
H	1.91987214811665	0.34975441436479	-0.42112726670299				

References:

1. Biswas, S.; Cokas, J.; Gee, W.; Paul, D.; Dias, N.; Morgan, H. W. T.; Finn, M. T.; Hudak, B. M.; Godbold, P. M.; Klug, C. A.; Epshteyn, A.; Alexandrova, A. N.; Ahmed, M.; Kaiser, R. I., Unconventional Low Temperature Decomposition of a Saturated Hydrocarbon over Atomically-Dispersed Titanium-Aluminum-Boron Catalyst. *Nat. Commun.* **2025**, *16*, 6793.
2. Finn, M. T.; Chaloux, B. L.; Epshteyn, A., Exploring the Effects of Reaction Conditions on Morphology and Stability of Sonochemically Generated Ti–Al–B Fuel Powders. *Energy Fuels* **2020**, *34*, 11373-11380.
3. Biswas, S.; Paul, D.; He, C.; Dias, N.; Ahmed, M.; Pantoya, M. L.; Kaiser, R. I., Counterintuitive Catalytic Reactivity of the Aluminum Oxide “Passivation” Shell of Aluminum Nanoparticles Facilitating the Thermal Decomposition of exo-Tetrahydrodicyclopentadiene (JP-10). *J. Phys. Chem. Lett.* **2023**, *14*, 9341-9350.
4. Biswas, S.; Paul, D.; Dias, N.; Lu, W.; Ahmed, M.; Pantoya, M. L.; Kaiser, R. I., Efficient Oxidative Decomposition of Jet-Fuel exo-Tetrahydrodicyclopentadiene (JP-10) by Aluminum Nanoparticles in a Catalytic Microreactor: An Online Vacuum Ultraviolet Photoionization Study. *J. Phys. Chem. A* **2024**, *128*, 1665-1684.
5. Biswas, S.; Paul, D.; Dias, N.; Kunzler, K.; Ahmed, M.; Pantoya, M. L.; Kaiser, R. I., Stress-Alteration Enhancement of the Reactivity of Aluminum Nanoparticles in the Catalytic Decomposition of exo-Tetrahydrodicyclopentadiene (JP-10). *J. Phys. Chem A* **2024**, *128*, 3613-3624.
6. Paul, D.; Biswas, S.; Dias, N.; Finn, M. T.; Lipton, A. S.; Epshteyn, A.; Ahmed, M.; Kaiser, R. I., A Synchrotron-Based Vacuum Ultraviolet Photoionization Mass Spectrometer-Coupled Microreactor To Probe Thermocatalysis. *Anal. Chem.* **2025**, *97*, 22846-22857.
7. The properties of elements. In *Geochemistry: An Introduction*, 2 ed.; Albarède, F., Ed. Cambridge University Press: Cambridge, 2009; pp 5-24.
8. Becke, A. D., Density-Functional Exchange-Energy Approximation with Correct Asymptotic Behavior. *Phys. Rev. A* **1988**, *38*, 3098-3100.
9. Lee, C.; Yang, W.; Parr, R. G., Development of the Colle-Salvetti Correlation-Energy Formula into a Functional of the Electron Density. *Phys. Rev. B* **1988**, *37*, 785-789.
10. Weigend, F.; Ahlrichs, R., Balanced Basis Sets of Split Valence, Triple Zeta Valence and Quadruple Zeta Valence Quality for H to Rn: Design and Assessment of Accuracy. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297-3305.
11. Weigend, F., Accurate Coulomb-Fitting Basis Sets for H to Rn. *Phys. Chem. Chem. Phys.* **2006**, *8*, 1057-1065.
12. Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H., A Consistent and Accurate ab initio Parametrization of Density Functional Dispersion Correction (DFT-D) for the 94 Elements H-Pu. *J. Chem. Phys.* **2010**, *132*, 154104.
13. Grimme, S.; Ehrlich, S.; Goerigk, L., Effect of the Damping Function in dispersion Corrected Density Functional Theory. *J. Comput. Chem.* **2011**, *32*, 1456-1465.
14. Henkelman, G.; Jónsson, H., Improved Tangent Estimate in the Nudged Elastic Band Method for Finding Minimum Energy Paths and Saddle Points. *J. Chem. Phys.* **2000**, *113*, 9978-9985.
15. Henkelman, G.; Uberuaga, B. P.; Jónsson, H., A Climbing Image Nudged Elastic Band Method for Finding Saddle Points and Minimum Energy Paths. *J. Chem. Phys.* **2000**, *113*, 9901-9904.
16. Grimme, S., Supramolecular Binding Thermodynamics by Dispersion-Corrected Density Functional Theory. *Chem. Eur. J.* **2012**, *18*, 9955-9964.
17. Grimus, W., 100th anniversary of the Sackur–Tetrode equation. *Ann. Phys. (Berlin)* **2013**, *525*, A32-A35.
18. Herzberg, G.; Crawford, B. L., Jr., Infrared and Raman Spectra of Polyatomic Molecules. *J. Phys. Chem.* **1946**, *50*, 288-288.