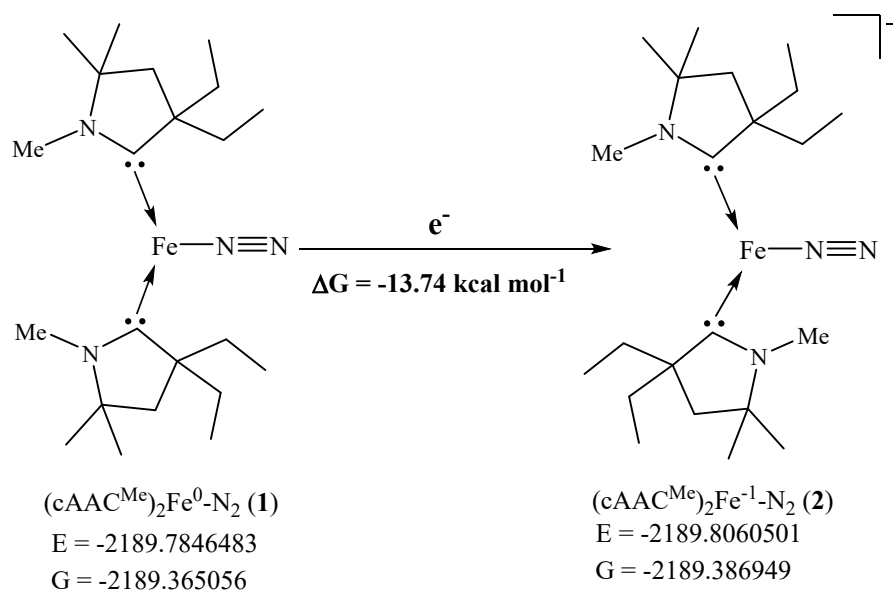


## Supporting Information

# Estimations of Fe<sup>0/-1</sup>-N<sub>2</sub> Interaction Energies of Iron(0)-Dicarbene and its Reduced Analogue by EDA-NOCV Analyses: Crucial Steps in Dinitrogen Activation Under Mild Condition

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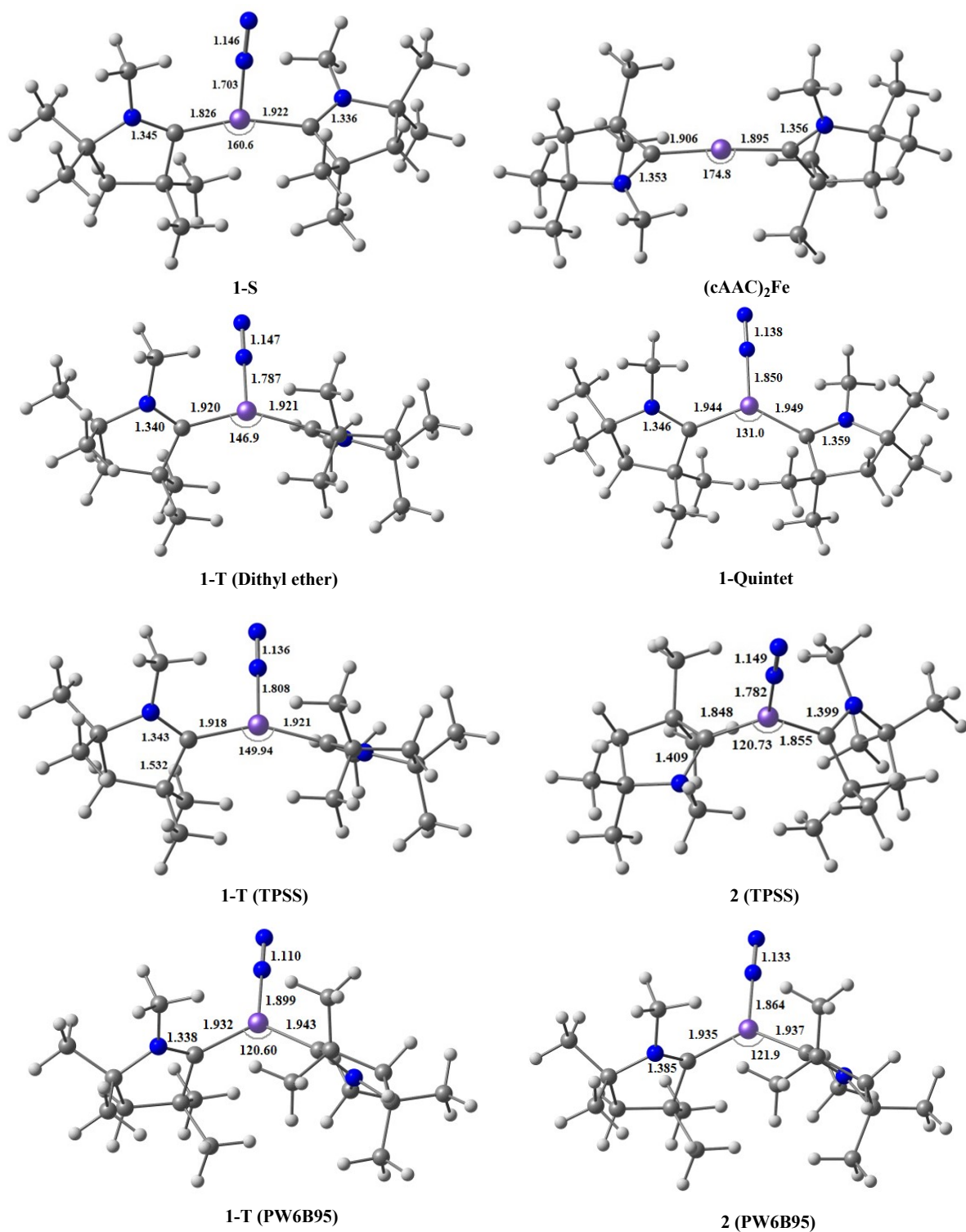
**Scheme S1.** The energetics of the reduction of complex **1** to form complex **2** calculated at BP86-D3(BJ)/Def2TZVPP level.  $\Delta E/\Delta G \text{ kcal mol}^{-1} = \Delta E/\Delta G \text{ Hatree} * 627.51$ .

**$\Delta G$  calculation for electron affinity:**

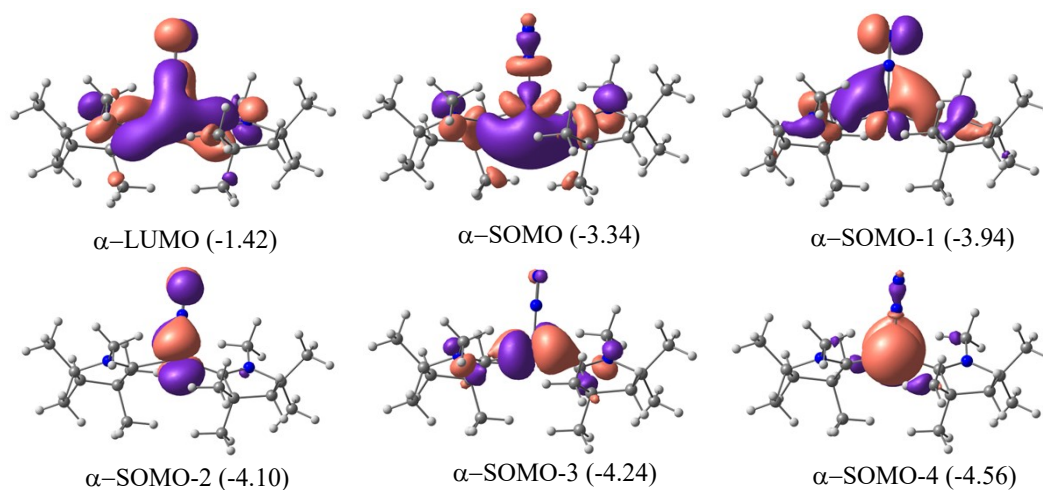
$$-2189.386949 + 2189.365056 = -0.021893 \text{ hatree} * 627.51 = -13.74 \text{ kcal mol}^{-1}$$

**Table S1.** The EDA-NOCV results at the BP86-D3(BJ)/TZ2P level of (cAAC)<sub>2</sub>Fe–N<sub>2</sub> bonds of complex **1** in gas phase and in solvent diethyl ether using neutral (cAAC)<sub>2</sub>Fe in electronic triplet state and neutral N<sub>2</sub> fragment electronic singlet state as interacting fragments. Energies are in kcal mol<sup>-1</sup>.

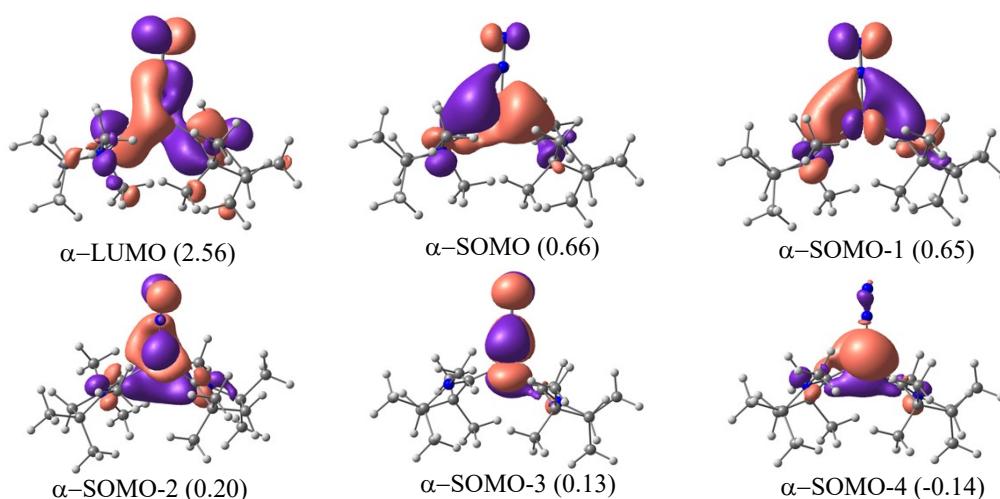
Complex <b>1</b>	Fragments	$\Delta E_{\text{int}}$	$\Delta E_{\text{pauli}}$	$\Delta E_{\text{elec}}$	$\Delta E_{\text{dis}}$	$\Delta E_{\text{orb}}$
Gas	(cAAC) <sub>2</sub> Fe (T) +	-87.9	190.2	-111.9	-5.2	-161.0
	[N <sub>2</sub> ] (S)					
Solvent	(cAAC) <sub>2</sub> Fe (T) +	-87.5	189.2	-112.0	-5.1	-159.7
	[N <sub>2</sub> ] (S)					



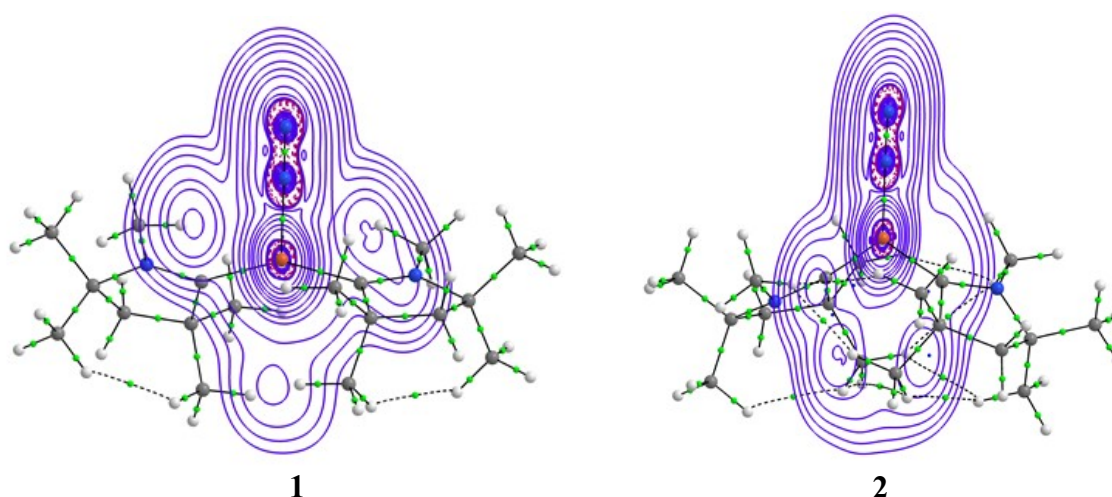
**Figure S1.** Optimized geometries of neutral singlet complex **1-S**, **1-T (Diethyl ether)**, **1-Quintet**, neutral triplet (cAAC)<sub>2</sub>Fe ligand at BP86-D3(BJ)/Def2TZVPP level and complexes **1-T** and **2** at TPSS-D3(BJ)/Def2TZVPP and PW6B95(D3)/Def2TZVPP levels.



**Figure S2.** MO of complex **1** at BP86-D3(BJ)/Def2TZVPP level.



**Figure S3.** MO of complex **2** at BP86-D3(BJ)/Def2TZVPP level.



**Figure S4.** Contour plot of Laplacian distribution [ $\nabla^2\rho(r)$ ] in the complexes **1** and **2** in Fe–N–N plane. Solid blue lines indicate the areas of charge concentration ( $\nabla^2\rho(r) < 0$ ) while dotted purple lines denote charge depletion ( $\nabla^2\rho(r) > 0$ ). Solid lines connecting atomic nuclei (black) are the bond paths, small green spheres along the bond path are bond critical points (BCP) and

those thick solid blue lines separating the atomic basins indicates the zero-flux surface crossing the molecular plane.

### Optimized coordinates

Electronic energies in Hartree

(cAAC)<sub>2</sub>Fe–N<sub>2</sub> (**1**) Triplet

Energy								-2189.7846483
26	0.005479000	0.532642000	-0.009758000	1	-0.835642000	-2.143134000	-1.469981000	
6	1.829153000	-0.022710000	0.077095000	1	-2.240170000	-2.613966000	-0.498070000	
6	-2.723525000	0.816627000	2.001471000	6	5.251935000	0.944641000	0.032122000	
6	-1.845580000	0.080710000	-0.162490000	1	5.531529000	1.392953000	-0.932153000	
6	2.861947000	1.245026000	-1.747128000	1	6.169576000	0.556323000	0.496408000	
6	2.292727000	-0.994166000	1.169440000	1	4.844864000	1.733317000	0.680043000	
6	-4.221535000	-0.220037000	0.203953000	6	4.776412000	-1.233576000	-1.134530000	
7	-2.888336000	0.272402000	0.665158000	1	4.069944000	-2.063582000	-1.260908000	
6	1.624358000	-0.639627000	2.505641000	1	5.730846000	-1.643084000	-0.774064000	
1	1.927319000	-1.340224000	3.299480000	1	4.960020000	-0.784468000	-2.121416000	
1	1.884748000	0.380566000	2.819264000	6	-3.930760000	-0.488380000	-1.288554000	
6	-5.300669000	0.855173000	0.383736000	1	-4.276851000	0.370662000	-1.882332000	
1	-5.534944000	1.033755000	1.442874000	1	-4.464135000	-1.377518000	-1.652804000	
1	-6.228777000	0.530905000	-0.108035000	6	-2.390546000	-0.617750000	-1.414677000	
1	-4.982559000	1.803256000	-0.071662000	6	1.889913000	-2.429192000	0.770932000	
7	2.923031000	0.340760000	-0.612290000	1	0.795586000	-2.510210000	0.715099000	
6	3.832670000	-0.812429000	1.216079000	1	2.292312000	-2.706700000	-0.212894000	
1	4.366869000	-1.753528000	1.407656000	7	0.060194000	2.311782000	0.261636000	
1	4.094516000	-0.113834000	2.024525000	7	0.106194000	3.440510000	0.415391000	
6	-4.614925000	-1.490388000	0.977307000	1	-0.750499000	0.022220000	-2.692766000	
1	-3.861794000	-2.279148000	0.855319000	1	-2.359968000	-2.625098000	-2.276933000	
1	-5.578881000	-1.873626000	0.613391000	1	2.263641000	-3.152077000	1.513679000	
1	-4.723459000	-1.281119000	2.051370000	1	0.527040000	-0.696666000	2.405487000	
6	-1.852076000	0.071321000	-2.676911000	1	-1.735668000	1.288707000	2.053662000	
1	-2.225988000	-0.421677000	-3.587979000	1	-3.490825000	1.572528000	2.217879000	
1	-2.145486000	1.129747000	-2.704480000	1	-2.781768000	0.027280000	2.768970000	
6	4.236568000	-0.192068000	-0.139936000	1	3.492066000	0.881265000	-2.572465000	
6	-1.931740000	-2.091016000	-1.413572000	1	1.820978000	1.296487000	-2.086869000	

1 3.189569000 2.259873000 -1.474705000  
 (cAAC)<sub>2</sub>Fe–N<sub>2</sub> (1)-Triplet  
 Solvent: Diethyl ether  
 Energy: -2189.7926593  
 26 -0.006479000 0.596044000 -0.012762000  
 6 -1.829137000 -0.001862000 -0.101823000  
 6 2.722776000 0.733002000 -2.026498000  
 6 1.841994000 0.106154000 0.174166000  
 6 -2.870821000 1.298660000 1.697512000  
 6 -2.283672000 -1.023211000 -1.153117000  
 6 4.205605000 -0.272225000 -0.200190000  
 7 2.877565000 0.234528000 -0.669666000  
 6 -1.651813000 -0.706720000 -2.516218000  
 1 -1.974400000 -1.435447000 -3.276073000  
 1 -1.932185000 0.299439000 -2.857631000  
 6 5.306306000 0.769054000 -0.435581000  
 1 5.526805000 0.902228000 -1.504052000  
 1 6.232656000 0.438165000 0.054635000  
 1 5.019260000 1.740575000 -0.009601000  
 7 -2.920350000 0.363994000 0.585198000  
 6 -3.828182000 -0.881562000 -1.181539000  
 1 -4.339856000 -1.841850000 -1.332484000  
 1 -4.119350000 -0.217687000 -2.008842000  
 6 4.558027000 -1.581359000 -0.926428000  
 1 3.785738000 -2.345038000 -0.769009000  
 1 5.513462000 -1.973281000 -0.550465000  
 1 4.666225000 -1.417238000 -2.008038000  
 6 1.880451000 0.188693000 2.694323000  
 1 2.268838000 -0.278612000 3.612680000  
 1 2.198245000 1.240590000 2.678081000  
 6 -4.227852000 -0.225946000 0.157526000  
 6 1.886418000 -2.018270000 1.508141000  
 1 0.790720000 -2.044219000 1.588356000  
 1 2.166588000 -2.581306000 0.607507000

6 -5.280424000 0.872490000 -0.034027000  
 1 -5.557575000 1.343819000 0.919633000  
 1 -6.191552000 0.437051000 -0.467763000  
 1 -4.910940000 1.650020000 -0.717136000  
 6 -4.715183000 -1.245326000 1.200486000  
 1 -3.980242000 -2.046924000 1.346912000  
 1 -5.659659000 -1.698451000 0.868098000  
 1 -4.900220000 -0.764281000 2.171562000  
 6 3.922555000 -0.473410000 1.303285000  
 1 4.296173000 0.399121000 1.859278000  
 1 4.435435000 -1.361218000 1.697657000  
 6 2.380853000 -0.557446000 1.448924000  
 6 -1.840810000 -2.433946000 -0.711188000  
 1 -0.743954000 -2.493527000 -0.678266000  
 1 -2.217704000 -2.685196000 0.289580000  
 7 -0.040584000 2.353668000 -0.334750000  
 7 -0.069476000 3.482927000 -0.531500000  
 1 0.779627000 0.163513000 2.740908000  
 1 2.318985000 -2.529672000 2.382537000  
 1 -2.215783000 -3.188812000 -1.420173000  
 1 -0.552508000 -0.753051000 -2.449163000  
 1 1.717701000 1.159447000 -2.119039000  
 1 3.464352000 1.512699000 -2.247447000  
 1 2.836088000 -0.076507000 -2.764612000  
 1 -3.431284000 0.910030000 2.560185000  
 1 -1.821821000 1.435803000 1.983089000  
 1 -3.292030000 2.276236000 1.419431000  
 (cAAC)<sub>2</sub>Fe–N<sub>2</sub> (1) Singlet  
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 26 -0.072374000 0.320858000 -0.158450000  
 6 -1.884390000 0.147438000 -0.016495000  
 6 2.658562000 1.585317000 -1.602763000  
 6 1.802738000 -0.076892000 -0.019568000  
 6 -3.130936000 1.985396000 1.042800000

6	-2.209590000	-1.205998000	-0.651213000	1	4.023848000	-0.198504000	1.985479000
6	4.207860000	0.158003000	-0.147172000	1	4.542012000	-1.634530000	1.084994000
7	2.832616000	0.560585000	-0.582249000	6	2.382792000	-1.146092000	0.912228000
6	-1.218314000	-1.394651000	-1.814795000	6	-2.016856000	-2.338578000	0.378349000
1	-1.198501000	-2.430523000	-2.190303000	1	-0.965306000	-2.402142000	0.691178000
1	-1.437023000	-0.713386000	-2.645607000	1	-2.612802000	-2.166482000	1.283348000
6	5.019845000	1.386018000	0.281271000	7	0.112484000	1.900954000	0.447886000
1	5.270413000	2.031948000	-0.572140000	7	0.281259000	2.971260000	0.822365000
1	5.964379000	1.061242000	0.740164000	1	0.592798000	-1.326946000	2.139010000
1	4.462497000	1.979222000	1.019322000	1	2.671514000	-3.309708000	0.857674000
7	-3.048250000	0.700619000	0.370497000	1	-2.311388000	-3.308219000	-0.055245000
6	-3.690874000	-1.061398000	-1.067581000	1	-0.156059000	-1.194363000	-1.500125000
1	-4.251727000	-2.005552000	-1.013056000	1	1.580826000	1.713068000	-1.763173000
1	-3.749108000	-0.695716000	-2.103536000	1	3.092356000	2.542144000	-1.279960000
6	4.927745000	-0.581983000	-1.286214000	1	3.132864000	1.280179000	-2.547936000
1	4.363965000	-1.468952000	-1.603199000	1	-3.959686000	1.985093000	1.765789000
1	5.922992000	-0.907520000	-0.952244000	1	-2.192967000	2.163595000	1.575925000
1	5.067245000	0.069418000	-2.160677000	1	-3.287358000	2.811055000	0.330108000
6	1.669299000	-1.145817000	2.271346000	(cAAC) <sub>2</sub> Fe–N <sub>2</sub> (1) Quintet			
1	2.088865000	-1.923029000	2.930570000	Energy: -2189.7512925			
1	1.773329000	-0.169991000	2.764620000	26	0.006251000	0.724190000	0.240226000
6	-4.284090000	0.014642000	-0.116660000	6	1.781918000	-0.058004000	0.056901000
6	2.209041000	-2.524484000	0.240128000	6	-2.886643000	1.520265000	1.537468000
1	1.143862000	-2.766852000	0.121886000	6	-1.761364000	-0.057253000	0.027048000
1	2.669876000	-2.554853000	-0.756906000	6	2.845688000	1.850612000	-1.092886000
6	-5.173975000	1.001463000	-0.885407000	6	2.260868000	-1.392880000	0.637653000
1	-5.595245000	1.771772000	-0.223897000	6	-4.184475000	-0.095699000	0.043988000
1	-6.013826000	0.462334000	-1.346575000	7	-2.890546000	0.448946000	0.557244000
1	-4.602682000	1.498496000	-1.681687000	6	1.479574000	-1.807497000	1.890320000
6	-5.073618000	-0.586973000	1.057208000	1	1.845058000	-2.771109000	2.280453000
1	-4.473345000	-1.317959000	1.612383000	1	1.580848000	-1.048638000	2.679160000
1	-5.980028000	-1.090160000	0.690622000	6	-5.090452000	1.044453000	-0.438847000
1	-5.390428000	0.197976000	1.759165000	1	-5.430593000	1.677224000	0.393376000
6	3.879562000	-0.758473000	1.050242000	1	-5.983184000	0.628575000	-0.927573000

1	-4.562044000	1.676675000	-1.165723000	1	-2.252936000	-3.384684000	-0.809084000
7	2.893762000	0.586810000	-0.383977000	1	2.534943000	-3.442937000	-0.083283000
6	3.754754000	-1.130443000	0.965750000	1	0.408266000	-1.907431000	1.666247000
1	4.380515000	-2.024310000	0.832287000	1	-1.944205000	1.468829000	2.103149000
1	3.842297000	-0.819816000	2.017389000	1	-2.948514000	2.511005000	1.062530000
6	-4.895672000	-0.906519000	1.139819000	1	-3.732529000	1.408203000	2.230452000
1	-4.269859000	-1.737186000	1.489152000	1	3.734139000	1.961987000	-1.729535000
1	-5.836248000	-1.321496000	0.750759000	1	1.947735000	1.869559000	-1.722186000
1	-5.145345000	-0.276317000	2.005670000	1	2.799704000	2.711830000	-0.404971000
6	-1.386775000	-1.169549000	-2.213986000	[(cAAC) <sub>2</sub> Fe(N <sub>2</sub> )] <sup>-</sup> (2) Doublet			
1	-1.692019000	-1.996691000	-2.874355000	Energy: -2189.8060501			
1	-1.554661000	-0.220840000	-2.743410000	26	-0.000019000	1.287448000	-0.048971000
6	4.208306000	0.029460000	0.053216000	6	-1.496820000	0.238577000	-0.256469000
6	-1.917516000	-2.545392000	-0.180029000	6	2.421761000	0.543708000	-1.988522000
1	-0.847537000	-2.674432000	0.023982000	6	1.595675000	0.432005000	0.310687000
1	-2.446126000	-2.600810000	0.781009000	6	-2.357124000	0.541721000	2.004618000
6	5.001061000	1.084903000	0.838154000	6	-1.898259000	-0.618420000	-1.471015000
1	5.319320000	1.918879000	0.196140000	6	3.553100000	-0.917020000	-0.247538000
1	5.905470000	0.630930000	1.268370000	7	2.604608000	0.150601000	-0.613271000
1	4.393083000	1.488420000	1.659971000	6	-1.636670000	0.112700000	-2.790685000
6	5.026230000	-0.446632000	-1.158712000	1	-1.922356000	-0.503161000	-3.662148000
1	4.488581000	-1.218832000	-1.722953000	1	-2.192135000	1.060764000	-2.820796000
1	5.985048000	-0.867832000	-0.823924000	6	4.983980000	-0.578977000	-0.693798000
1	5.251159000	0.385009000	-1.842046000	1	5.086306000	-0.601585000	-1.789571000
6	-3.691677000	-0.969613000	-1.128843000	1	5.696037000	-1.310226000	-0.279649000
1	-3.834452000	-0.422530000	-2.072320000	1	5.263910000	0.422826000	-0.338159000
1	-4.257147000	-1.908816000	-1.203413000	7	-2.383082000	-0.179709000	0.753560000
6	-2.174709000	-1.203786000	-0.897161000	6	-3.406120000	-0.893254000	-1.250683000
6	2.117735000	-2.488425000	-0.442110000	1	-3.725779000	-1.877837000	-1.629880000
1	1.061737000	-2.648368000	-0.694725000	1	-3.993724000	-0.131054000	-1.785714000
1	2.637299000	-2.210572000	-1.368812000	6	3.141449000	-2.276153000	-0.853983000
7	-0.217292000	2.509031000	-0.190151000	1	2.108683000	-2.527769000	-0.582878000
7	-0.379227000	3.604263000	-0.455515000	1	3.802704000	-3.084050000	-0.501632000
1	-0.308337000	-1.253760000	-2.017346000	1	3.203167000	-2.243935000	-1.952604000



				(cAAC) <sub>2</sub> Fe -Triplet		
				Energy: -2080.1616961		
6	2.035074000	0.640986000	2.790584000			
1	2.339546000	0.128981000	3.721332000			
1	2.726471000	1.474350000	2.599422000	26	-0.007807000	-0.068795000
6	-3.660833000	-0.756243000	0.273734000	6	1.896164000	-0.016699000
6	1.014794000	-1.460975000	1.892675000	6	-2.596519000	-1.276628000
1	-0.001380000	-1.059797000	1.993862000	6	-1.889940000	-0.060217000
1	0.978651000	-2.189369000	1.072004000	6	2.372462000	-2.062862000
6	-4.850067000	0.189853000	0.531242000	6	2.709990000	1.133749000
1	-5.065915000	0.293881000	1.605616000	6	-4.277594000	-0.394627000
1	-5.758266000	-0.195110000	0.040982000	7	-2.873874000	-0.622326000
1	-4.630764000	1.187062000	0.123129000	6	2.219067000	1.450893000
6	-3.923626000	-2.112050000	0.953255000	1	2.815805000	2.259795000
1	-3.110134000	-2.815034000	0.729570000	1	2.288144000	0.564175000
1	-4.875109000	-2.552727000	0.610830000	6	-5.072830000	-1.707090000
1	-3.980179000	-1.993874000	2.046681000	1	-5.264283000	-2.095182000
6	3.426142000	-0.885557000	1.291879000	1	-6.048904000	-1.539211000
1	4.190786000	-0.200768000	1.692440000	1	-4.534635000	-2.473200000
1	3.602728000	-1.877007000	1.738703000	7	2.789230000	-0.895781000
6	2.011904000	-0.323444000	1.595486000	6	4.174708000	0.622112000
6	-1.090754000	-1.933861000	-1.450671000	1	4.901949000	1.412198000
1	-0.021922000	-1.709742000	-1.571686000	1	4.426078000	0.228853000
1	-1.209470000	-2.448742000	-0.486647000	6	-4.976174000	0.616943000
7	0.013435000	3.058303000	-0.254403000	1	-4.431695000	1.569227000
7	0.031549000	4.198335000	-0.421811000	1	-5.999273000	0.813408000
1	1.034991000	1.074795000	2.940062000	1	-5.044776000	0.229095000
1	1.293806000	-1.995105000	2.819440000	6	-1.900974000	0.325195000
1	-1.410465000	-2.617875000	-2.258191000	1	-2.413036000	0.821508000
1	-0.566826000	0.357239000	-2.875835000	1	-1.904813000	-0.759441000
1	1.895992000	1.512656000	-1.979722000	6	4.231994000	-0.529330000
1	3.387175000	0.653660000	-2.508068000	6	-2.492398000	2.184421000
1	1.794879000	-0.168758000	-2.562677000	1	-1.438901000	2.497930000
1	-2.962116000	0.029771000	2.770651000	1	-2.946913000	2.476517000
1	-1.316993000	0.590388000	2.361855000	6	5.070465000	-1.705790000
1	-2.709021000	1.589231000	1.899223000	1	5.131086000	-2.523118000

1	6.096946000	-1.368136000	-0.527361000	1	2.576060000	3.422241000	1.106892000
1	4.647782000	-2.101275000	-1.259580000	1	2.513566000	2.952383000	-0.623710000
6	4.757393000	-0.080173000	1.566437000	6	-5.443147000	0.300384000	-0.915074000
1	4.176729000	0.766010000	1.955051000	1	-5.573920000	1.237500000	-1.477873000
1	5.809863000	0.228351000	1.489432000	1	-6.324868000	0.177535000	-0.266632000
1	4.702521000	-0.899628000	2.297758000	1	-5.414393000	-0.534174000	-1.630770000
6	-4.046189000	0.153178000	1.188472000	7	2.945602000	-0.294447000	-0.925874000
1	-4.168975000	-0.666283000	1.912565000	6	3.975177000	0.994470000	0.710964000
1	-4.775692000	0.933370000	1.448159000	1	4.424215000	0.937143000	1.714771000
6	-2.581730000	0.662192000	1.228304000	1	4.482871000	1.808241000	0.168556000
6	2.533801000	2.387564000	0.047301000	6	-4.159128000	1.548587000	0.856467000
1	1.473525000	2.677547000	0.076172000	1	-3.206361000	1.606635000	1.400671000
1	2.853731000	2.206674000	1.082555000	1	-4.984382000	1.496103000	1.584030000
1	-0.852413000	0.662326000	2.556734000	1	-4.274494000	2.478603000	0.278638000
1	-3.004919000	2.730745000	1.801970000	6	-2.124382000	-2.718031000	0.380334000
1	3.122725000	3.227507000	-0.355392000	1	-2.572106000	-3.421821000	1.107451000
1	1.166166000	1.772123000	-2.231269000	1	-2.509861000	-2.952018000	-0.623183000
1	-1.535817000	-1.564118000	-1.948524000	6	4.159519000	-0.318673000	-0.074831000
1	-3.209239000	-2.181431000	-2.067906000	6	-1.839657000	-0.966415000	2.136114000
1	-2.782436000	-0.609708000	-2.805675000	1	-0.744797000	-1.066242000	2.081107000
1	2.515668000	-1.918699000	2.125425000	1	-2.057218000	0.060076000	2.463612000
1	1.302867000	-2.221197000	0.842907000	6	5.442719000	-0.303725000	-0.914835000
1	2.930458000	-2.958316000	0.730913000	1	5.572425000	-1.241009000	-1.477601000
[(cAAC) <sub>2</sub> Fe]- Doublet				1	6.324430000	-0.182022000	-0.266163000
Energy: -2080.1666907				1	5.415233000	0.530875000	-1.630534000
26	-0.000039000	0.001250000	-0.565126000	6	4.156542000	-1.550279000	0.856326000
6	1.845617000	0.317141000	-0.317283000	1	3.203504000	-1.607085000	1.400189000
6	-2.712234000	1.387665000	-1.846815000	1	4.981615000	-1.498910000	1.584173000
6	-1.845399000	-0.315877000	-0.316813000	1	4.270876000	-2.480425000	0.278501000
6	2.710610000	-1.387328000	-1.847297000	6	-3.974282000	-0.995908000	0.711068000
6	2.441566000	1.256849000	0.748040000	1	-4.480798000	-1.810339000	0.168550000
6	-4.160179000	0.317008000	-0.074747000	1	-4.423610000	-0.939175000	1.714779000
7	-2.946041000	0.294451000	-0.925483000	6	-2.440340000	-1.256291000	0.748455000
6	2.127574000	2.718969000	0.379743000	6	1.840270000	0.967862000	2.135619000

1	0.745537000	1.069004000	2.080418000	6	-3.865199000	-0.690237000	-1.269987000
1	2.056531000	-0.058856000	2.463266000	1	-4.405429000	-1.604750000	-1.533147000
1	-1.033591000	-2.862652000	0.360451000	1	-4.126533000	0.074143000	-2.009674000
1	-2.234828000	-1.669552000	2.893159000	6	4.673755000	-1.366653000	-1.093476000
1	2.236168000	1.670599000	2.892658000	1	3.940027000	-2.175420000	-1.058397000
1	1.036980000	2.865010000	0.359633000	1	5.638028000	-1.758021000	-0.753373000
1	-1.863288000	1.108530000	-2.487395000	1	4.790053000	-1.050505000	-2.135377000
1	-3.601991000	1.574641000	-2.471657000	6	1.833292000	-0.211279000	2.654008000
1	-2.428974000	2.329107000	-1.332628000	1	2.192154000	-0.792435000	3.512114000
1	2.425777000	-2.328356000	-1.333218000	1	2.120459000	0.835169000	2.793618000
1	1.862326000	-1.107006000	-2.488230000	6	-4.251688000	-0.185491000	0.136511000
1	3.600374000	-1.575568000	-2.471748000	6	1.957268000	-2.236772000	1.187663000
N <sub>2</sub> Singlet				1	0.865604000	-2.301648000	1.222420000
Energy: -109.5749788				1	2.285579000	-2.662325000	0.234960000
7	0.000000000	0.000000000	0.551559000	6	-5.256710000	0.971812000	0.073862000
7	0.000000000	0.000000000	-0.551559000	1	-5.514333000	1.337633000	1.073336000
(cAAC) <sub>2</sub> Fe–N <sub>2</sub> (1) Triplet-TPSS-D3(BJ)				1	-6.180452000	0.631535000	-0.405059000
Energy: -2189.7800793				1	-4.849834000	1.802910000	-0.510047000
26	-0.004173000	0.510259000	0.039812000	6	-4.793927000	-1.301728000	1.044938000
6	-1.843106000	-0.019382000	-0.084226000	1	-4.098743000	-2.143236000	1.091105000
6	2.755276000	1.018638000	-1.906154000	1	-5.753138000	-1.664211000	0.661189000
6	1.855974000	0.044788000	0.155236000	1	-4.959628000	-0.934404000	2.063219000
6	-2.850276000	1.096187000	1.851474000	6	3.937733000	-0.606333000	1.247488000
6	-2.327614000	-0.886630000	-1.250668000	1	4.263628000	0.189900000	1.925466000
6	4.241940000	-0.186915000	-0.205576000	1	4.474642000	-1.518553000	1.524923000
7	2.905742000	0.322457000	-0.637067000	6	2.398689000	-0.765323000	1.337548000
6	-1.663065000	-0.423960000	-2.555913000	6	-1.933060000	-2.354749000	-0.984255000
1	-1.966344000	-1.056227000	-3.399166000	1	-0.843341000	-2.444865000	-0.948962000
1	-1.925256000	0.613704000	-2.782571000	1	-2.328040000	-2.711603000	-0.028666000
6	5.297715000	0.924326000	-0.267195000	7	-0.049098000	2.314232000	-0.072463000
1	5.521889000	1.216634000	-1.298196000	7	-0.085170000	3.448763000	-0.126910000
1	6.228518000	0.569251000	0.186598000	1	0.736467000	-0.267212000	2.640406000
1	4.959134000	1.806928000	0.283796000	1	2.377504000	-2.842438000	2.000335000
7	-2.929681000	0.293688000	0.640030000	1	-2.318934000	-3.001562000	-1.782075000

1	-0.570292000	-0.488787000	-2.459399000	1	2.814975000	1.728320000	2.405170000
1	1.720576000	1.356506000	-1.975759000	6	-3.727344000	-0.682217000	0.353352000
1	3.419366000	1.886845000	-1.957533000	6	1.147426000	-1.287826000	2.055600000
1	2.977250000	0.354198000	-2.750204000	1	0.133429000	-0.891297000	2.147699000
1	-3.444409000	0.644744000	2.653456000	1	1.102335000	-2.094847000	1.319357000
1	-1.803385000	1.139119000	2.155711000	6	-4.868706000	0.332833000	0.558253000
1	-3.208815000	2.116494000	1.677048000	1	-5.052011000	0.525901000	1.621780000
[(cAAC) <sub>2</sub> Fe(N <sub>2</sub> )] <sup>-</sup> (2) Doublet-TPSS-D3(BJ)				1	-5.798904000	-0.049228000	0.119451000
Energy: -2189.7912104				1	-4.617705000	1.280426000	0.071205000
26	0.002485000	1.208200000	-0.147190000	6	-4.042384000	-1.971749000	1.132266000
6	-1.524452000	0.174539000	-0.265976000	1	-3.269919000	-2.723649000	0.949837000
6	2.422549000	0.374888000	-2.044060000	1	-5.015180000	-2.385837000	0.834272000
6	1.638152000	0.438704000	0.269310000	1	-4.076383000	-1.771044000	2.209886000
6	-2.346254000	0.673140000	1.976877000	6	3.528973000	-0.731939000	1.326217000
6	-1.983376000	-0.747382000	-1.408780000	1	4.285440000	-0.003381000	1.643307000
6	3.622528000	-0.900131000	-0.204861000	1	3.731576000	-1.672290000	1.853674000
7	2.653685000	0.122110000	-0.640043000	6	2.110779000	-0.170224000	1.608617000
6	-1.702010000	-0.128120000	-2.780842000	6	-1.236712000	-2.094645000	-1.298107000
1	-2.005559000	-0.798907000	-3.598420000	1	-0.166262000	-1.931983000	-1.454549000
1	-2.229321000	0.825290000	-2.885362000	1	-1.362262000	-2.523290000	-0.298728000
6	5.036496000	-0.586884000	-0.716451000	7	-0.021929000	2.955876000	-0.496422000
1	5.104442000	-0.692878000	-1.805469000	7	-0.027054000	4.075564000	-0.752789000
1	5.763381000	-1.276686000	-0.270030000	1	1.142453000	1.341549000	2.822494000
1	5.313968000	0.437294000	-0.447819000	1	1.464674000	-1.712962000	3.020604000
7	-2.419378000	-0.133558000	0.778172000	1	-1.604768000	-2.818526000	-2.041972000
6	-3.498922000	-0.937247000	-1.158127000	1	-0.629559000	0.075114000	-2.879732000
1	-3.864121000	-1.927329000	-1.460655000	1	1.866762000	1.318001000	-2.110183000
1	-4.056605000	-0.191357000	-1.736818000	1	3.368881000	0.466081000	-2.591370000
6	3.212141000	-2.311542000	-0.677093000	1	1.812906000	-0.409763000	-2.523885000
1	2.189688000	-2.539246000	-0.367753000	1	-2.921075000	0.215698000	2.792641000
1	3.883422000	-3.074272000	-0.262603000	1	-1.295705000	0.737704000	2.280499000
1	3.258425000	-2.378268000	-1.770413000	1	-2.703592000	1.704984000	1.815522000
6	2.143414000	0.914291000	2.697014000	(cAAC) <sub>2</sub> Fe–N <sub>2</sub> (1) Triplet-PW6B95-D3			
1	2.476481000	0.506589000	3.663605000	Energy: -2191.3578227			

26	0.002869000	1.214660000	0.308781000	6	-3.823172000	-2.336810000	0.275026000
6	-1.642747000	0.283226000	-0.089658000	1	-2.928541000	-2.835449000	-0.080349000
6	2.533718000	0.954272000	-1.811652000	1	-4.682145000	-2.772542000	-0.228626000
6	1.695041000	0.260446000	0.347057000	1	-3.927166000	-2.541358000	1.337979000
6	-2.602626000	-0.055912000	2.113985000	6	3.498868000	-1.171629000	1.061572000
6	-1.977558000	-0.132777000	-1.512825000	1	4.193684000	-0.606508000	1.678893000
6	3.714529000	-0.790463000	-0.404356000	1	3.689978000	-2.227038000	1.235658000
7	2.654294000	0.214512000	-0.584890000	6	2.056937000	-0.766306000	1.406226000
6	-1.689803000	0.985268000	-2.503039000	6	-1.124102000	-1.349101000	-1.886561000
1	-1.918557000	0.676251000	-3.521579000	1	-0.074452000	-1.069291000	-1.923424000
1	-2.268523000	1.873974000	-2.269927000	1	-1.218546000	-2.144603000	-1.154114000
6	5.095197000	-0.187119000	-0.619647000	7	-0.005149000	3.109830000	0.433603000
1	5.277424000	0.055954000	-1.663080000	7	-0.011007000	4.213155000	0.551816000
1	5.855472000	-0.901786000	-0.316112000	1	0.926717000	0.158205000	2.990428000
1	5.215100000	0.713556000	-0.024665000	1	1.376656000	-2.714773000	2.052775000
7	-2.602998000	-0.230971000	0.687599000	1	-1.420944000	-1.736554000	-2.860375000
6	-3.469601000	-0.491130000	-1.449850000	1	-0.633977000	1.255136000	-2.466724000
1	-3.734640000	-1.305571000	-2.118809000	1	2.045553000	1.901435000	-1.596631000
1	-4.060455000	0.375590000	-1.737823000	1	3.508987000	1.153774000	-2.243363000
6	3.512107000	-1.952917000	-1.371353000	1	1.932173000	0.419992000	-2.548953000
1	2.535201000	-2.406976000	-1.244627000	1	-3.109222000	-0.883665000	2.602886000
1	4.269936000	-2.715587000	-1.212793000	1	-1.574272000	-0.026390000	2.462758000
1	3.595432000	-1.611417000	-2.400782000	1	-3.093790000	0.871361000	2.410420000
6	1.950302000	-0.161832000	2.799337000	[(cAAC) <sub>2</sub> Fe(N <sub>2</sub> )] <sup>-</sup> (2) Doublet- PW6B95-D3			
1	2.222002000	-0.888827000	3.562784000	Energy: -2191.3543137			
1	2.596141000	0.705599000	2.900004000	26	0.021293000	1.249235000	-0.138920000
6	-3.764401000	-0.835989000	0.012631000	6	-1.610456000	0.220896000	-0.296586000
6	1.100718000	-1.958388000	1.319017000	6	2.582321000	0.524105000	-1.966503000
1	0.080874000	-1.634246000	1.506535000	6	1.719826000	0.419936000	0.285857000
1	1.115157000	-2.415754000	0.335031000	6	-2.440803000	0.660731000	1.943832000
6	-5.056032000	-0.187485000	0.492221000	6	-2.013785000	-0.701009000	-1.431484000
1	-5.254752000	-0.417820000	1.536242000	6	3.649928000	-0.905756000	-0.213145000
1	-5.894550000	-0.555484000	-0.092828000	7	2.777491000	0.207717000	-0.582197000
1	-5.006784000	0.891857000	0.379202000	6	-1.757582000	-0.083114000	-2.795089000

1	-2.034491000	-0.765218000	-3.601183000	1	-0.157937000	-1.787841000	-1.472298000
1	-2.315843000	0.842616000	-2.906537000	1	-1.318602000	-2.436031000	-0.329665000
6	5.095439000	-0.637110000	-0.607760000	7	0.008142000	3.102280000	-0.337599000
1	5.219749000	-0.625317000	-1.688542000	7	0.018267000	4.229163000	-0.458365000
1	5.746526000	-1.414071000	-0.211372000	1	1.124888000	1.109478000	2.873812000
1	5.417496000	0.322344000	-0.212645000	1	1.273314000	-1.878001000	2.839673000
7	-2.477599000	-0.105621000	0.733405000	1	-1.540005000	-2.735061000	-2.062421000
6	-3.508525000	-0.953805000	-1.183115000	1	-0.701272000	0.160652000	-2.890479000
1	-3.828055000	-1.949247000	-1.489621000	1	2.114876000	1.503885000	-2.029157000
1	-4.091504000	-0.234261000	-1.755346000	1	3.528923000	0.547510000	-2.503803000
6	3.185834000	-2.213217000	-0.857905000	1	1.911871000	-0.186728000	-2.466027000
1	2.133201000	-2.384544000	-0.658748000	1	-2.974572000	0.149813000	2.744986000
1	3.756196000	-3.059284000	-0.479346000	1	-1.403545000	0.791283000	2.243084000
1	3.318983000	-2.174864000	-1.937515000	1	-2.868921000	1.662064000	1.821168000
6	2.109401000	0.665008000	2.745904000				
1	2.394409000	0.163659000	3.673677000				
1	2.810170000	1.473320000	2.553726000				
6	-3.742306000	-0.717421000	0.315465000				
6	1.052188000	-1.398245000	1.883502000				
1	0.055438000	-0.966981000	1.919341000				
1	1.033796000	-2.163781000	1.114145000				
6	-4.921340000	0.229667000	0.531384000				
1	-5.111471000	0.397059000	1.589815000				
1	-5.825113000	-0.185669000	0.089647000				
1	-4.717517000	1.189203000	0.063010000				
6	-3.988572000	-2.011892000	1.084835000				
1	-3.192812000	-2.724575000	0.893486000				
1	-4.937377000	-2.462594000	0.796332000				
1	-4.021483000	-1.819875000	2.155748000				
6	3.475103000	-0.905440000	1.305679000				
1	4.238554000	-0.263475000	1.743048000				
1	3.599887000	-1.900455000	1.729706000				
6	2.080735000	-0.309206000	1.571959000				
6	-1.213323000	-2.002446000	-1.320912000				