Supplementary Information

How to capture C_2O_2: Structures and bonding of neutral and charged complexes [(NHC)-C_2O_2-(NHC)]^q (NHC = N-heterocyclic carbene; q = 0, 1+, 2+)

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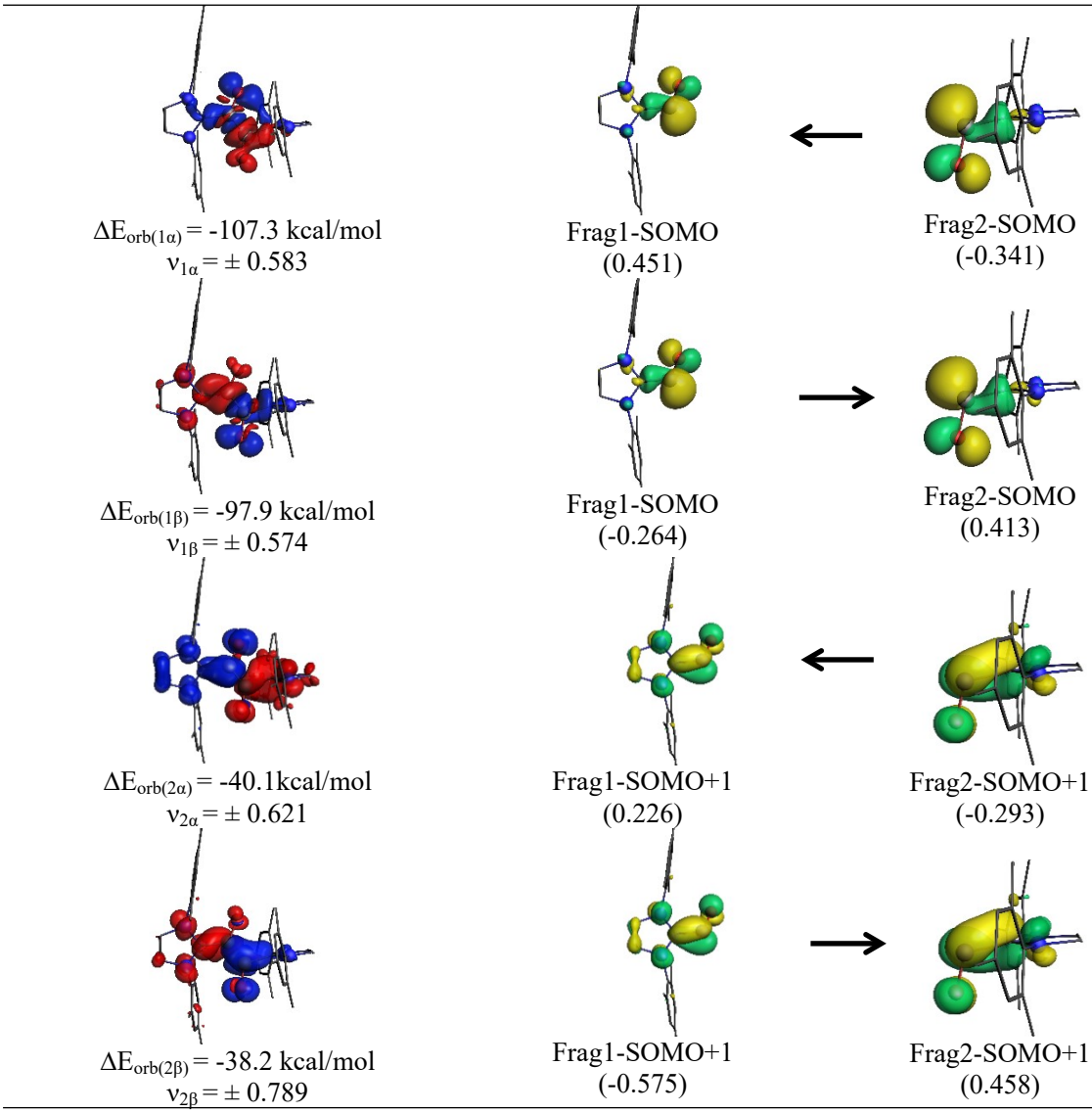

Figure S1. Plot of the deformation densities Δρ of the pairwise orbital interactions of the α and β electrons and the associated most important interacting MOs of the two fragments [NHC-CO](T) in [NHC-C_2O_2-NHC] (**1**). The direction of the charge flow is red→blue. The eigenvalues υ give the amount of charge flow.

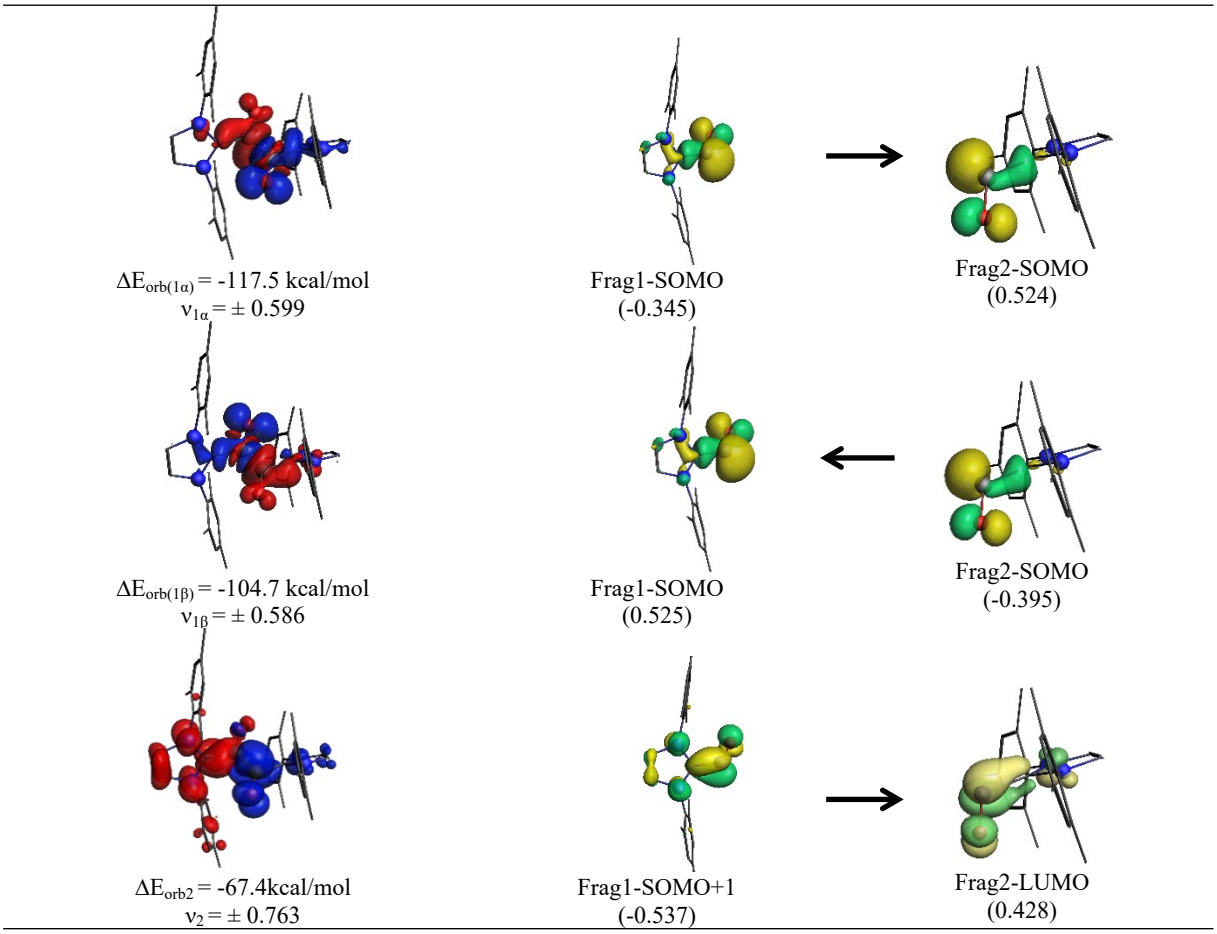

Figure S2. Plot of the deformation densities Δρ of the pairwise orbital interactions of the α and β electrons and the associated most important interacting MOs of the two fragments $[NHC\text{-}CO]^+$ (D) and [NHC-CO] (T) in $[NHC\text{-}C_2O_2\text{-}NHC]^+$ (**1**$^+$). The direction of the charge flow is red→blue. The eigenvalues υ give the amount of charge flow.

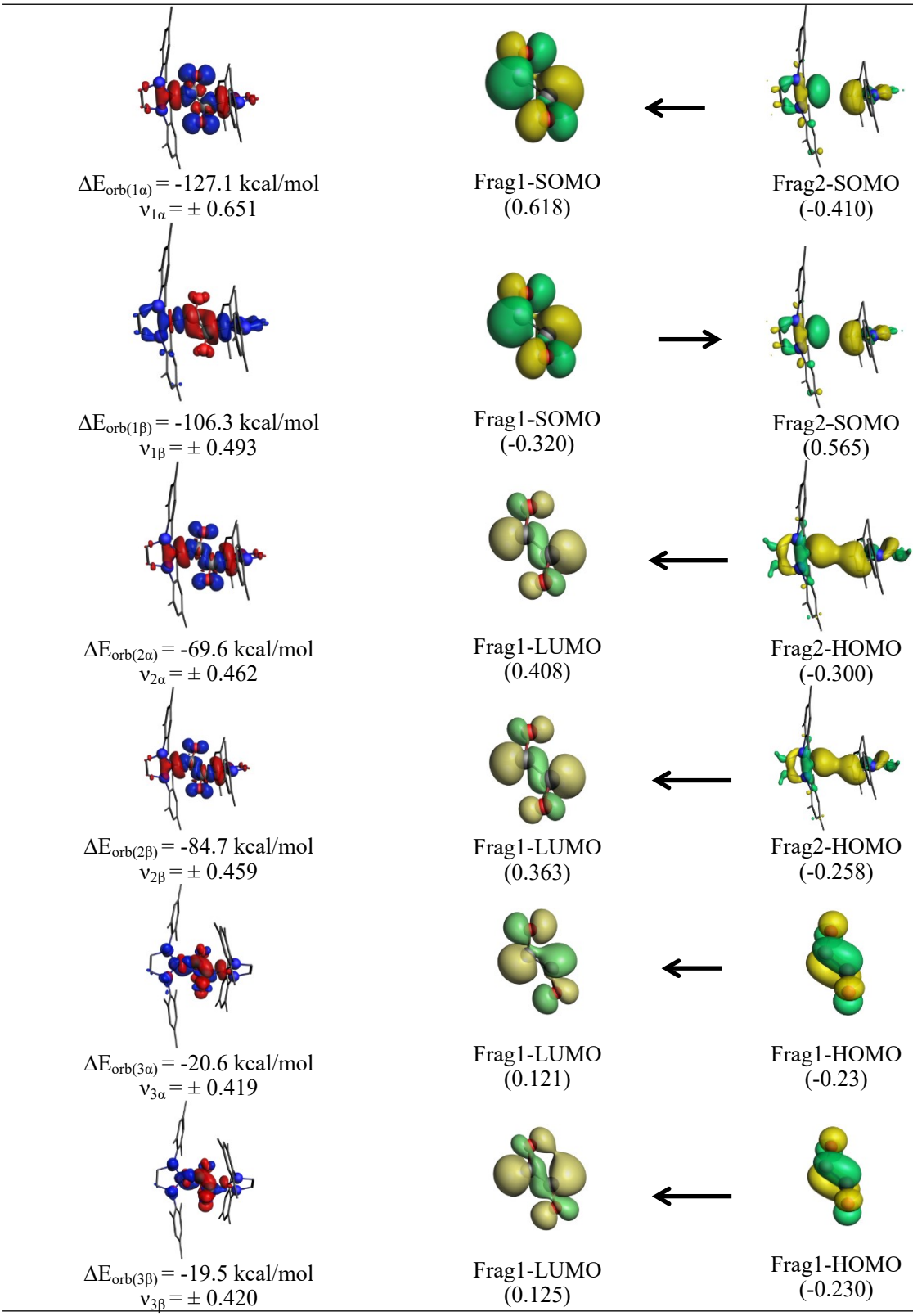

Figure S3. Plot of deformation densities Δρ of the pairwise orbital interactions of the α and β electrons and the associated most important interacting MOs of the two fragments $[C_2O_2]^-$ (D) and $[2NHC]^+$ (D) in [NHC-C_2O_2-NHC] (**1**). The direction of the charge flow is red→blue. The eigenvalues υ give the amount of charge flow.

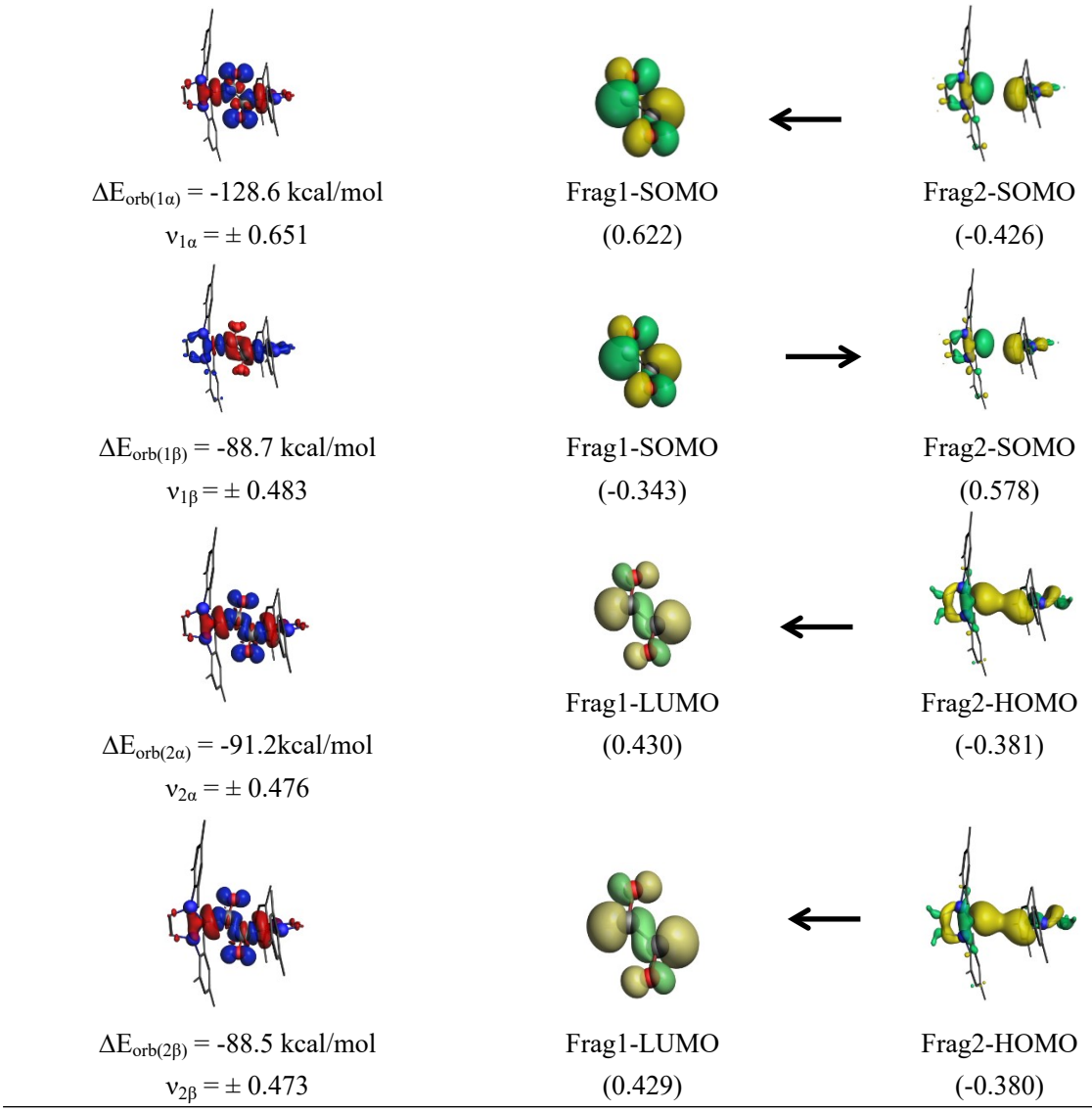

Figure S4. Plot of deformation densities Δρ of the pairwise orbital interactions of the α and β electrons and the associated interaction energies (ΔE_{orb}) between fragments, as well as the shape of the two fragments $[C_2O_2]^0$ (T) and $[2NHC]^+$ (D) in $[NHC\text{-}C_2O_2\text{-}NHC]^+$ (**1**$^+$). The direction of the charge flow is red→blue. The eigenvalues υ give the amount of charge flow.

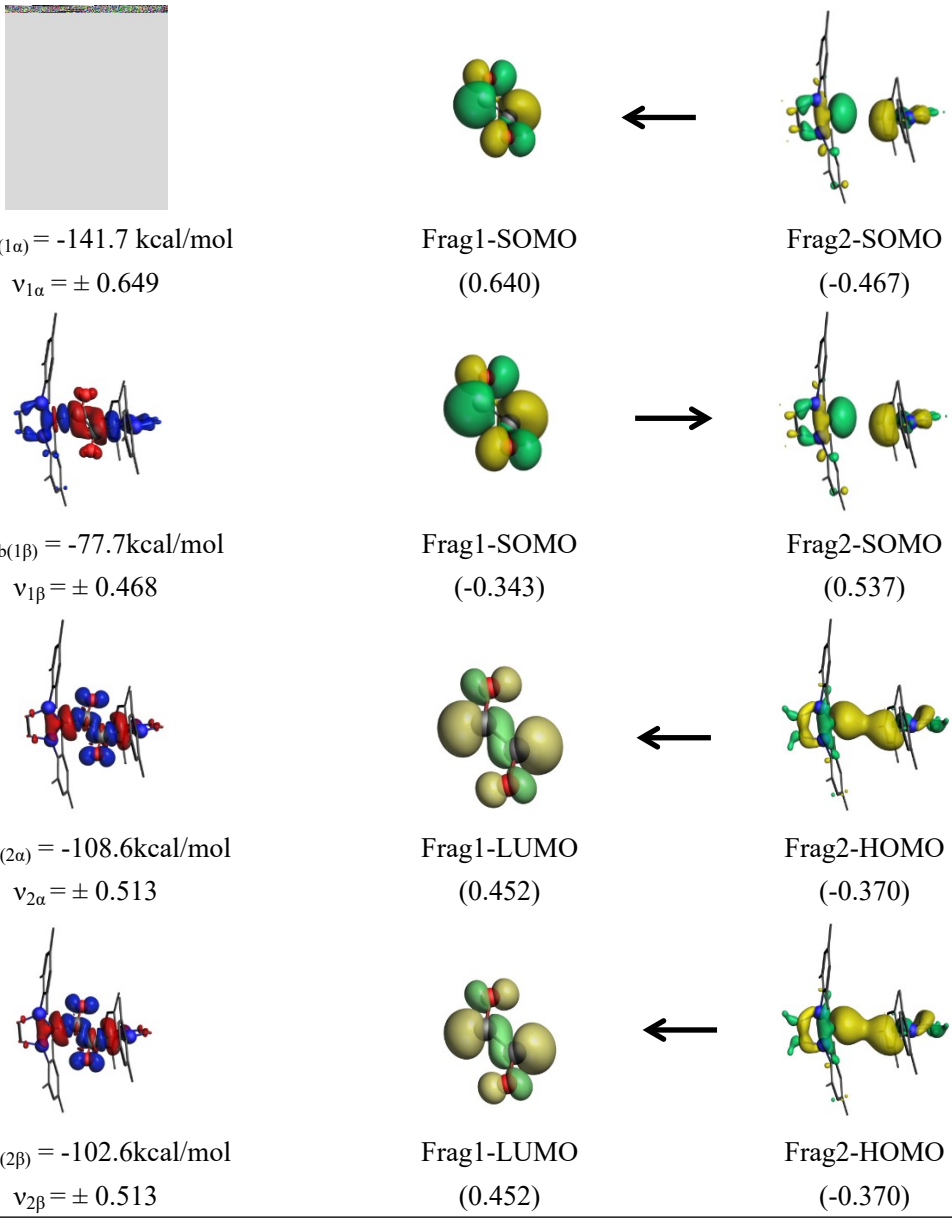

Figure S5. Plot of deformation densities Δρ of the pairwise orbital interactions of the α and β electrons and the associated interaction energies (ΔE_{orb}) between fragments, as well as the shape of the most important interacting MOs of the two fragments $[C_2O_2]^+$ (D) and $[2NHC]^+$ (D) in $[NHC\text{-}C_2O_2\text{-}NHC]^{2+}$ (**1**$^{2+}$). The direction of the charge flow is red→blue. The eigenvalues υ give the amount of charge flow.

Table S1. EDA-NOCV results of 1, 1^+ and 1^{2+} at the BP86+D3(BJ)/TZ2P//BP86-D3(BJ) /def2-TZVPP level of theory using fragments in the electronic singlet (S) or doublet (D) state. Energy values are given in kcal·mol^{-1}.

Fragments	**1** $[C_2O_2]$ (S) + $[NHC_2]$ (S)	**1^+** $[C_2O_2]^+$(D) + $[NHC_2]$ (S)	**1^{2+}** $[C_2O_2]^{2+}$ (S) + $[NHC_2]$ (S)
ΔE_{int}	-207.6	-316.1	-529.9
ΔE_{Pauli}	862.6	782.1	791.2
ΔE_{disp}[a]	-22.7(2.1%)	-21.7(2.0%)	-21.6(1.6%)
ΔE_{elstat}[a]	-436.2 (40.8%)	-430.9(39.2%)	-475.3(36.0%)
ΔE_{orb}[a]	-611.1(57.1%)	-645.7(58.8%)	-824.2(62.4%)
ΔE_{orb1}[b]	-293.3(48.0%)	-307.8(47.6%)	-342.6(41.6%)
ΔE_{orb2}[b]	-189.9(31.0%)	-206.4(32.0%)	-249.1(30.2%)
ΔE_{rest}	- 127.9(20.9%)	-131.5(20.4%)	-232.5(28.2%)

[a]The values in parentheses give the percentage contribution to the total attractive interactions $\Delta E_{elstat} + \Delta E_{orb} + \Delta E_{disp}$.

[b]The values in parentheses give the percentage contribution to the total orbital interactions ΔE_{orb}.

Table S2. Coordinates and energies (a.u) of the structures optimized at the BP86-D3(BJ)/ def2-TZVPP level by the Gaussian 16 software.

1 (NHC-C_2O_2-NHC)^0 (S)

E = -2076.024080

O	-0.3077	-0.77049	-1.53479
N	0.726567	-2.04849	1.67166
N	-1.06348	-2.68806	0.57129
C	2.247625	-0.77718	3.10377
C	2.019853	-1.47305	1.905489
C	-0.01047	-0.58991	-0.26718
C	-0.10052	-1.70822	0.633383
C	3.540656	-0.28866	3.333076
C	4.300669	-1.18092	1.231968
C	3.024433	-1.67393	0.942962
C	4.576154	-0.47902	2.412913
C	0.263692	-3.22135	2.272152
C	-2.32099	-2.50608	-0.10492
C	-2.5137	-3.07021	-1.37454
C	-3.30608	-1.75219	0.549627
C	1.133112	-0.53441	4.08183
C	-0.85057	-3.61107	1.594067
C	2.755339	-2.38898	-0.35331
C	5.951571	0.085614	2.661434
C	-4.80198	-2.20471	-1.33274
C	-4.55288	-1.63561	-0.08006
C	-3.02112	-1.05878	1.855341
C	-3.76841	-2.90769	-1.96915
C	-1.37618	-3.74559	-2.08414
C	-6.14509	-2.04722	-2.0006
O	0.38888	1.038323	1.545704
N	1.094405	2.139834	-1.59791
N	-0.79197	2.736197	-0.69793
C	2.377886	0.641324	-3.03873
C	2.305309	1.408434	-1.86545
C	0.242409	0.673315	0.317078
C	0.172362	1.780634	-0.67196
C	3.580641	-0.03211	-3.28732
C	4.543905	0.83134	-1.2555
C	3.360995	1.51134	-0.94594
C	4.669347	0.051483	-2.41158
C	0.70454	3.322709	-2.22001
C	-2.03562	2.627993	0.021325
C	-2.15448	3.255712	1.268888
C	-3.05776	1.859147	-0.55932
C	1.19607	0.515661	-3.96046
C	-0.48227	3.693675	-1.6573
C	3.225029	2.298773	0.327627
C	5.937793	-0.71762	-2.67872
C	-4.44539	2.40756	1.38355
C	-4.26906	1.786861	0.142202
C	-2.849	1.119767	-1.84942
C	-3.37983	3.132741	1.934203
C	-0.98552	3.976676	1.88064
C	-5.74324	2.259138	2.136699
H	3.735616	0.262694	4.256038
H	5.101606	-1.35681	0.511587
H	0.799216	-3.68199	3.092038
H	0.321164	-0.00441	3.560386
H	1.483322	0.079774	4.921115
H	0.724074	-1.46943	4.494436
H	-1.51762	-4.45122	1.739344
H	2.174042	-3.31014	-0.19965
H	3.698877	-2.65443	-0.84648
H	2.174344	-1.75572	-1.04128
H	6.088725	1.039847	2.125983
H	6.737031	-0.59794	2.308692
H	6.12026	0.283114	3.728489
H	-5.34355	-1.07586	0.423685
H	-2.62043	-1.75113	2.610982
H	-3.93252	-0.59857	2.255072
H	-2.2718	-0.26272	1.719666
H	-3.93845	-3.33365	-2.96101
H	-0.5907	-2.98929	-2.25368
H	-1.70227	-4.16185	-3.04563
H	-0.93765	-4.55639	-1.484
H	-6.84919	-1.50173	-1.3584
H	-6.59138	-3.02419	-2.23967
H	-6.05453	-1.49452	-2.94847
H	3.65983	-0.64554	-4.18779
H	5.385791	0.910453	-0.56538
H	1.31277	3.786208	-2.9857
H	0.338441	0.133611	-3.38243
H	1.41999	-0.18027	-4.77859
H	0.914372	1.48233	-4.40606

H	-1.13595	4.534901	-1.84812
H	2.864411	3.320854	0.135839
H	4.191621	2.365236	0.841514
H	2.498724	1.825972	1.010746
H	5.925311	-1.6866	-2.15297
H	6.822504	-0.16919	-2.32657
H	6.064531	-0.92884	-3.74893
H	-5.08761	1.212566	-0.29461
H	-2.56197	1.801406	-2.66557
H	-3.76687	0.596427	-2.14288
H	-2.03275	0.370591	-1.76167
H	-3.49814	3.608964	2.910259
H	-0.1636	3.256485	2.028451
H	-1.2607	4.414962	2.847981
H	-0.61423	4.783911	1.231289
H	-6.57499	2.022579	1.459577
H	-5.99696	3.174659	2.688873
H	-5.6764	1.443486	2.875015

1^+ [NHC-C_2O_2-NHC]$^+$ (D)

E = -2075.866728

O	-0.09317	0.653806	1.640188
N	0.917507	2.403037	-1.21147
N	-1.03302	2.764706	-0.31013
C	2.413018	1.305209	-2.80803
C	2.202263	1.818632	-1.51618
C	0.034732	0.602732	0.383012
C	-0.01711	1.871952	-0.38943
C	3.680243	0.785356	-3.08645
C	4.451442	1.331883	-0.87239
C	3.194371	1.840081	-0.5249
C	4.711646	0.79382	-2.13625
C	0.487255	3.648008	-1.65483
C	-2.29685	2.518586	0.346469
C	-2.47885	2.979202	1.658863
C	-3.28087	1.825435	-0.37419
C	1.323288	1.304092	-3.84551
C	-0.7386	3.870668	-1.09491
C	2.937058	2.373034	0.858933
C	6.063763	0.219487	-2.46721
C	-4.75515	2.083684	1.56364
C	-4.51449	1.636237	0.259206
C	-3.01966	1.286415	-1.75528
C	-3.72378	2.741127	2.249454
C	-1.36532	3.659111	2.406335
C	-6.09914	1.880054	2.21255
O	0.072599	-0.67838	-1.65321
N	1.00247	-2.39015	1.209456
N	-0.95123	-2.77462	0.327834
C	2.468273	-1.24134	2.79707
C	2.276614	-1.78161	1.513454
C	0.097918	-0.60639	-0.39351
C	0.056446	-1.87332	0.393505
C	3.727387	-0.70231	3.078095
C	4.526169	-1.28135	0.881744
C	3.278982	-1.81117	0.532209
C	4.767745	-0.71679	2.138302
C	0.588147	-3.63672	1.664219
C	-2.21466	-2.55055	-0.33775
C	-2.37283	-3.00372	-1.65617
C	-3.22203	-1.88745	0.379673
C	1.368148	-1.23424	3.823776
C	-0.64004	-3.87421	1.115877
C	3.039536	-2.37376	-0.84273
C	6.108015	-0.11424	2.466829
C	-4.66853	-2.1572	-1.57778
C	-4.45221	-1.71886	-0.26601
C	-2.99032	-1.36192	1.770875
C	-3.61608	-2.78575	-2.25844
C	-1.24014	-3.66069	-2.39585
C	-6.00906	-1.97448	-2.23987
H	3.867237	0.369677	-4.07882
H	5.248077	1.361302	-0.12789
H	1.101084	4.256277	-2.30645
H	0.412181	0.841279	-3.44298
H	1.638943	0.739194	-4.73047
H	1.071829	2.323179	-4.17646
H	-1.42971	4.699327	-1.18228
H	2.358263	3.307495	0.84265
H	3.88453	2.568809	1.374528
H	2.371524	1.649184	1.465078
H	6.014753	-0.8778	-2.54976
H	6.804995	0.46609	-1.69653
H	6.434342	0.594491	-3.4314
H	-5.30569	1.120489	-0.28675
H	-2.65255	2.066541	-2.43852
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H	-2.26062	0.488796	-1.73985

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H	3.900507	-0.2673	4.064641
H	5.330307	-1.31496	0.145263
H	1.21236	-4.23404	2.316155
H	0.455577	-0.78806	3.405543
H	1.669737	-0.6527	4.70284
H	1.123884	-2.25077	4.167832
H	-1.32185	-4.70955	1.21209
H	2.486395	-3.32335	-0.81104
H	3.993102	-2.55258	-1.35314
H	2.453939	-1.67626	-1.46084
H	6.068582	0.985312	2.404515
H	6.885039	-0.45886	1.772675
H	6.422901	-0.36439	3.488962
H	-5.25997	-1.22513	0.275933
H	-2.66719	-2.15663	2.459945
H	-3.90885	-0.91791	2.170303
H	-2.20874	-0.58634	1.785752
H	-3.76518	-3.11985	-3.28726
H	-0.40821	-2.95004	-2.51467
H	-1.56451	-3.98956	-3.38988
H	-0.85481	-4.53942	-1.85776
H	-6.59692	-1.18719	-1.7501
H	-6.59824	-2.90331	-2.19017
H	-5.90068	-1.71734	-3.30233

1^{2+} $[NHC\text{-}C_2O_2\text{-}NHC]^{2+}$ (S)

E = -2075.553777

O	-0.15739	-1.14052	-1.29374
N	0.894643	-1.75566	2.039478
N	-0.949	-2.58235	1.187518
C	2.256369	-0.10116	3.224406
C	2.135208	-1.02283	2.165588
C	0.079913	-0.74932	-0.16296
C	0.039115	-1.67028	0.996655
C	3.483293	0.553155	3.353081
C	4.396755	-0.66073	1.483095
C	3.180779	-1.323	1.274083
C	4.569878	0.279147	2.504274
C	0.452127	-2.74183	2.899953
C	-2.15775	-2.67701	0.39019
C	-2.18537	-3.57016	-0.69179
C	-3.23466	-1.85094	0.750867
C	1.130517	0.17323	4.185951
C	-0.71397	-3.24458	2.374487
C	3.045437	-2.31932	0.152223
C	5.89068	0.966064	2.711288
C	-4.48168	-2.82832	-1.12046
C	-4.39212	-1.95204	-0.02939
C	-3.16166	-0.90356	1.920084
C	-3.36844	-3.62154	-1.4362
C	-0.99621	-4.42271	-1.03881
C	-5.75152	-2.9388	-1.91891
O	-0.15735	1.140528	1.293747
N	0.894633	1.755662	-2.03949
N	-0.949	2.582355	-1.18752
C	2.256375	0.101178	-3.22443
C	2.135194	1.022824	-2.16559
C	0.079921	0.749328	0.162962
C	0.039121	1.6703	-0.99665
C	3.483303	-0.55312	-3.35311
C	4.396737	0.660717	-1.48309
C	3.180753	1.322976	-1.27407
C	4.569878	-0.27913	-2.50428
C	0.452127	2.741837	-2.89995
C	-2.15775	2.677009	-0.39019
C	-2.18537	3.570146	0.691801
C	-3.23466	1.850947	-0.75088
C	1.130537	-0.17319	-4.186
C	-0.71398	3.244585	-2.37449
C	3.045407	2.319278	-0.1522
C	5.890668	-0.96608	-2.71128
C	-4.48168	2.828306	1.120463
C	-4.39212	1.952035	0.029381
C	-3.16166	0.903587	-1.9201
C	-3.36843	3.621517	1.436217
C	-0.99621	4.422694	1.038831
C	-5.75152	2.938767	1.918919
H	3.600975	1.288161	4.151714
H	5.237706	-0.9055	0.833619
H	1.016192	-3.01721	3.782633
H	0.15913	0.223628	3.678113

H	1.29519	1.125599	4.702938
H	1.06648	-0.60516	4.961739
H	-1.39305	-4.00641	2.738863
H	2.366522	-3.14697	0.397854
H	4.023719	-2.75195	-0.08773
H	2.676521	-1.83995	-0.76843
H	5.761922	2.050374	2.836314
H	6.577439	0.788947	1.874652
H	6.379092	0.59747	3.626208
H	-5.25164	-1.33168	0.23107
H	-2.97021	-1.43386	2.865035
H	-4.10569	-0.3597	2.030382
H	-2.36591	-0.15223	1.801968
H	-3.42185	-4.3056	-2.28517
H	-0.13622	-3.79809	-1.325
H	-1.22631	-5.08589	-1.87992
H	-0.68285	-5.05287	-0.19337
H	-6.39016	-2.05582	-1.7911
H	-6.33362	-3.81488	-1.5935
H	-5.54401	-3.07051	-2.98905
H	3.601002	-1.2881	-4.15177
H	5.237682	0.905487	-0.8336
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H	-2.97037	1.433915	-2.86507
H	-4.10563	0.35961	-2.03031
H	-2.3658	0.15235	-1.80207
H	-3.42185	4.30557	2.285194
H	-0.13623	3.798076	1.325055
H	-1.22632	5.085897	1.879925
H	-0.68283	5.052837	0.193394
H	-6.39014	2.055775	1.791129
H	-6.33364	3.81483	1.593488
H	-5.54401	3.070506	2.989061

NHC-CO (S)

E = -1037.938161

O	-0.19666	-1.14276	2.1426
N	-1.08568	0.470808	-0.72655
N	1.109771	0.447743	-0.76119
C	-3.2747	1.214532	0.073588
C	-2.42446	0.17298	-0.3426
C	0.027141	-0.19413	1.442439
C	0.018584	-0.06373	-0.07677
C	-4.58669	0.886204	0.439326
C	-4.16234	-1.44517	0.04703
C	-2.84767	-1.17253	-0.33894
C	-5.05232	-0.43168	0.428601
C	-0.67051	1.380022	-1.71245
C	2.452085	0.177917	-0.36259
C	2.973107	-1.11537	-0.54679
C	3.193465	1.196381	0.264193
C	-2.79619	2.641062	0.172865
C	0.686033	1.359692	-1.73513
C	-1.91694	-2.2909	-0.72641
C	-6.47044	-0.76105	0.819544
C	5.070426	-0.36112	0.464478
C	4.50442	0.905078	0.657224
C	2.577909	2.542896	0.545256
C	4.285563	-1.35866	-0.12779
C	2.13994	-2.20753	-1.16246
C	6.493733	-0.6413	0.874639
H	-5.25392	1.686759	0.767931
H	-4.50114	-2.48405	0.047531
H	-1.38033	1.898242	-2.34329
H	-1.76576	2.691509	0.548827
H	-3.44234	3.209739	0.853722
H	-2.81201	3.155831	-0.80076
H	1.390387	1.857546	-2.3892
H	-1.34328	-2.04244	-1.63039
H	-2.48226	-3.21338	-0.91104
H	-1.19036	-2.48766	0.076481
H	-6.97287	0.105332	1.269353
H	-6.50376	-1.5891	1.542361
H	-7.0607	-1.07236	-0.05662
H	5.090097	1.684594	1.150536
H	2.444194	3.138138	-0.37115
H	3.212781	3.119299	1.229797
H	1.585884	2.424595	1.004192

H	4.705031	-2.35773	-0.26848
H	1.363105	-2.55129	-0.46331
H	2.764842	-3.06853	-1.43088
H	1.619539	-1.85474	-2.06408
H	6.801091	-0.00438	1.715099
H	7.188708	-0.44468	0.04252
H	6.626852	-1.69072	1.170638

NHC-CO (T)

E = -1037.933045

O	0.771255	-0.94511	-2.16731
N	-1.15193	0.358328	0.653916
N	1.075856	0.372821	0.65353
C	-3.05265	-1.15436	0.373094
C	-2.51183	0.139684	0.273201
C	-0.10531	-0.5841	-1.38262
C	-0.04265	-0.01614	-0.11298
C	-4.3927	-1.33108	0.014913
C	-4.60727	1.004654	-0.52474
C	-3.26854	1.231183	-0.1855
C	-5.18785	-0.26582	-0.42867
C	-0.72599	0.984717	1.816267
C	2.440878	0.15279	0.301544
C	3.233084	1.25629	-0.06333
C	2.953941	-1.15673	0.324469
C	-2.20685	-2.30995	0.830843
C	0.636578	0.994477	1.817798
C	-2.64065	2.590761	-0.34562
C	-6.63867	-0.48146	-0.77711
C	5.126762	-0.26297	-0.36296
C	4.298813	-1.33701	-0.01331
C	2.07914	-2.3272	0.678844
C	4.574511	1.023834	-0.38404
C	2.641976	2.639092	-0.15153
C	6.580881	-0.4854	-0.69267
H	-4.82658	-2.33157	0.084166
H	-5.20616	1.841625	-0.89188
H	-1.43354	1.339867	2.554407
H	-1.44753	-2.55259	0.070663
H	-2.82224	-3.20096	1.006249
H	-1.66473	-2.07075	1.757261
H	1.335813	1.355277	2.561852
H	-2.3687	3.037684	0.622864
H	-3.32894	3.278143	-0.85278
H	-1.7156	2.525749	-0.93692
H	-6.79727	-1.46383	-1.24293
H	-7.00361	0.290106	-1.46819
H	-7.27054	-0.44201	0.124675
H	4.709801	-2.34941	-0.00366
H	1.446755	-2.10977	1.551294
H	2.686324	-3.21401	0.899561
H	1.407156	-2.57043	-0.1583
H	5.198646	1.870403	-0.68047
H	1.708516	2.630914	-0.7325
H	3.345134	3.328847	-0.63463
H	2.395513	3.050133	0.839543
H	6.736498	-1.45617	-1.18284
H	7.198427	-0.47672	0.219923
H	6.965652	0.300695	-1.35635

NHC-CO$^+$ (D)

E = -1037.743424

O	-0.72678	-0.87717	-2.09558
N	1.136931	0.354392	0.71836
N	-1.06381	0.347955	0.72307
C	3.268888	1.244799	-0.08342
C	2.501219	0.128966	0.293548
C	0.114362	-0.40477	-1.39702
C	0.040405	0.015926	-0.01334
C	4.582757	0.999451	-0.48943
C	4.311788	-1.36931	-0.13237
C	2.986449	-1.18938	0.276268
C	5.12486	-0.29443	-0.51581
C	0.730113	0.891737	1.913928
C	-2.43795	0.147005	0.319216
C	-2.97313	-1.1481	0.406442
C	-3.1597	1.257564	-0.1487
C	2.699379	2.639379	-0.0867
C	-0.64853	0.901724	1.910645
C	2.133886	-2.36716	0.672714
C	6.554212	-0.51807	-0.92682
C	-5.07754	-0.23499	-0.45212
C	-4.48517	1.033613	-0.53141
C	-2.53255	2.62249	-0.26309
C	-4.30576	-1.30768	0.015925
C	-2.15372	-2.31838	0.881436
C	-6.51634	-0.43612	-0.84201
H	5.198424	1.844077	-0.8044

H	4.719497	-2.3817	-0.15134
H	1.442272	1.199427	2.669672
H	1.727771	2.681435	-0.60096
H	3.379407	3.328626	-0.59981
H	2.54856	3.026826	0.93231
H	-1.35962	1.238789	2.655655
H	1.50776	-2.15317	1.550472
H	2.764252	-3.23103	0.913189
H	1.464668	-2.67415	-0.14625
H	6.867488	0.200133	-1.69558
H	6.708423	-1.53344	-1.31283
H	7.226548	-0.38707	-0.06434
H	-5.06882	1.874445	-0.91076
H	-2.30409	3.056696	0.722026
H	-3.21036	3.313668	-0.77635
H	-1.59179	2.592871	-0.83338
H	-4.75207	-2.30205	0.076046
H	-1.43882	-2.64262	0.109534
H	-2.80009	-3.17425	1.106478
H	-1.57951	-2.08286	1.789172
H	-6.82376	0.271463	-1.62255
H	-7.17539	-0.2745	0.025514
H	-6.69598	-1.45632	-1.20421

NHC (S)

E = -924.583095

N	-1.0631	0.007142	0.593044
N	1.063095	-0.00712	0.593038
C	-3.12433	-1.20306	0.079158
C	-2.43133	0.014279	0.160559
C	-6E-06	-0.0001	-0.27884
C	-4.46163	-1.17074	-0.33444
C	-4.36916	1.220653	-0.58679
C	-3.03084	1.237492	-0.17682
C	-5.10233	0.029705	-0.66517
C	-0.6805	0.004788	1.936643
C	2.431328	-0.01426	0.160551
C	3.124268	1.203087	0.078915
C	3.030903	-1.23752	-0.17658
C	-2.43245	-2.5025	0.39507
C	0.6805	-0.00459	1.936639
C	-2.24139	2.517785	-0.12305
C	-6.55257	0.042749	-1.0785
C	5.10234	-0.02973	-0.66514
C	4.369214	-1.2207	-0.58654
C	2.2415	-2.51784	-0.12255
C	4.461579	1.170746	-0.33466
C	2.432334	2.50256	0.394566
C	6.55257	-0.04282	-1.07848
H	-5.01251	-2.11152	-0.4101
H	-4.84839	2.164583	-0.85806
H	-1.39627	0.011009	2.750276
H	-1.53143	-2.62121	-0.22452
H	-3.09959	-3.35428	0.213305
H	-2.1011	-2.54309	1.443496
H	1.39628	-0.01068	2.750269
H	-1.82679	2.693586	0.880819
H	-2.8686	3.376142	-0.39428
H	-1.38606	2.469811	-0.81313
H	-6.84536	-0.90816	-1.54397
H	-6.75911	0.852885	-1.79125
H	-7.20939	0.197929	-0.20754
H	4.848493	-2.16467	-0.85761
H	1.827069	-2.69354	0.881405
H	2.868707	-3.3762	-0.39378
H	1.386061	-2.46997	-0.81251
H	5.012421	2.11153	-0.4105
H	1.53128	2.62109	-0.22501
H	3.099422	3.354336	0.212588
H	2.101023	2.543368	1.442996
H	6.758762	-0.85202	-1.79242
H	7.209311	-0.1996	-0.20775
H	6.845792	0.908629	-1.54256

NHC^{+} (D)

E = -924.320966

N	-1.09641	-0.44775	0.490503
N	1.074796	-0.46105	0.548228
C	-3.42657	-1.11548	0.062842
C	-2.43682	-0.11609	0.140485
C	0.035559	-0.03214	-0.17192
C	-4.71226	-0.70373	-0.29673
C	-4.0073	1.590653	-0.54407
C	-2.70939	1.244361	-0.16858
C	-5.03169	0.638295	-0.59133
C	-0.71479	-1.22531	1.590136
C	2.439011	-0.16313	0.162561
C	3.002931	1.050802	0.593124

C	3.13042	-1.1006	-0.62698				
C	-3.14608	-2.57904	0.287129	**$C_2O_2^+$ (D)**			
C	0.648623	-1.22749	1.633319	**E**= -226.320985			
C	-1.61466	2.254679	-0.10969	C	-0.168234	0.698563	0
C	-6.43762	1.020356	-0.94684	C	0.168234	-0.698563	0
C	5.063031	0.402295	-0.56117	O	-0.168234	-1.795423	0
C	4.446467	-0.79235	-0.97395	O	0.168234	1.795423	0
C	2.473094	-2.37482	-1.08309				
C	4.324302	1.306915	0.217488	**$C_2O_2^{2+}$ (S)**			
C	2.219375	2.043123	1.410591	**E**= -225.669322			
C	6.489623	0.690865	-0.93113	C	0	0	0.723611
H	-5.49371	-1.46147	-0.38348	C	0	0	-0.723611
H	-4.22583	2.630794	-0.79052	O	0	0	-1.84367
H	-1.44146	-1.68335	2.247175	O	0	0	1.84367
H	-2.14113	-2.86478	-0.05009				
H	-3.87455	-3.18756	-0.26189	**C_2O_2 (T)**			
H	-3.23354	-2.85669	1.348719	**E**= -226.675403			
H	1.343304	-1.72011	2.303443	C	0	0	0.645944
H	-1.28083	2.443472	0.922275	C	0	0	-0.645944
H	-1.90075	3.202583	-0.57883	O	0	0	-1.843436
H	-0.71238	1.84624	-0.63645	O	0	0	1.843436
H	-6.8615	0.326084	-1.68668				
H	-6.4935	2.039136	-1.34785	**CO (S)**			
H	-7.08725	0.970341	-0.05832	**E**= -113.359803			
H	5.008579	-1.4997	-1.58661	C	0	0	-0.649693
H	2.151137	-2.99437	-0.23219	O	0	0	0.48727
H	3.163701	-2.97204	-1.68891				
H	1.578787	-2.16687	-1.68894	**CO (T)**			
H	4.791387	2.239335	0.539804	**E**= -113.1495591			
H	1.47066	2.561033	0.792117	C	0.0	0.0	-0.693926
H	2.884012	2.805299	1.833146	O	0.0	0.0	0.520445
H	1.682229	1.561939	2.240128	**CO^+ (D)**			
H	6.72068	0.338034	-1.94519	**E**= -112.845786			
H	7.176077	0.168512	-0.24491	C	0	0	-0.641584
H	6.715707	1.762565	-0.87022	O	0	0	0.481188