

Supplementary Information

Supplementary Data:

		$[\text{UO}_2(\text{BTP})_2]^{2+}$	UO_2IA	$\text{UO}_2\text{IA}'$
ρ_{BCP}	PBE	0.300	0.299	0.290
	B3LYP	0.318	0.316	0.308
$\nabla^2\rho_{\text{BCP}}$	PBE	0.317	0.314	0.316
	B3LYP	0.268	0.264	0.267
H_{BCP}	PBE	-0.270	-0.270	-0.254
	B3LYP	-0.306	-0.302	-0.287
$\delta(\text{U},\text{O})$	PBE	1.961	1.976	1.928*
	B3LYP	1.932	1.937	1.897*

Table S1. QTAIM-derived properties of the U-O bond of the three complexes considered in this study. Data from complexes optimised with the inclusion of solvation effects. All reported quantities are in atomic units. * Average over both U-O bonds.

		[UO ₂ (BTP) ₂] ²⁺		UO ₂ IA			UO ₂ IA'		
		U-N _T	U-N _P	U-N _A	U-N _B	U-N _C	U-N _A	U-N _B	U-N _C
ρ_{BCP}	PBE	0.050	0.047	0.050	0.027	0.034	0.054, 0.054	0.041, 0.037	0.037, 0.042
	B3LYP	0.047	0.045	0.049	0.026	0.034	0.052, 0.052	0.035, 0.036	0.039, 0.040
$\nabla^2\rho_{\text{BCP}}$	PBE	0.121	0.116	0.118	0.066	0.081	0.130, 0.131	0.100, 0.092	0.090, 0.100
	B3LYP	0.120	0.115	0.120	0.068	0.085	0.130, 0.130	0.089, 0.090	0.100, 0.101
H_{BCP}	PBE	-0.005	-0.004	-0.005	-0.001	-0.002	-0.006, -0.006	-0.003, -0.002	-0.002, -0.003
	B3LYP	-0.005	-0.004	-0.005	-0.000	-0.002	-0.006, -0.006	-0.002, -0.002	-0.003, -0.003
$\delta(\text{U,N})$	PBE	0.318	0.303	0.367	0.233	0.276	0.375, 0.371	0.286, 0.290	0.296, 0.304
	B3LYP	0.284	0.273	0.330	0.207	0.251	0.337, 0.335	0.253, 0.257	0.267, 0.273

Table S2. QTAIM–derived properties of the U-N bond of the three complexes considered in this study. Data from complexes optimised with the inclusion of solvation effects. All reported quantities are in atomic units.

		[UO ₂ (BTP) ₂] ²⁺			UO ₂ IA			UO ₂ IA'		
		UO ₂ ²⁺	Complex	Δ	UO ₂ ²⁺	Complex	Δ	UO ₂ ²⁺	Complex	Δ
PBE, DCM	<i>N</i> (U)	88.76	89.21	0.45	88.75	89.16	0.41	88.77	89.18	0.41
	<i>N</i> (O)	8.62	8.83	0.21	8.62	8.86	0.23	8.62	8.89	0.27
	<i>N</i> (UO ₂)	106.00	106.88	0.88	106.00	106.88	0.88	106.00	106.95	0.95
	<i>λ</i> (U)	86.53	86.12	-0.41	86.52	86.16	-0.36	86.54	86.12	-0.42
	<i>λ</i> (O)	7.44	7.66	0.23	7.44	7.71	0.27	7.43*	7.75*	0.31
	<i>λ</i> (UO ₂)	106.00	105.46	-0.54	106.00	105.65	-0.35	106.00	105.56	-0.44
	<i>δ</i> (U,O)	2.23	1.96	-0.27	2.23	1.98	-0.25	2.23*	1.93*	-0.30

Table S3: QTAIM–derived properties of isolated and complexed uranyl. Isolated uranyl simulated at the complexed geometry. Δ gives the difference between isolated and complexed values. *Values averaged over both O centres. Properties derived from PBE/def(2)-TZVP/SARC-TZVP solvated densities. All quantities are in atomic units.

		[UO ₂ (BTP) ₂] ²⁺			UO ₂ IA			UO ₂ IA'		
		UO ₂ ²⁺	Complex	Δ	UO ₂ ²⁺	Complex	Δ	UO ₂ ²⁺	Complex	Δ
B3LYP, Gas Phase	<i>N</i> (U)	88.79	88.99	0.20	88.79	88.95	0.16	88.62	88.96	0.34
	<i>N</i> (O)	8.61	8.85	0.25	8.61	8.87	0.27	8.69	8.89	0.20
	<i>N</i> (UO ₂)	106.00	106.70	0.70	106.00	106.69	0.69	106.00	106.74	0.74
	<i>λ</i> (U)	86.52	86.09	-0.42	86.52	86.13	-0.39	86.44	86.09	-0.35
	<i>λ</i> (O)	7.41	7.70	0.29	7.41	7.74	0.33	7.54*	7.76*	0.22
	<i>λ</i> (UO ₂)	106.00	105.51	-0.49	106.00	105.65	-0.35	106.00	105.59	-0.41
	<i>δ</i> (U,O)	2.27	1.96	-0.31	2.27	1.97	-0.30	2.18*	1.94*	-0.24

Table S4: QTAIM–derived properties of isolated and complexed uranyl. Isolated uranyl simulated at the complexed geometry. Δ gives the difference between isolated and complexed values. *Values averaged over both O centres. Properties derived from B3LYP/def(2)-TZVP/SARC-TZVP gas phase densities. All quantities are in atomic units.

		[UO ₂ (BTP) ₂] ²⁺			UO ₂ IA			UO ₂ IA'		
		UO ₂ ²⁺	Complex	Δ	UO ₂ ²⁺	Complex	Δ	UO ₂ ²⁺	Complex	Δ
B3LYP, DCM	<i>N</i> (U)	88.62	88.99	0.37	88.62	88.95	0.33	88.63	88.96	0.33
	<i>N</i> (O)	8.69	8.88	0.19	8.69	8.90	0.21	8.69	8.92	0.24
	<i>N</i> (UO ₂)	106.00	106.74	0.74	106.00	106.75	0.75	106.00	106.81	0.81
	<i>λ</i> (U)	86.44	86.08	-0.36	86.44	86.11	-0.33	86.45	86.08	-0.38
	<i>λ</i> (O)	7.54	7.73	0.19	7.54	7.78	0.24	7.54*	7.81*	0.27
	<i>λ</i> (UO ₂)	106.00	105.50	-0.50	106.00	105.65	-0.35	106.00	105.59	-0.41
	<i>δ</i> (U,O)	2.18	1.93	-0.25	2.18	1.94	-0.24	2.18*	1.90*	-0.28

Table S5: QTAIM–derived properties of isolated and complexed uranyl. Isolated uranyl simulated at the complexed geometry. Δ gives the difference between isolated and complexed values. *Values averaged over both O centres. Properties derived from B3LYP/def(2)-TZVP/SARC-TZVP solvated densities. All quantities are in atomic units.

		[UO ₂ (BTP) ₂] ²⁺		UO ₂ IA			UO ₂ IA'		
		U-N _T	U-N _P	U-N _A	U-N _B	U-N _C	U-N _A	U-N _B	U-N _C
PBE	DCM	0.208	0.193	0.214	0.117	0.157	0.219,	0.161,	0.179,
							0.219	0.158	0.174
B3LYP	GP	0.175	0.164	0.189	0.103	0.139	0.193,	0.134,	0.152,
	DCM	0.185	0.174	0.200	0.109	0.146	0.193	0.135	0.154
							0.205,	0.146,	0.163,
							0.205	0.143	0.160

Table S6: Critical values of the ELF, n_c , calculated in the U-N bonding regions. Properties derived from PBE/def(2)-TZVP/SARC-TZVP solvated densities and B3LYP/def(2)-TZVP/SARC-TZVP gas phase and solvated densities.

Energies and Optimised Structures (as taken from optimised TURBOMOLE coord file):

[UO₂(BTP)₂]²⁺

PBE, Gas Phase:

Energy: -60926.0133569 eV

Coordinates:

0.00000000000000	0.00000000000000	0.00000000000000	u
0.56263894403026	-3.31200589292661	0.00000000000000	o
-0.56263894403026	3.31200589292661	0.00000000000000	o
5.01651300137727	-0.07904082339670	0.00000000000000	n
6.25641802173637	-0.49275128355283	2.18316024482077	c
6.25641802173637	-0.49275128355283	-2.18316024482077	c
8.70266115659874	-1.49505511429381	2.27067622267989	c
4.93929233467588	0.41626697853100	4.46101574349342	c
8.70266115659874	-1.49505511429381	-2.27067622267989	c
4.93929233467588	0.41626697853100	-4.46101574349342	c
9.91462901758077	-2.05775443807843	0.00000000000000	c
9.61233502336070	-1.77949818110672	4.09601515416219	h
6.21546139809251	0.60463388243412	6.63825541660607	n
2.51279419951991	1.13555551420680	4.14313345249785	n
9.61233502336070	-1.77949818110672	-4.09601515416219	h
2.51279419951991	1.13555551420680	-4.14313345249785	n
6.21546139809251	0.60463388243412	-6.63825541660607	n
11.81047817511002	-2.86569201993635	0.00000000000000	h
5.04321315819913	1.82074366308574	8.49253076663807	c
1.36679281918833	2.42818297689126	5.96100066397672	n
1.36679281918833	2.42818297689126	-5.96100066397672	n
5.04321315819913	1.82074366308574	-8.49253076663807	c
2.63982379974978	2.88139855729268	8.08630931874934	c
6.00634014290757	1.95872866636340	10.31571010523555	h
2.63982379974978	2.88139855729268	-8.08630931874934	c
6.00634014290757	1.95872866636340	-10.31571010523555	h
1.68211900932273	4.04757010085845	9.49170476295234	h
1.68211900932273	4.04757010085845	-9.49170476295234	h
-5.01651300137727	0.07904082339670	0.00000000000000	n

-6.25641802173637	0.49275128355283	-2.18316024482077	c
-6.25641802173637	0.49275128355283	2.18316024482077	c
-8.70266115659874	1.49505511429381	-2.27067622267989	c
-4.93929233467588	-0.41626697853100	-4.46101574349342	c
-8.70266115659874	1.49505511429381	2.27067622267989	c
-4.93929233467588	-0.41626697853100	4.46101574349342	c
-9.91462901758077	2.05775443807843	0.00000000000000	c
-9.61233502336070	1.77949818110672	-4.09601515416219	h
-6.21546139809251	-0.60463388243412	-6.63825541660607	n
-2.51279419951991	-1.13555551420680	-4.14313345249785	n
-9.61233502336070	1.77949818110672	4.09601515416219	h
-2.51279419951991	-1.13555551420680	4.14313345249785	n
-6.21546139809251	-0.60463388243412	6.63825541660607	n
-11.81047817511002	2.86569201993635	0.00000000000000	h
-5.04321315819913	-1.82074366308574	-8.49253076663807	c
-1.36679281918833	-2.42818297689126	-5.96100066397672	n
-1.36679281918833	-2.42818297689126	5.96100066397672	n
-5.04321315819913	-1.82074366308574	8.49253076663807	c
-2.63982379974978	-2.88139855729268	-8.08630931874934	c
-6.00634014290757	-1.95872866636340	-10.31571010523555	h
-2.63982379974978	-2.88139855729268	8.08630931874934	c
-6.00634014290757	-1.95872866636340	10.31571010523555	h
-1.68211900932273	-4.04757010085845	-9.49170476295234	h
-1.68211900932273	-4.04757010085845	9.49170476295234	h

PBE, DCM:

Energy: -60930.8769351 eV

Coordinates:

0.00000000000000	0.00000000000000	0.00000000000000	u
0.56308668503927	-3.32831806166456	0.00000000000000	o
-0.56308668503927	3.32831806166456	0.00000000000000	o
4.98052307109254	-0.08495873360402	0.00000000000000	n
6.21973726970155	-0.49218793785511	2.18290028708554	c
6.21973726970155	-0.49218793785511	-2.18290028708554	c

8.67333567991639	-1.47019986474197	2.27178489323182	c
4.88658788926455	0.39254717785283	4.45791047230418	c
8.67333567991639	-1.47019986474197	-2.27178489323182	c
4.88658788926455	0.39254717785283	-4.45791047230418	c
9.89165709332148	-2.01391930292155	0.00000000000000	c
9.58852706702226	-1.75632618076775	4.09262699742831	h
6.11653381401198	0.51713551426131	6.66777804732425	n
2.47952562496319	1.15272816220543	4.11042068450111	n
9.58852706702226	-1.75632618076775	-4.09262699742831	h
2.47952562496319	1.15272816220543	-4.11042068450111	n
6.11653381401198	0.51713551426131	-6.66777804732425	n
11.79673708968499	-2.79693972267347	0.00000000000000	h
4.91679055782906	1.71090956419482	8.51882756357737	c
1.31929445152609	2.44756416345442	5.91802982054711	n
1.31929445152609	2.44756416345442	-5.91802982054711	n
4.91679055782906	1.71090956419482	-8.51882756357737	c
2.55001832701931	2.83696331712955	8.07765160343277	c
5.82095876883618	1.78997541997450	10.37380592657992	h
2.55001832701931	2.83696331712955	-8.07765160343277	c
5.82095876883618	1.78997541997450	-10.37380592657992	h
1.59198977681396	3.99374647775330	9.48879427969003	h
1.59198977681396	3.99374647775330	-9.48879427969003	h
-4.98052307109254	0.08495873360402	0.00000000000000	n
-6.21973726970155	0.49218793785511	-2.18290028708554	c
-6.21973726970155	0.49218793785511	2.18290028708554	c
-8.67333567991639	1.47019986474197	-2.27178489323182	c
-4.88658788926455	-0.39254717785283	-4.45791047230418	c
-8.67333567991639	1.47019986474197	2.27178489323182	c
-4.88658788926455	-0.39254717785283	4.45791047230418	c
-9.89165709332148	2.01391930292155	0.00000000000000	c
-9.58852706702226	1.75632618076775	-4.09262699742831	h
-6.11653381401198	-0.51713551426131	-6.66777804732425	n
-2.47952562496319	-1.15272816220543	-4.11042068450111	n
-9.58852706702226	1.75632618076775	4.09262699742831	h

-2.47952562496319	-1.15272816220543	4.11042068450111	n
-6.11653381401198	-0.51713551426131	6.66777804732425	n
-11.79673708968499	2.79693972267347	0.00000000000000	h
-4.91679055782906	-1.71090956419482	-8.51882756357737	c
-1.31929445152609	-2.44756416345442	-5.91802982054711	n
-1.31929445152609	-2.44756416345442	5.91802982054711	n
-4.91679055782906	-1.71090956419482	8.51882756357737	c
-2.55001832701931	-2.83696331712955	-8.07765160343277	c
-5.82095876883618	-1.78997541997450	-10.37380592657992	h
-2.55001832701931	-2.83696331712955	8.07765160343277	c
-5.82095876883618	-1.78997541997450	10.37380592657992	h
-1.59198977681396	-3.99374647775330	-9.48879427969003	h
-1.59198977681396	-3.99374647775330	9.48879427969003	h

B3LYP, Gas Phase:

Energy: -60951.3884195 eV

Coordinates:

0.00000000000000	0.00000000000000	0.00000000000000	u
0.56395619281114	-3.27055395733715	0.00000000000000	o
-0.56395619281114	3.27055395733715	0.00000000000000	o
5.05562210683290	-0.07444415177508	0.00000000000000	n
6.27973127114111	-0.49068695486163	2.17462749236962	c
6.27973127114111	-0.49068695486163	-2.17462749236962	c
8.70392581982580	-1.50989903262438	2.26213170453210	c
4.97472313800473	0.44319806080080	4.45304365960640	c
8.70392581982580	-1.50989903262438	-2.26213170453210	c
4.97472313800473	0.44319806080080	-4.45304365960640	c
9.90261893443931	-2.08277833870457	0.00000000000000	c
9.61310986753984	-1.79954332823430	4.06724891899528	h
6.28261017167568	0.69518541347070	6.59268347893170	n
2.56204994140170	1.13216699632679	4.16639962834575	n
9.61310986753984	-1.79954332823430	-4.06724891899528	h
2.56204994140170	1.13216699632679	-4.16639962834575	n
6.28261017167568	0.69518541347070	-6.59268347893170	n

11.77652423771655	-2.90085806298961	0.00000000000000	h
5.13110738380194	1.88883889793073	8.44886703539163	c
1.41422285449573	2.38134944441115	6.00273717385276	n
1.41422285449573	2.38134944441115	-6.00273717385276	n
5.13110738380194	1.88883889793073	-8.44886703539163	c
2.68407054265967	2.84573155745295	8.10089876933457	c
6.13182451755918	2.10176916697623	10.22486333943123	h
2.68407054265967	2.84573155745295	-8.10089876933457	c
6.13182451755918	2.10176916697623	-10.22486333943123	h
1.71996780376165	3.94656721571989	9.52992344145550	h
1.71996780376165	3.94656721571989	-9.52992344145550	h
-5.05562210683290	0.07444415177508	0.00000000000000	n
-6.27973127114111	0.49068695486163	-2.17462749236962	c
-6.27973127114111	0.49068695486163	2.17462749236962	c
-8.70392581982580	1.50989903262438	-2.26213170453210	c
-4.97472313800473	-0.44319806080080	-4.45304365960640	c
-8.70392581982580	1.50989903262438	2.26213170453210	c
-4.97472313800473	-0.44319806080080	4.45304365960640	c
-9.90261893443931	2.08277833870457	0.00000000000000	c
-9.61310986753984	1.79954332823430	-4.06724891899528	h
-6.28261017167568	-0.69518541347070	-6.59268347893170	n
-2.56204994140170	-1.13216699632679	-4.16639962834575	n
-9.61310986753984	1.79954332823430	4.06724891899528	h
-2.56204994140170	-1.13216699632679	4.16639962834575	n
-6.28261017167568	-0.69518541347070	6.59268347893170	n
-11.77652423771655	2.90085806298961	0.00000000000000	h
-5.13110738380194	-1.88883889793073	-8.44886703539163	c
-1.41422285449573	-2.38134944441115	-6.00273717385276	n
-1.41422285449573	-2.38134944441115	6.00273717385276	n
-5.13110738380194	-1.88883889793073	8.44886703539163	c
-2.68407054265967	-2.84573155745295	-8.10089876933457	c
-6.13182451755918	-2.10176916697623	-10.22486333943123	h
-2.68407054265967	-2.84573155745295	8.10089876933457	c
-6.13182451755918	-2.10176916697623	10.22486333943123	h

-1.71996780376165 -3.94656721571989 -9.52992344145550 h
-1.71996780376165 -3.94656721571989 9.52992344145550 h

B3LYP, DCM:

Energy: -60956.2678320 eV

Coordinates:

0.000000000000000	0.000000000000000	0.000000000000000	u
0.56397262873999	-3.28507659459633	0.000000000000000	o
-0.56397262873999	3.28507659459633	0.000000000000000	o
5.01776315027946	-0.08746040241977	0.000000000000000	n
6.24187464281393	-0.49614514605228	2.17420990326905	c
6.24187464281393	-0.49614514605228	-2.17420990326905	c
8.67330825109281	-1.49223024195778	2.26305130708170	c
4.92348018608243	0.41978329238075	4.44906979454795	c
8.67330825109281	-1.49223024195778	-2.26305130708170	c
4.92348018608243	0.41978329238075	-4.44906979454795	c
9.87802540722060	-2.04766026117723	0.000000000000000	c
9.58736746671781	-1.78402683325298	4.06392855450276	h
6.19252843370863	0.61710125475089	6.61989774643042	n
2.52889834040565	1.14755700291351	4.13351291358594	n
9.58736746671781	-1.78402683325298	-4.06392855450276	h
2.52889834040565	1.14755700291351	-4.13351291358594	n
6.19252843370863	0.61710125475089	-6.61989774643042	n
11.76052479329935	-2.84315560781032	0.000000000000000	h
5.02087166861103	1.80354570970477	8.46796732798293	c
1.37094420130560	2.41113484454734	5.95528121522287	n
1.37094420130560	2.41113484454734	-5.95528121522287	n
5.02087166861103	1.80354570970477	-8.46796732798293	c
2.60823186026930	2.82911304770381	8.07953110684048	c
5.97224979655798	1.96862243791557	10.27367653974280	h
2.60823186026930	2.82911304770381	-8.07953110684048	c
5.97224979655798	1.96862243791557	-10.27367653974280	h
1.64693592191210	3.93207804476846	9.50681028250362	h
1.64693592191210	3.93207804476846	-9.50681028250362	h

-5.01776315027946	0.08746040241977	0.000000000000000	n
-6.24187464281393	0.49614514605228	-2.17420990326905	c
-6.24187464281393	0.49614514605228	2.17420990326905	c
-8.67330825109281	1.49223024195778	-2.26305130708170	c
-4.92348018608243	-0.41978329238075	-4.44906979454795	c
-8.67330825109281	1.49223024195778	2.26305130708170	c
-4.92348018608243	-0.41978329238075	4.44906979454795	c
-9.87802540722060	2.04766026117723	0.000000000000000	c
-9.58736746671781	1.78402683325298	-4.06392855450276	h
-6.19252843370863	-0.61710125475089	-6.61989774643042	n
-2.52889834040565	-1.14755700291351	-4.13351291358594	n
-9.58736746671781	1.78402683325298	4.06392855450276	h
-2.52889834040565	-1.14755700291351	4.13351291358594	n
-6.19252843370863	-0.61710125475089	6.61989774643042	n
-11.76052479329935	2.84315560781032	0.000000000000000	h
-5.02087166861103	-1.80354570970477	-8.46796732798293	c
-1.37094420130560	-2.41113484454734	-5.95528121522287	n
-1.37094420130560	-2.41113484454734	5.95528121522287	n
-5.02087166861103	-1.80354570970477	8.46796732798293	c
-2.60823186026930	-2.82911304770381	-8.07953110684048	c
-5.97224979655798	-1.96862243791557	-10.27367653974280	h
-2.60823186026930	-2.82911304770381	8.07953110684048	c
-5.97224979655798	-1.96862243791557	10.27367653974280	h
-1.64693592191210	-3.93207804476846	-9.50681028250362	h
-1.64693592191210	-3.93207804476846	9.50681028250362	h

UO₂IA

PBE, Gas Phase:

Energy: -53175.8092376 eV

Coordinates:

0.0000000000000000	0.0000000000000000	0.15238939228987	u
0.0000000000000000	-2.70555104221326	-4.38383081237821	n
0.0000000000000000	-5.17231988571899	-5.19356403724126	c
0.0000000000000000	-1.32358519038959	-6.52367145801020	c
0.0000000000000000	-5.29155361838826	-7.91985712095309	c
0.0000000000000000	-2.87667719412782	-8.76063737556609	c
0.0000000000000000	-7.01502779659644	-9.00962661881453	h
0.0000000000000000	-2.21162121621938	-10.68452755147755	h
0.0000000000000000	-5.48990238397223	0.48831500799316	n
0.0000000000000000	-7.49209703549428	-1.12189456887295	c
0.0000000000000000	-6.52814409892264	2.82343199962809	c
0.0000000000000000	-9.85580704191424	0.25590745452467	c
0.0000000000000000	-9.24607889157955	2.74597919441275	c
0.0000000000000000	-11.70990917083357	-0.59354909586160	h
0.0000000000000000	-10.49416218665091	4.35652139122560	h
0.0000000000000000	-2.42172423752552	4.49729157898798	n
0.0000000000000000	-4.92609235923399	4.91572897014801	c
0.0000000000000000	-1.31132317302703	6.80621580798038	c
0.0000000000000000	-5.46529989178258	7.58694783541689	c
0.0000000000000000	-3.18051179767365	8.77837679471413	c
0.0000000000000000	-7.31749200206670	8.43635540920234	h
0.0000000000000000	-2.81224897680788	10.78257221635600	h
0.0000000000000000	5.48990238397223	0.48831500799316	n
0.0000000000000000	6.52814409892264	2.82343199962809	c
0.0000000000000000	7.49209703549428	-1.12189456887295	c
0.0000000000000000	9.24607889157955	2.74597919441275	c
0.0000000000000000	9.85580704191424	0.25590745452467	c
0.0000000000000000	10.49416218665091	4.35652139122560	h
0.0000000000000000	11.70990917083357	-0.59354909586160	h
0.0000000000000000	2.42172423752552	4.49729157898798	n

0.0000000000000000	4.92609235923399	4.91572897014801	c
0.0000000000000000	1.31132317302703	6.80621580798038	c
0.0000000000000000	5.46529989178258	7.58694783541689	c
0.0000000000000000	3.18051179767365	8.77837679471413	c
0.0000000000000000	7.31749200206670	8.43635540920234	h
0.0000000000000000	2.81224897680788	10.78257221635600	h
0.0000000000000000	2.70555104221326	-4.38383081237821	n
0.0000000000000000	5.17231988571899	-5.19356403724126	c
0.0000000000000000	1.32358519038959	-6.52367145801020	c
0.0000000000000000	5.29155361838826	-7.91985712095309	c
0.0000000000000000	2.87667719412782	-8.76063737556609	c
0.0000000000000000	7.01502779659644	-9.00962661881453	h
0.0000000000000000	2.21162121621938	-10.68452755147755	h
-3.32222910310247	0.0000000000000000	0.12956645192698	o
3.32222910310247	0.0000000000000000	0.12956645192698	o
0.0000000000000000	7.33816923910446	-3.73310617376048	c
0.0000000000000000	-7.33816923910446	-3.73310617376048	c
0.0000000000000000	9.11183703730846	-4.75513999572595	h
0.0000000000000000	-9.11183703730846	-4.75513999572595	h

PBE, DCM:

Energy: -53176.3437668 eV

Coordinates:

-0.00860220437794	-0.00013475736056	0.17071013223382	u
-0.04322961520766	-2.71930449752683	-4.35030216242328	n
0.03765554072916	-5.19218730555564	-5.19108491725663	c
-0.22216571877480	-1.33374966472260	-6.50578125358337	c
-0.10702432056753	-5.30962215508606	-7.91909723257709	c
-0.28694074009069	-2.88014437300356	-8.75245856637022	c
-0.07782092088391	-7.04708535354052	-9.01675676429837	h
-0.43184886851836	-2.20163670244519	-10.68403146676765	h
0.11976587299565	-5.48452594614818	0.48244080137405	n
0.25546518267262	-7.51161467873364	-1.12215383335280	c
0.10946715349488	-6.54016147307834	2.83177084131996	c

0.35559371540305	-9.87549854826038	0.26412599318893	c
0.25505627215386	-9.25912353996004	2.76813809149402	c
0.47184365255797	-11.73986922380132	-0.59411432803119	h
0.27548337928965	-10.50731246455472	4.39928702753136	h
-0.10740236268513	-2.40996234484000	4.47883443958863	n
-0.04001971114054	-4.93329680715497	4.92165405147295	c
-0.21997811089570	-1.30812822731006	6.80993877566395	c
-0.12715051978986	-5.47399697837468	7.59235293628705	c
-0.24640354865775	-3.17334520502344	8.78766939545549	c
-0.10056748954300	-7.34173224825067	8.44695976643978	h
-0.33309398967821	-2.79590729133388	10.80485263125744	h
0.12104626501453	5.48573274721979	0.46943295178744	n
0.12793105816448	6.54613208422019	2.81659766124527	c
0.24254012552505	7.50968193271909	-1.14027683120990	c
0.27342356528821	9.26496124972668	2.74639151217188	c
0.35290520525060	9.87638897772282	0.24042167439179	c
0.30661276458596	10.51644513755481	4.37480036048358	h
0.46145268265815	11.73910868216927	-0.62241000830875	h
-0.09616092406370	2.42006410297529	4.47338040245828	n
-0.01604579576770	4.94402548337620	4.91053006187228	c
-0.21211636057148	1.32396926093930	6.80704692194196	c
-0.09586668922433	5.49097656305234	7.58016724576803	c
-0.22596110702405	3.19362151954398	8.78069237913333	c
-0.05873252769237	7.36040930545002	8.43066280906849	h
-0.31280487687581	2.82118089064828	10.79880564496452	h
-0.05842711361873	2.70962453286363	-4.35663476859205	n
0.00351166341637	5.18116481451575	-5.20291379195282	c
-0.23223529630713	1.31818569582624	-6.50870633174613	c
-0.15092414732604	5.29180593296624	-7.93068849498289	c
-0.31391709042850	2.85924909481709	-8.75852057927452	c
-0.13705595691655	7.02707481452564	-9.03211602443685	h
-0.45705226874766	2.17551750138991	-10.68839261009852	h
-3.38435142929873	-0.00087852857342	0.10042856865063	o
3.36789082914703	0.00028038623812	0.16522832648196	o

0.18642592857203	7.36535842560389	-3.76038415858329	c
0.22054689143232	-7.37264403672756	-3.74291695061229	c
0.25577450068093	9.14686960395960	-4.79758874914036	h
0.30350745564120	-9.15596638865790	-4.77599158012771	h

B3LYP, Gas Phase:

Energy: -53196.7792241 eV

Coordinates:

0.00000000000000	0.00000000000000	0.15298531927827	u
0.00000000000000	-2.70440356018573	-4.38544748254982	n
0.00000000000000	-5.17150894260380	-5.19416197155119	c
0.00000000000000	-1.32361660445845	-6.52595027110335	c
0.00000000000000	-5.29224252643514	-7.92026237699297	c
0.00000000000000	-2.87770764949998	-8.76217769492253	c
0.00000000000000	-7.01668801989583	-9.00890663459748	h
0.00000000000000	-2.21319511878513	-10.68648144327589	h
0.00000000000000	-5.48802135903423	0.48901059338935	n
0.00000000000000	-7.49013956790375	-1.12176118309432	c
0.00000000000000	-6.52738474178757	2.82372901000293	c
0.00000000000000	-9.85420251285911	0.25507473227099	c
0.00000000000000	-9.24532476367542	2.74528829572276	c
0.00000000000000	-11.70794405107864	-0.59577427823432	h
0.00000000000000	-10.49399131900445	4.35562389007402	h
0.00000000000000	-2.42160676413803	4.49849789935908	n
0.00000000000000	-4.92605683044872	4.91662513737168	c
0.00000000000000	-1.31135649861429	6.80751967782944	c
0.00000000000000	-5.46549547623489	7.58775599119522	c
0.00000000000000	-3.18089922762721	8.77933606459153	c
0.00000000000000	-7.31773135824879	8.43757738380966	h
0.00000000000000	-2.81339843667381	10.78390987312133	h
0.00000000000000	5.48802135903423	0.48901059338935	n
0.00000000000000	6.52738474178757	2.82372901000293	c

0.0000000000000000	7.49013956790375	-1.12176118309432	c
0.0000000000000000	9.24532476367542	2.74528829572276	c
0.0000000000000000	9.85420251285911	0.25507473227099	c
0.0000000000000000	10.49399131900445	4.35562389007402	h
0.0000000000000000	11.70794405107864	-0.59577427823432	h
0.0000000000000000	2.42160676413803	4.49849789935908	n
0.0000000000000000	4.92605683044872	4.91662513737168	c
0.0000000000000000	1.31135649861429	6.80751967782944	c
0.0000000000000000	5.46549547623489	7.58775599119522	c
0.0000000000000000	3.18089922762721	8.77933606459153	c
0.0000000000000000	7.31773135824879	8.43757738380966	h
0.0000000000000000	2.81339843667381	10.78390987312133	h
0.0000000000000000	2.70440356018573	-4.38544748254982	n
0.0000000000000000	5.17150894260380	-5.19416197155119	c
0.0000000000000000	1.32361660445845	-6.52595027110335	c
0.0000000000000000	5.29224252643514	-7.92026237699297	c
0.0000000000000000	2.87770764949998	-8.76217769492253	c
0.0000000000000000	7.01668801989583	-9.00890663459748	h
0.0000000000000000	2.21319511878513	-10.68648144327589	h
-3.32214135577701	0.0000000000000000	0.13165480016375	o
3.32214135577701	0.0000000000000000	0.13165480016375	o
0.0000000000000000	7.33661111431522	-3.73287092340491	c
0.0000000000000000	-7.33661111431522	-3.73287092340491	c
0.0000000000000000	9.11063829323154	-4.75430174881407	h
0.0000000000000000	-9.11063829323154	-4.75430174881407	h

B3LYP, DCM:

Energy: -53197.2340551 eV

Coordinates:

0.00789771323548	0.00105367853823	0.16040040851845	u
-0.02692479961063	-2.70676891807304	-4.35974458809597	n
0.03943330931112	-5.17488888957010	-5.17856867679597	c
-0.22465610012363	-1.32995834715565	-6.49952760090668	c
-0.13485472942102	-5.29562356266743	-7.89788852085789	c

-0.31761843904873	-2.88290028033083	-8.73202627241517	c
-0.12346881630244	-7.02053498502777	-8.98590364796913	h
-0.48239349274512	-2.21831806036427	-10.64972579152326	h
0.14009475523845	-5.47435276310442	0.48716409500665	n
0.27878802532101	-7.48155095979794	-1.11824346162568	c
0.13251340680832	-6.51586600036183	2.82605798479495	c
0.38814660988829	-9.83820869621723	0.26506182845751	c
0.28794293185490	-9.22757015734172	2.75517111596980	c
0.50945540832114	-11.68865540631820	-0.58440623593523	h
0.31349864864951	-10.47016528325717	4.37042159107488	h
-0.10418593638659	-2.41009693492219	4.48086349323345	n
-0.03229130070348	-4.91638707837483	4.91013759820288	c
-0.23755168705344	-1.30180166152637	6.79209965001551	c
-0.13937824183523	-5.45357827515494	7.57777894371950	c
-0.27555993180324	-3.16831391827143	8.76405901782092	c
-0.11477181173768	-7.30553958674477	8.42838538472945	h
-0.38045981566171	-2.79683983913114	10.76528223768075	h
0.14001025739275	5.47569929259904	0.47466098862599	n
0.14411169822497	6.52245785183789	2.81127636544323	c
0.26789299348918	7.47958953539109	-1.13591734965519	c
0.29938124360099	9.23391157972263	2.73364088610193	c
0.38417462937779	9.83921682829829	0.24163340134194	c
0.33455778677164	10.47998522043566	4.34602358055662	h
0.49939126768443	11.68790791824514	-0.61249544930025	h
-0.09749032439277	2.42094416209576	4.47555870542264	n
-0.01648129448398	4.92787913890937	4.89943328910622	c
-0.23228809333806	1.31799668703342	6.78933722915091	c
-0.11736238330462	5.47106599409505	7.56601896051494	c
-0.26096178886408	3.18879591215204	8.75730871980303	c
-0.08464401356453	7.32468018897573	8.41273187722623	h
-0.36576570790975	2.82207545760652	10.75942588477237	h
-0.03797948127626	2.69695029549008	-4.36588404460937	n
0.01427950835516	5.16363015676957	-5.19016967758538	c
-0.23191355874720	1.31448312007526	-6.50241375428039	c

-0.16664582436746	5.27763478927572	-7.90928577659825	c
-0.33718942445381	2.86213072926080	-8.73800559413273	c
-0.16612173577236	7.00023625263698	-9.00101517593373	h
-0.50083089528641	2.19265204482890	-10.65411023596104	h
-3.32935058436319	-0.00460183322238	0.07996371968574	o
3.34618206526548	-0.00137384407076	0.18538157563747	o
0.20476450998369	7.33209127515960	-3.74637200623383	c
0.23045970230897	-7.33967227786255	-3.72934814808194	c
0.27016198374640	9.10126975479510	-4.77263657675104	h
0.30600175772746	-9.11077030535897	-4.75158994736571	h

UO₂IA'

PBE, Gas Phase:

Energy: -72410.9739259 eV

Coordinates:

-0.54613201733617	0.05793865194181	-0.17148992374564	u
-0.06755136890132	-2.53456953972056	-4.56856165667727	n
0.91488828019082	-4.86619512621540	-5.14478654005420	c
-0.02315051244172	-1.23062528723090	-6.77925756308372	c
1.82780798896716	-4.93657240945194	-7.73909515263859	c
1.21862328776061	-2.63641255230287	-8.78767260688874	c
3.24133781785265	-7.07124411766278	-8.94472895511121	c
1.97457728168634	-1.72928783297015	-11.36106181659301	c
-1.02573263349256	-5.14205236306297	0.24115037552778	n
-0.41948370920209	-7.15255153532951	-1.25320383630456	c
-1.95266505044853	-6.16586091714670	2.43124741912632	c
-1.03819096198419	-9.53061776447950	-0.02174580426527	c
-2.06362733920976	-8.91662764998861	2.28858485479941	c
-0.55085675381896	-12.11443184123626	-1.07815284932341	c
-2.93142647055427	-10.78012925918927	4.22520775604401	c
-1.01815025770593	-2.20440126004753	4.13590180570156	n
-2.12706023453690	-4.49385482337815	4.51340995723196	c
-0.79442770824202	-1.08406708187327	6.44018003623015	c
-2.89888865733234	-4.73983166490276	7.14329804251998	c
-1.99936383157686	-2.60595558290174	8.36892425702342	c

-4.57949972078163	-6.67740858640483	8.32999774533879	c
-2.48449940580955	-1.94325742151884	11.08232300445422	c
-0.20103249093824	5.26388618783528	0.09864444892770	n
0.80321284377660	6.38297550266075	2.20449292286749	c
-1.07259195658333	7.20416904909271	-1.35791130380652	c
0.65908106178784	9.12887821785942	2.05697009488731	c
-0.58848125844252	9.63579721777366	-0.17018173692769	c
1.48451966835456	11.06054654734365	3.94423447916221	c
-1.26960914042688	12.16383844903108	-1.24796241921749	c
0.28457810142455	2.40775506658723	4.03259561348627	n
1.30838430708570	4.75359108872474	4.26514498319273	c
0.38955302090467	1.30723949925429	6.35503537567495	c
2.38573560307070	5.06647898606639	6.77525778842323	c
1.75817028353000	2.90334418915749	8.11166648601652	c
4.09452369697909	7.11537346243855	7.71953715049189	c
2.70279264339078	2.24219367941446	10.70086801447502	c
-1.19535449434320	2.52422227671847	-4.60227346002943	n
-2.29548393633228	4.79515497516803	-5.20463868420393	c
-1.13224633023060	1.20822444224745	-6.80640605113562	c
-3.14672050173129	4.81462091238479	-7.81799336358245	c
-2.37413319679860	2.55472568066986	-8.85309319848239	c
-4.53889033765739	6.91436001647286	-9.10689993299417	c
-2.99861586564896	1.62483577746290	-11.44997344156118	c
-3.91447646275773	0.26972556642292	-0.08023269766541	o
2.82217832539461	-0.14802102750267	-0.30000686145650	o
-2.24697626963049	6.94430570896701	-3.70054165873175	c
0.68575000205837	-7.00124613525687	-3.63997228580450	c
-3.03743469317267	8.65951151873363	-4.52778283438909	h
1.28839637019975	-8.78245020507659	-4.48672421206815	h
-2.65589499378610	-12.71693709578290	3.53348714044879	h
-4.94568404139679	-10.56897203593542	4.68787976121706	h
-1.87094776837700	-10.60626917141624	6.00391723387925	h
2.10575910879255	-13.12741238064693	-0.46822909638195	c
-0.82400747230568	-12.09421128955222	-3.14181534467728	h
-1.97318679381818	-13.44477106737111	-0.34391663996370	h
3.11189955797954	-6.90286574724023	-11.01436234599860	h

2.32542840004467	-8.88272720449937	-8.46976405435923	h
6.03819665543029	-7.18720660812455	-8.15539598436437	c
3.77994190117752	-2.58773840767193	-11.92536887241137	h
2.22717265190275	0.32898785001278	-11.39929272436055	h
0.58467062275819	-2.21469855943296	-12.83190025275499	h
-4.78373226502809	2.47000868249327	-12.09875821653832	h
-3.22924799444424	-0.43625414274775	-11.49165638587633	h
-1.55138567285830	2.11991799096232	-12.86073149927804	h
-5.94068918193106	6.09422119269779	-10.41366725085778	h
-2.81080730587452	8.71661747315925	-10.59751993569791	c
-5.63716589627052	7.99966136299031	-7.71179535623655	h
0.76300756346429	13.25496513682252	-3.01772756211455	c
-1.61350924638297	13.50921216988679	0.30336768149490	h
-3.07496405900593	12.02774760826364	-2.27715678616597	h
0.79611215524417	12.94093789188386	3.39816859662114	h
3.55387072231438	11.18948732302970	4.10089806181744	h
0.74897539819349	10.65440660877347	5.84326418609844	h
3.06737177866658	8.66158018073522	8.66139536329779	h
5.20112367827793	7.95413371216341	6.18070640110327	h
5.43922027178561	6.35256768761849	9.10565967974610	h
1.22431223676209	1.29746629900278	11.80736585061351	h
3.14548873417616	3.99298352147494	11.73346060208541	h
5.06360184530016	0.54333957780491	10.63097084529054	c
-2.26193519823009	0.10349588609127	11.35509324334489	h
-0.83757075702717	-3.39696799112265	12.98366763562588	c
-4.48744784343800	-2.33939182471935	11.50967703082364	h
-6.00915577571854	-7.37293049366821	6.99934656472798	h
-5.58305097785257	-5.85106104324871	9.95179905068870	h
-3.54119028937404	-8.33090380439089	9.04928253171665	h
7.03021954922054	-5.43787825520896	-8.67724656708146	h
7.00457119981471	-8.77930952096193	-9.07830606767295	h
6.22507069060608	-7.41604549747648	-6.09948395883954	h
3.57914956148651	-11.86864897807446	-1.21783643016683	h
2.38937693804524	-15.01633095768356	-1.28861472493063	h
2.39401440148538	-13.26426243270008	1.58482627760516	h
-1.76230635217723	7.69389283629249	-12.07064483077955	h

-1.41430891532615	9.61698077533127	-9.34939384956520	h
-3.91763605261363	10.21639694814314	-11.51755339838712	h
2.56402288685425	13.50573655270887	-2.01271109295773	h
0.18005810748757	15.10244699278905	-3.77193633885371	h
1.11739069973920	11.98219791192731	-4.62140060370316	h
1.18445268509837	-3.05808582600676	12.65283053613544	h
-1.15620631057775	-5.44391173636132	12.82845738450967	h
-1.27806140452424	-2.82840686935758	14.93423027979027	h
4.66760386328703	-1.24239964324197	9.64657307267661	h
5.71398848427189	0.09682826246061	12.55457055643376	h
6.62266320232638	1.47435946354635	9.62096883832170	h

PBE, DCM:

Energy: -72411.6239880 eV

Coordinates:

-0.54457200063141	0.05680462731332	-0.16441032124863	u
-0.04081429534965	-2.52006268928499	-4.54466180818741	n
0.97498128687733	-4.84277386914051	-5.11741912123701	c
0.00286923571197	-1.21796689422612	-6.76500459894355	c
1.90602680535963	-4.90255107368819	-7.70462739726305	c
1.27166113487845	-2.60996124096456	-8.76219469165716	c
3.34143794737622	-7.02599253528605	-8.90236105012776	c
2.01056567563253	-1.70864697592135	-11.34146296392879	c
-1.02767175588738	-5.11274990355883	0.23167342929127	n
-0.40580267467242	-7.13157438603806	-1.25397139637179	c
-1.99839637910365	-6.14161385046338	2.40970011282484	c
-1.06582094519646	-9.50516066611417	-0.03893598254877	c
-2.13560681321490	-8.88866949685177	2.25374399475592	c
-0.57413563589711	-12.08978834549396	-1.09031443567648	c
-3.07379596377141	-10.74825712833298	4.15987106569823	c
-1.03440692399603	-2.19106015390648	4.11894567025184	n
-2.17066709036258	-4.47516362691822	4.49348956879272	c
-0.80006992324822	-1.08208453850310	6.43386011241635	c
-2.94525446133652	-4.71932303587751	7.12076795605651	c
-2.01891756313504	-2.59822748271776	8.35495941090980	c

-4.62274415187928	-6.65616543443733	8.30968308548184	c
-2.47279087345630	-1.95684441249324	11.07803343908017	c
-0.20606012343656	5.23020381769729	0.09475695969979	n
0.84289391256723	6.35861408714217	2.18344061944754	c
-1.10798844262487	7.17597821960374	-1.34527439431810	c
0.71219131003071	9.10257791485146	2.02571933910328	c
-0.58947981969905	9.60665187042085	-0.17432500369254	c
1.61004613385829	11.03926595113056	3.87331252030011	c
-1.28597522360492	12.13334750594847	-1.24465104923057	c
0.30460489987733	2.39041521285682	4.01560369467558	n
1.35452299101332	4.73243811262768	4.24246111073058	c
0.40632942044122	1.29699683850629	6.34763148400360	c
2.43852528648414	5.04134565912805	6.74776648936763	c
1.79000232147247	2.88671559874959	8.09400447121026	c
4.14574101254425	7.08818730142229	7.69491756090297	c
2.71124168816225	2.24265232239343	10.69517260938807	c
-1.22131029838657	2.50790250840233	-4.57321999988886	n
-2.36073462679011	4.76560163503589	-5.16947832122381	c
-1.13821466803611	1.20333861797410	-6.79224576160387	c
-3.21216463144519	4.78198015726533	-7.78181101133959	c
-2.39690383212284	2.54009147430435	-8.83084160359962	c
-4.62589933748833	6.87061455064043	-9.06384838015284	c
-2.97980071122904	1.63075063492879	-11.44366353682374	c
-3.93683799015137	0.26598401976309	-0.07686536470005	o
2.84668811310189	-0.14426792459941	-0.30030944423852	o
-2.32688516839554	6.91504729566438	-3.66473521865081	c
0.74161397394240	-6.98335384724172	-3.62065265023707	c
-3.15175414892112	8.62197620003335	-4.47399551944141	h
1.35580911871025	-8.76217567978227	-4.46235524981948	h
-2.82685615667268	-12.68333121701344	3.45454554601724	h
-5.09029615360806	-10.49173580076668	4.58640052965466	h
-2.04049306489991	-10.60884796348646	5.95678665140377	h
2.05547352283035	-13.12655482468633	-0.40429415047116	c
-0.78503271954885	-12.06213046213005	-3.16041100598210	h
-2.02694148804341	-13.40690095039617	-0.39560267824135	h
3.20615222136626	-6.86718954905873	-10.97132186632640	h

2.45093657811123	-8.84517465090899	-8.41262761633467	h
6.14253822337685	-7.10069039366786	-8.11987513777854	c
3.82335227692763	-2.55216281726157	-11.90269865173056	h
2.23475011523072	0.35210372970762	-11.39790752234058	h
0.62056152938328	-2.22766820005327	-12.79961259271176	h
-4.76851656188867	2.46121888035628	-12.09966117834178	h
-3.17619508115947	-0.43262906339352	-11.51666242890371	h
-1.52168599399877	2.16997011705162	-12.82568418126283	h
-6.02373186970905	6.03742498704479	-10.36538897706462	h
-2.91196387023020	8.67948323819360	-10.56469358049229	c
-5.72223176015603	7.95221173241366	-7.66542594006237	h
0.72223285881534	13.21661401349326	-3.04825258272280	c
-1.59732124860224	13.47981548086338	0.31124738823944	h
-3.10607117145384	11.99759382278626	-2.24590610763997	h
0.94194793538125	12.92369299271027	3.31866846862273	h
3.68433404901907	11.12635505458874	3.97867253706108	h
0.91083137154958	10.66582842851056	5.79209850233738	h
3.10797949185486	8.62340260610307	8.64196072812491	h
5.24958067445028	7.93588345568527	6.15984554843349	h
5.48656648791339	6.32160046814034	9.08199054819290	h
1.22711840916842	1.29181253851657	11.78731076920317	h
3.13147094388925	4.00094149842808	11.72229502437497	h
5.08728179781096	0.56307863803214	10.65607270743789	c
-2.24338913637134	0.08608007320825	11.36981658795475	h
-0.80417076222675	-3.43369671394604	12.94346795647691	c
-4.46941841572778	-2.36008989428916	11.52220533466181	h
-6.05288798247568	-7.35655494011145	6.98324058060036	h
-5.61822067061878	-5.82870622521624	9.93513393051090	h
-3.57216147056507	-8.30264502619020	9.02572129923422	h
7.11167905320070	-5.34262551247637	-8.65734961325128	h
7.11810703083784	-8.68630383021783	-9.04306058989994	h
6.34090197597765	-7.32625594986487	-6.06374679513046	h
3.56344280146698	-11.88391031252275	-1.11296782844847	h
2.33691620641879	-15.01543798989745	-1.22404383421861	h
2.28086544868793	-13.27413244872945	1.65631313627700	h
-1.86626229414082	7.66104969364664	-12.04321261647581	h

-1.51744828496128	9.59430142015282	-9.32384562891257	h
-4.03879739921806	10.16774734061175	-11.47776768279372	h
2.53920543762862	13.46835573178009	-2.07164839607094	h
0.12338480135073	15.06354950240243	-3.78965513444924	h
1.04535359653309	11.94547258325893	-4.66081523403554	h
1.21496071267796	-3.09530404873217	12.59229367674216	h
-1.13339663773260	-5.47814413075277	12.77534588090809	h
-1.22315050654453	-2.87486424237020	14.90084524214244	h
4.71803836726830	-1.23404842995882	9.68030458956688	h
5.71324657555305	0.13425935691175	12.59110923282949	h
6.65115441130224	1.50684126153882	9.66456872684753	h

B3LYP, Gas Phase:

Energy: -72445.5313924 eV

Coordinates:

-0.53432627176528	0.05327179380630	-0.17329598582464	u
-0.12642411313873	-2.55650476759667	-4.59695062553928	n
0.80269147912315	-4.89828562939272	-5.17522486453343	c
-0.09800977036026	-1.25818319327701	-6.79011099709350	c
1.66382216670809	-4.98204363966639	-7.77987108461907	c
1.08432817932939	-2.68719621424523	-8.81124325483081	c
3.01584046235582	-7.13953072528671	-9.01885593362237	c
1.82462574098779	-1.79516836087001	-11.39668229103408	c
-0.99230116246259	-5.18110552666661	0.25753430037895	n
-0.40948399209502	-7.17125123066408	-1.24673245659808	c
-1.83957991552018	-6.19534210377958	2.46553492626536	c
-0.94686844171023	-9.54708916344289	0.01305718580287	c
-1.89660153061363	-8.94305897961934	2.33847290172127	c
-0.45928830197889	-12.13076713811473	-1.04883407777175	c
-2.64396030748602	-10.81091639067629	4.32376290875829	c
-0.97600314131288	-2.22557943221149	4.16073317341126	n
-2.02930225455832	-4.52195498944210	4.53284395881489	c
-0.79505774786328	-1.08489799584143	6.44329469518341	c
-2.82508094767591	-4.76301464609702	7.15253712709331	c

-1.98979711259691	-2.62026876947175	8.36552728779011	c
-4.50385940816227	-6.71927467200262	8.31634619498490	c
-2.53909669698545	-1.93753729223837	11.06325323253685	c
-0.17344133857212	5.29702107717750	0.10419205105350	n
0.74993633847118	6.39663319904206	2.23717806866457	c
-0.97646750721083	7.22526151377009	-1.38209590450294	c
0.60349650671524	9.13730877575916	2.09049674282002	c
-0.53491412161651	9.64762860029656	-0.17349613129559	c
1.32739422708735	11.06479655241225	4.02627931496134	c
-1.17321634306005	12.18310990550333	-1.26452248692027	c
0.23714717087017	2.42741683046847	4.06081496052174	n
1.21875650282167	4.77107897090551	4.29836540069531	c
0.33537675365066	1.31881308757225	6.36494570532234	c
2.27364411708013	5.08694928800709	6.81427377210319	c
1.67144090242336	2.92824794436391	8.13050404920614	c
3.96423966295264	7.14996724683665	7.76647216687817	c
2.61370083438920	2.27228440235927	10.72290668283511	c
-1.14101338813913	2.53648159650754	-4.63945329691186	n
-2.16595121181059	4.83069494473227	-5.24151535723642	c
-1.14280147010602	1.20274740752457	-6.81248427259451	c
-3.03728075017990	4.85055280212592	-7.84156354588140	c
-2.36829943194526	2.56687881034923	-8.85046087042795	c
-4.38452414263535	6.97645010528065	-9.13914569486659	c
-3.07737525813437	1.62280423322930	-11.42302152859303	c
-3.86398534713563	0.25982416128552	-0.08428847891354	o
2.79516588214439	-0.15075944322904	-0.29263498353695	o
-2.07761663602011	6.97145633740628	-3.74983712105768	c
0.60646915822839	-7.01444073605546	-3.66234965501625	c
-2.80989075657353	8.68338756746095	-4.59140119124909	h
1.18269696686352	-8.78072912240667	-4.51376698887482	h
-2.25602406737488	-12.72806947900829	3.68192390245424	h
-4.65162645650696	-10.71397366938365	4.78371499328069	h
-1.59491045372992	-10.53082989784239	6.07635541572058	h
2.21960467964172	-13.12173465124843	-0.51655246698455	c
-0.78726578192767	-12.12060945526349	-3.08764922042727	h
-1.83530295607848	-13.46273687143069	-0.27788469951349	h

2.80225520742813	-6.99326156179706	-11.06673429416032	h
2.11976984264884	-8.92627189182147	-8.49056087290438	h
5.84262926418263	-7.26833949118428	-8.35694879723793	c
3.60782808993328	-2.65955763245758	-11.96512517314452	h
2.09090108983004	0.24506074437330	-11.44552912526376	h
0.42934940159418	-2.27785230399811	-12.84070627614985	h
-4.85843400333854	2.47541673623258	-12.02089561912361	h
-3.33520557100546	-0.41927494179033	-11.43915158701086	h
-1.67538391039925	2.08701354940958	-12.86608618403770	h
-5.82906664537122	6.19027110910690	-10.39228407263885	h
-2.63684728804819	8.69802520721305	-10.69613581925826	c
-5.40726924410460	8.11357140002235	-7.75279490729260	h
0.95597313154835	13.32986992417533	-2.87418893352469	c
-1.63674507224560	13.49264217589917	0.26381972717261	h
-2.88664843293084	12.04217827050639	-2.40912169606093	h
0.59812982849231	12.91649385747447	3.49649068581294	h
3.37227067046012	11.25458532809991	4.22779199008600	h
0.56351896557146	10.61050029881265	5.88497742548784	h
2.92999349206269	8.65974775808007	8.72403260623904	h
5.04071118493964	8.00715430819270	6.23787654975650	h
5.32069454010145	6.39564110753884	9.12149301813302	h
1.16426581455561	1.29160722066736	11.80163912068642	h
3.00013635607927	4.01300734829489	11.76191442868002	h
5.01731804940523	0.63764097554193	10.67241446967153	c
-2.32284400382597	0.09362173561109	11.32475287666538	h
-0.94345624789355	-3.37179154047994	13.01865616300986	c
-4.53571222102016	-2.32575247477336	11.44283404630369	h
-5.86030433812733	-7.45774175077551	6.95721345629870	h
-5.57641383905159	-5.89381366360887	9.87250584049879	h
-3.46167157427582	-8.32320998620513	9.09280270596649	h
6.81745121423089	-5.54585282557340	-8.93875899334582	h
6.74353265951952	-8.86634074655413	-9.30350042959460	h
6.12164358483833	-7.48150812782591	-6.32511332860074	h
3.65168677124931	-11.86555666811648	-1.30796560531551	h
2.48563412443827	-14.99697446913602	-1.33807132745459	h
2.56807270198835	-13.25541386235946	1.51234083326530	h

-1.66611111375622	7.63002755934892	-12.16956801220913	h
-1.19435951427486	9.56785230130691	-9.50514817055269	h
-3.71423181931376	10.20646328968485	-11.60461890521352	h
2.66644426195799	13.59723117354529	-1.75241118594983	h
0.39435103318544	15.16511897127933	-3.63510358505057	h
1.43720642156750	12.09736899450323	-4.45667764125287	h
1.07243012739254	-3.04902934660863	12.73324423938945	h
-1.26774710701321	-5.40426621662429	12.88962450418955	h
-1.42456475082640	-2.77423808148257	14.93534592565045	h
4.68097000278201	-1.14575126522194	9.69349540983746	h
5.65266695183282	0.21195362023684	12.59010570329090	h
6.55175271620549	1.60352091552506	9.68843316326809	h

B3LYP, DCM:

Energy: -72446.1258162 eV

Coordinates:

-0.53800024727059	0.05595229456620	-0.16455350307129	u
-0.08357236038555	-2.53901883497367	-4.57025769011340	n
0.87457997638829	-4.87524453652170	-5.14155601506333	c
-0.03059062528167	-1.23901693870857	-6.77041943043532	c
1.78189134176189	-4.94604696100872	-7.73001997548663	c
1.19686953529499	-2.65392112944059	-8.77041950726846	c
3.16381476849211	-7.09456993810073	-8.95015896877083	c
1.95299475187534	-1.76081678537082	-11.35016746935667	c
-1.01426869537264	-5.14710086686859	0.24570906938411	n
-0.43246275872430	-7.14712287408622	-1.25384924556832	c
-1.91685376305100	-6.16362218753471	2.44081226226388	c
-1.04174027956976	-9.51617057439450	-0.01839085150924	c
-2.03350938539787	-8.90688911633954	2.29079670945976	c
-0.57987899922713	-12.10253529342030	-1.08509142534018	c
-2.88557103545241	-10.77253947757683	4.23466020719845	c
-0.98967490508524	-2.21177857622907	4.14070816603879	n
-2.07981043129508	-4.49896063853912	4.51397320312469	c
-0.77335209125965	-1.08729073059154	6.43373950167149	c
-2.85381645264619	-4.73962309605942	7.13888403090166	c

-1.96991358097109	-2.61636434911945	8.35641099406857	c
-4.52492684782824	-6.68946539079180	8.32148709285208	c
-2.45678506948388	-1.95731211545043	11.07147146088382	c
-0.20268115399381	5.26495098611581	0.10060004880988	n
0.76301079531892	6.37795695636313	2.21693671493217	c
-1.05429008838012	7.19495136189556	-1.36594924295337	c
0.60619336835547	9.11535084753209	2.06712732424586	c
-0.59682945975221	9.61749017768011	-0.16810026626575	c
1.39106851553355	11.05046882250082	3.97073707589929	c
-1.27460729542931	12.14882315685949	-1.24515832183020	c
0.26370295892754	2.41063230728863	4.03995467029853	n
1.25997489632533	4.75566555140880	4.27110703612091	c
0.37962067315808	1.30452820070831	6.35034664148248	c
2.33634157804128	5.06778455137620	6.77515045973617	c
1.73617018688327	2.90998246092362	8.09961270458969	c
4.02131158286182	7.13658059793248	7.72166172207309	c
2.68254216155615	2.26644134641609	10.69333837267367	c
-1.16127550713612	2.52124267753607	-4.60993607745402	n
-2.23835614216675	4.79610383484555	-5.21136692276640	c
-1.11264092202256	1.20220568188736	-6.80048040619559	c
-3.08669293841365	4.81067467098581	-7.81753049845131	c
-2.34482457783105	2.55206635495990	-8.83922085607334	c
-4.46433025964323	6.91662395991155	-9.11529711928488	c
-2.97768407929714	1.62674376997174	-11.43764361816616	c
-3.88862939974689	0.25849745835576	-0.07868165374030	o
2.81168833552256	-0.14208607358601	-0.28911669282796	o
-2.19165346546031	6.93580582068359	-3.71525749531038	c
0.64397949285552	-6.99836790455895	-3.64373866011267	c
-2.96993090636362	8.63496924743472	-4.53993076505620	h
1.22550574941040	-8.76539884037654	-4.48837752401851	h
-2.59776346327793	-12.69210896326230	3.55055295695134	h
-4.88642420030121	-10.57216910127791	4.68653994559759	h
-1.82979838610861	-10.58466496267655	5.99513837883823	h
2.05288101961053	-13.16115821279026	-0.45824394271876	c
-0.82830720193573	-12.06917052804103	-3.13400767137880	h
-2.01394668557766	-13.40418425124665	-0.37258980131963	h

2.96968932228484	-6.95273744870000	-10.99928601526955	h
2.28061736621675	-8.88698704616997	-8.42276947515233	h
5.98597633806854	-7.19311224787887	-8.26092044285629	c
3.74946470946196	-2.61092510800694	-11.89629445092829	h
2.19536614673220	0.28191287459572	-11.40600750724085	h
0.57453266367630	-2.26890625664202	-12.80045645989010	h
-4.75253833735881	2.46684211600879	-12.06847722863652	h
-3.20581061846524	-0.41819551640325	-11.48580524796885	h
-1.54288445313679	2.12979880160133	-12.83356362080238	h
-5.88837779547966	6.10677826074199	-10.37559945612789	h
-2.73521341752916	8.66484884808794	-10.66456764627089	c
-5.50705275619032	8.03716321696735	-7.73133112936762	h
0.82239887470583	13.31386740699190	-2.88488498586562	c
-1.72068370077042	13.45016581174191	0.29408797424615	h
-3.00255854310680	11.99425559278960	-2.36444432498608	h
0.67410725400595	12.90476071979577	3.43577003834174	h
3.44197010131871	11.20952196896619	4.12513774807686	h
0.65987703740846	10.62140938519826	5.84816576316259	h
2.97605085721546	8.63277891765772	8.68719608832079	h
5.08476858156610	8.00466984691085	6.19070746727647	h
5.38400131668369	6.38483063484684	9.07102210509863	h
1.24140478201025	1.27468032901918	11.77145571051636	h
3.05385125270804	4.01243104588279	11.72685958280388	h
5.10281627988142	0.65573810750847	10.64449610196889	c
-2.23058220324073	0.06993880557221	11.35039435100766	h
-0.81634112016788	-3.41673585502094	12.97124469395549	c
-4.44286059809429	-2.35128603350251	11.49113655478857	h
-5.92343211753170	-7.39868648192077	6.99049647161981	h
-5.54262815373829	-5.86901666232217	9.91554380358386	h
-3.47317440203459	-8.30875640054140	9.04972480383124	h
6.95010588634903	-5.46334093039323	-8.84072312235119	h
6.90354894681876	-8.78543111526964	-9.19967687514436	h
6.24979643592871	-7.40731971814121	-6.22618147116180	h
3.54557155513160	-11.93798608668024	-1.18919383796913	h
2.29697582450033	-15.03537190039889	-1.28731570387278	h
2.31844116670118	-13.32110674566068	1.58167664553214	h

-1.74509889181124	7.61335354395575	-12.13736623330890	h
-1.31226215156100	9.55946757990971	-9.46734210400525	h
-3.83865997431899	10.15445385399878	-11.57146517617277	h
2.54702255155240	13.59586797017764	-1.78784543430154	h
0.22777221201738	15.14463590844999	-3.62969855347713	h
1.28686575019279	12.09113874132727	-4.48094045800472	h
1.19339925424682	-3.09556427625638	12.64073546217987	h
-1.15311328225318	-5.44665337583813	12.83102118741174	h
-1.25184679233382	-2.83077522856920	14.90164668115461	h
4.78553820449672	-1.13605358044038	9.67267753030223	h
5.73548670040823	0.24298709855861	12.56521350895192	h
6.62895390980224	1.63887678029777	9.66380155481223	h