

## Supporting Information (SI)

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### Molecular Orbital and Topological electronic density study of $n \rightarrow \pi^*$ interactions: Amides and Thioamides, cases.

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## Set B3LYP/6-311+G(2d,p)

### Proline 1, *endo*

C	-0.01533718	-0.01333504	-0.08711317
H	1.06982928	-0.09766223	-0.12132600
C	-1.48527530	1.93353725	0.03618745
H	-2.35093918	2.16668165	-0.58578271
H	-1.08597733	2.87482787	0.43085693
C	-1.83745616	0.95869455	1.16819762
H	-2.65735704	0.31098666	0.85403118
H	-2.14154428	1.47669101	2.07849574
C	-0.55545476	0.13327840	1.35117698
H	0.17700042	0.68267767	1.94770844
H	-0.72535231	-0.82836424	1.83554873
N	-0.45632920	1.21715526	-0.73054054
C	0.03461057	1.55305314	-1.95808419
O	0.85607709	0.84409779	-2.52520803
C	-0.48509362	2.83605297	-2.57433294
H	-1.53718982	2.72668642	-2.85159394
H	-0.40869744	3.68041730	-1.88519910
H	0.09561914	3.04253042	-3.47021137
C	-0.60578814	-1.24624673	-0.77324577
O	0.20345044	-2.30801355	-0.61624252
C	-0.25914284	-3.54032983	-1.20005172
H	-0.39190535	-3.41844285	-2.27452199
H	0.51783360	-4.27075463	-0.98921394
H	-1.20517167	-3.84256629	-0.75081091
O	-1.67376018	-1.28509567	-1.33045901

H	1.07159545	2.18944075	1.84270219
H	0.70154026	3.19650352	0.43282918
C	-1.66589534	1.76633268	0.60995346
C	-0.6441929	-1.02424267	1.07611354
O	-2.57803211	0.99420874	0.34234387
O	-0.6822818	-0.89395076	2.27290156
C	-1.92297027	3.19384265	1.05041462
H	-1.55219257	3.90750017	0.30955952
H	-2.9968672	3.32446479	1.15969693
H	-1.43130689	3.41340253	2.00107286
N	-0.36564934	1.36889954	0.51775613
O	-1.04466015	-2.12523354	0.41942657
H	-2.49889646	-2.79414964	1.74869544
H	-1.87282259	-3.96586996	0.54828379
H	-0.8864213	-3.51107106	1.97316012
C	-1.61197991	-3.16597946	1.23662442

### Proline 1, *exo*

C	-0.05429223	-0.00024655	0.10980482
C	1.49229867	-0.04807586	0.12476342
C	1.91330442	1.42199368	-0.01594917
C	0.83463238	2.16941866	0.77227484
H	-0.45994176	-0.19753917	-0.88415167
H	1.83721042	-0.44242623	1.08331868
H	1.88330245	-0.68792355	-0.66572048
H	2.91729413	1.61239522	0.36558459
H	1.88515619	1.72881255	-1.06474282

### Proline 2, *endo*

C	0.00000000	0.00000000	0.00000000
H	1.08394000	0.00000000	0.00000000
C	-1.52692807	1.91884645	0.00000000
H	-2.39902836	2.08206040	-0.63154887
H	-1.15158043	2.89515874	0.31944096
C	-1.84977246	1.02196100	1.20174312
H	-2.66330735	0.34777706	0.94891180
H	-2.13395242	1.60409792	2.07693035
C	-0.56122891	0.21560526	1.42063251
H	0.16113791	0.79380651	1.99887873
H	-0.73708990	-0.72215090	1.94278869
N	-0.47898683	1.18318390	-0.72302547
C	0.07435861	1.53054998	-1.91272366
S	0.97538351	0.86574428	-2.41957561
C	-0.47208271	2.77395492	-2.58424033
H	-1.52206453	2.64087041	-2.84877157
H	-0.40543199	3.64476104	-1.93071219
H	0.10339619	2.95406251	-3.48626787
C	-0.56979996	-1.29292801	-0.61712498
O	0.29927965	-2.26820014	-0.99647519
C	-0.23859102	-3.54875185	-1.43956176
H	-0.15046049	-3.65332577	-2.52382115
H	0.31316260	-4.36219363	-0.96615096
H	-1.28587945	-3.60735731	-1.16589212
O	-1.78782489	-1.43097546	-0.68516920

### Proline 2, *exo*

C	-0.10828261	0.00615451	0.10121985
C	1.43954302	-0.05843545	0.08642343
C	1.87965595	1.40948922	0.01622062
C	0.81075055	2.13059058	0.83557829
H	-0.54098767	-0.17848337	-0.88282571
H	1.80065931	-0.51020045	1.01290392
H	1.80422918	-0.65924597	-0.74575639
H	2.88402935	1.56948739	0.41027989
H	1.85907797	1.76839656	-1.0159438
H	1.02394726	2.07055861	1.90894094
H	0.70346383	3.17869467	0.56460999
C	-1.66878159	1.85788205	0.55625748
C	-0.67387528	-1.02169873	1.07947253
S	-2.99431581	0.94712976	0.10882853
O	-0.73356440	-0.86678150	2.27244989
C	-1.82783368	3.28504833	1.02270724
H	-1.35685228	3.98171428	0.32173990
H	-2.88432832	3.52511228	1.08922899
H	-1.36432842	3.43514360	2.00227741
N	-0.41415091	1.37711862	0.52179405
O	-0.98627062	-2.16008820	0.44157404
H	-2.42694743	-2.89796171	1.74853239
H	-1.68257737	-4.05225945	0.59995202
H	-0.77375144	-3.48900539	2.03790885
C	-1.50057704	-3.21785322	1.27234203

### Proline 3, *endo*

C	0.05750000	0.45230000	0.71050000
H	-0.19320000	-0.12300000	1.59430000
C	2.27590000	0.95470000	-0.20590000
H	2.61100000	0.86580000	-1.23830000
H	3.15090000	0.86460000	0.44400000
C	1.52680000	2.27010000	0.04190000
H	1.04950000	2.59970000	-0.87670000
H	2.19340000	3.05580000	0.39390000
C	0.45370000	1.89780000	1.07550000
H	0.87180000	1.90280000	2.08330000
H	-0.39630000	2.57620000	1.06030000
N	1.28950000	-0.08510000	0.12270000
C	1.45160000	-1.42460000	-0.02460000
O	0.57670000	-2.21790000	0.31590000
C	2.75980000	-1.89300000	-0.62860000
H	2.86270000	-1.53450000	-1.65380000
H	3.61700000	-1.52430000	-0.06370000
H	2.76570000	-2.97800000	-0.62740000
C	-1.09220000	0.44870000	-0.31680000
N	-2.25640000	-0.17170000	0.01500000
C	-3.39450000	-0.04940000	-0.88790000
H	-3.55990000	-0.98170000	-1.43360000
H	-4.29390000	0.18230000	-0.31550000
H	-3.19830000	0.74360000	-1.60050000
C	-2.42230000	-1.08650000	1.14430000
H	-3.20820000	-1.79600000	0.89190000
H	-1.51360000	-1.65540000	1.31510000
H	-2.72310000	-0.56290000	2.05530000
O	-0.94740000	1.06070000	-1.37120000

### Proline 3, *exo*

C	0.09900000	-0.65180000	-0.49790000
C	0.56890000	-2.12220000	-0.40410000
C	2.10240000	-2.04070000	-0.40610000
C	2.38040000	-0.74400000	0.35590000
H	-0.13750000	-0.37530000	-1.52130000
H	0.22190000	-2.54550000	0.53670000
H	0.17320000	-2.72390000	-1.21980000
H	2.57020000	-2.90630000	0.05990000
H	2.48330000	-1.95780000	-1.42530000
H	2.35050000	-0.91000000	1.43630000
H	3.34030000	-0.30200000	0.10000000
C	1.24850000	1.47450000	-0.09790000
C	-1.08890000	-0.40290000	0.45210000
O	0.26410000	2.08050000	-0.51470000
O	-0.92910000	-0.59170000	1.65250000
C	2.48130000	2.20530000	0.39550000
H	3.33780000	2.01420000	-0.25320000
H	2.26620000	3.26890000	0.39040000
H	2.75190000	1.89370000	1.40460000
C	-3.40990000	0.17910000	0.81060000
H	-3.19950000	-0.29240000	1.76390000
H	-3.56630000	1.24840000	0.97530000
H	-4.31710000	-0.24640000	0.38140000
N	1.27440000	0.11850000	-0.06580000
N	-2.28590000	-0.05170000	-0.08990000
C	-2.44230000	0.41160000	-1.47030000
H	-2.27570000	-0.39120000	-2.18930000
H	-3.46590000	0.75400000	-1.59690000
H	-1.76890000	1.24110000	-1.68150000

### Proline 4, *endo*

C	0.07840000	0.55070000	-0.66830000
H	0.24770000	-0.10980000	-1.51060000
C	-1.99180000	1.51570000	0.19280000
H	-2.33340000	1.49520000	1.22580000
H	-2.86610000	1.60930000	-0.45580000
C	-0.97910000	2.63810000	-0.05820000
H	-0.45440000	2.87120000	0.86510000
H	-1.45930000	3.54470000	-0.42200000
C	-0.00390000	2.03390000	-1.07800000
H	-0.40940000	2.10330000	-2.08850000
H	0.96910000	2.52100000	-1.07270000
N	-1.25840000	0.27780000	-0.13610000
C	-1.72690000	-0.96530000	0.03230000
C	-3.12150000	-1.07670000	0.59510000
H	-3.14960000	-0.69180000	1.61700000
H	-3.83700000	-0.49760000	0.00750000
H	-3.42710000	-2.11580000	0.60530000
C	1.13760000	0.33740000	0.43350000
N	2.36240000	-0.11840000	0.05010000
C	3.35860000	-0.38700000	1.08110000
H	3.46200000	-1.46210000	1.24870000
H	4.32540000	0.01490000	0.77650000
H	3.04210000	0.08350000	2.00500000
C	2.65050000	-0.64400000	-1.28190000
H	3.72710000	-0.76890000	-1.37190000
H	2.17050000	-1.61070000	-1.44900000
H	2.33990000	0.04730000	-2.06220000
O	0.87390000	0.65280000	1.58730000
S	-0.84230000	-2.33680000	-0.34410000

### Proline 4, *exo*

C	0.00460000	0.72560000	-0.49470000
C	-0.22360000	2.25710000	-0.53500000
C	-1.74830000	2.42790000	-0.48080000
C	-2.19790000	1.24870000	0.37900000
H	0.20040000	0.31230000	-1.47930000
H	0.23040000	2.71480000	0.34250000
H	0.22280000	2.70540000	-1.42020000
H	-2.04950000	3.38590000	-0.06080000
H	-2.18310000	2.34390000	-1.47780000
H	-2.06960000	1.46200000	1.44330000
H	-3.22990000	0.96240000	0.20160000
C	-1.52910000	-1.13680000	0.00540000
C	1.12510000	0.38470000	0.50850000
O	0.88330000	0.46830000	1.70550000
C	-2.87300000	-1.55300000	0.55240000
H	-3.68330000	-1.20180000	-0.09070000
H	-2.91970000	-2.63390000	0.60530000
H	-3.03610000	-1.13800000	1.54880000
C	3.41440000	-0.25710000	0.95820000
H	3.11980000	0.05610000	1.95330000
H	3.56770000	-1.33950000	0.96050000
H	4.34910000	0.23000000	0.68020000
N	-1.27630000	0.17700000	-0.02620000
N	2.36530000	0.11580000	0.01580000
C	2.63220000	-0.16040000	-1.39300000
H	2.25400000	0.63230000	-2.03530000
H	3.70980000	-0.20180000	-1.53260000
H	2.19840000	-1.11290000	-1.70400000
S	-0.43730000	-2.28710000	-0.53170000

### Proline 5, *endo*

C	-0.13730000	-0.25180000	0.85190000
H	0.05490000	0.46110000	1.64580000
C	-2.34560000	-0.94540000	0.03310000
H	-2.64400000	-1.06600000	-1.00750000
H	-3.24110000	-0.73160000	0.62240000
C	-1.60940000	-2.18650000	0.55640000
H	-1.17450000	-2.73170000	-0.27560000
H	-2.27830000	-2.85350000	1.09800000
C	-0.49340000	-1.62950000	1.45490000
H	-0.86130000	-1.47490000	2.47020000
H	0.36770000	-2.29120000	1.50610000
N	-1.37280000	0.14670000	0.17730000
C	-1.55510000	1.44150000	-0.18760000
C	-2.85900000	1.78180000	-0.87760000
H	-2.93420000	1.26050000	-1.83300000
H	-3.72050000	1.49130000	-0.27500000
H	-2.88360000	2.85260000	-1.05130000
C	1.06710000	-0.30640000	-0.10300000
N	2.16980000	0.36580000	0.26490000
C	3.38940000	0.25430000	-0.53440000
H	3.32360000	0.87060000	-1.43350000
H	4.23270000	0.58010000	0.06890000
H	3.53140000	-0.77540000	-0.84840000
C	2.18600000	1.37570000	1.33610000
H	3.07930000	1.98030000	1.21540000
H	1.31910000	2.02640000	1.25290000
H	2.22110000	0.91460000	2.32450000
S	0.98410000	-1.22850000	-1.49980000
O	-0.69660000	2.29420000	0.03030000

### Proline 5, *exo*

C	0.17120000	-0.45780000	-0.72730000
C	0.58890000	-1.92910000	-0.97650000
C	2.12130000	-1.92430000	-0.86620000
C	2.39110000	-0.85130000	0.19060000
H	0.01110000	0.05120000	-1.67280000
H	0.16190000	-2.55770000	-0.19910000
H	0.23370000	-2.28330000	-1.94260000
H	2.52170000	-2.89660000	-0.58420000
H	2.57800000	-1.63200000	-1.81310000
H	2.26810000	-1.25360000	1.19910000
H	3.38260000	-0.41420000	0.10540000
C	1.41250000	1.48320000	0.09890000
C	-1.08170000	-0.34660000	0.15660000
C	2.64990000	2.03480000	0.77760000
H	3.52770000	1.92510000	0.13850000
H	2.48570000	3.09020000	0.96910000
H	2.85380000	1.52050000	1.71660000
C	-3.41740000	0.26350000	0.38550000
H	-3.56290000	-0.67380000	0.91440000
H	-3.37860000	1.06260000	1.12850000
H	-4.24530000	0.43980000	-0.29590000
N	1.35240000	0.14170000	-0.09210000
N	-2.17600000	0.20870000	-0.38540000
C	-2.16050000	0.95040000	-1.65620000
H	-2.08570000	0.27920000	-2.51290000
H	-3.09390000	1.49770000	-1.73980000
H	-1.33990000	1.66390000	-1.66280000
S	-1.03700000	-0.95990000	1.71500000
O	0.49840000	2.21880000	-0.26800000

### Proline 6, *endo*

C	0.00470000	0.39470000	-0.81910000
H	0.10100000	-0.37250000	-1.57840000
C	-2.03640000	1.52050000	-0.07860000
H	-2.33310000	1.68230000	0.95580000
H	-2.93620000	1.50170000	-0.69740000
C	-1.03950000	2.57990000	-0.56020000
H	-0.51670000	3.00450000	0.29200000
H	-1.53580000	3.38550000	-1.09860000
C	-0.05630000	1.80390000	-1.44870000
H	-0.44280000	1.71560000	-2.46500000
H	0.92280000	2.27470000	-1.50120000
N	-1.31830000	0.23800000	-0.21340000
C	-1.82190000	-0.96120000	0.10720000
C	-3.19930000	-0.95820000	0.71960000
H	-3.18970000	-0.42140000	1.67090000
H	-3.92270000	-0.46010000	0.07040000
H	-3.52230000	-1.97720000	0.89390000
C	1.14340000	0.26290000	0.20410000
N	2.27040000	-0.32680000	-0.22850000
C	3.41650000	-0.43030000	0.67520000
H	3.20400000	-1.12330000	1.49080000
H	4.27740000	-0.77920000	0.11290000
H	3.63050000	0.54010000	1.11660000
C	2.35760000	-1.03390000	-1.51360000
H	3.34150000	-1.48310000	-1.59280000
H	1.60870000	-1.82470000	-1.56690000
H	2.23130000	-0.35360000	-2.35560000
S	-0.99770000	-2.39930000	-0.13480000
S	0.98540000	0.91450000	1.73680000

### Proline 6, *exo*

C	0.04910000	-0.60110000	-0.68020000
C	0.22440000	-2.11930000	-0.94260000
C	1.73870000	-2.35730000	-0.86200000
C	2.19720000	-1.33690000	0.17820000
H	-0.06530000	-0.05490000	-1.61140000
H	-0.28370000	-2.68100000	-0.16200000
H	-0.19960000	-2.40600000	-1.90320000
H	1.98680000	-3.37820000	-0.57720000
H	2.21610000	-2.14760000	-1.82010000
H	2.01920000	-1.69600000	1.19420000
H	3.24380000	-1.06870000	0.07620000
C	1.65760000	1.10730000	0.07180000
C	-1.13980000	-0.33130000	0.25360000
C	2.99140000	1.38590000	0.72080000
H	3.81460000	1.06460000	0.07830000
H	3.08950000	2.45020000	0.89730000
H	3.08230000	0.85380000	1.66950000
C	-3.45140000	0.33070000	0.52850000
H	-3.62750000	-0.53770000	1.15860000
H	-3.29730000	1.18900000	1.18420000
H	-4.31200000	0.50710000	-0.10980000
N	1.33000000	-0.17980000	-0.09360000
N	-2.27510000	0.10570000	-0.31210000
C	-2.35330000	0.53750000	-1.71330000
H	-2.15190000	-0.28700000	-2.39690000
H	-3.35940000	0.89280000	-1.90800000
H	-1.65180000	1.35080000	-1.90130000
S	0.66700000	2.37170000	-0.40260000
S	-1.00260000	-0.69830000	1.88030000

## Set B3LYP D3/6-311+G(2d,p)

### Proline 1, *endo*

C	0.01063442	-0.00073022	-0.05152441
H	1.09454446	-0.09598049	-0.06979033
C	-1.46780844	1.93550658	0.04502352
H	-2.31844535	2.15817055	-0.59980065
H	-1.08863127	2.87978645	0.45049105
C	-1.83860723	0.95382106	1.16368868
H	-2.64183427	0.29912783	0.82402316
H	-2.17006814	1.46439672	2.06799251
C	-0.55510501	0.13983317	1.37394627
H	0.16113876	0.69513282	1.98367973
H	-0.72703000	-0.82427755	1.85168229
N	-0.41250883	1.23314914	-0.69458487
C	0.03858631	1.52151791	-1.94663402
O	0.83945115	0.78808239	-2.51193748
C	-0.49935951	2.78190557	-2.58749678
H	-1.55006782	2.64595278	-2.85777271
H	-0.43668584	3.64000768	-1.91483595
H	0.07381307	2.97901108	-3.48999112
C	-0.58818083	-1.21400487	-0.75636623
O	0.20866620	-2.28569646	-0.62089492
C	-0.27040142	-3.49654438	-1.23370300
H	-0.40297791	-3.34437794	-2.30418143
H	0.49674398	-4.24211660	-1.04235675
H	-1.22021359	-3.79552663	-0.79072110
O	-1.65900420	-1.22958928	-1.30967023

### Proline 1, *exo*

C	-0.03585518	-0.00243046	0.08159938
C	1.50787917	-0.04176563	0.12529484
C	1.92117861	1.42892527	-0.01692428
C	0.82799354	2.17026803	0.75377285
H	-0.42535137	-0.21173377	-0.91562181
H	1.83325667	-0.42538930	1.09446154
H	1.91739997	-0.68537408	-0.65186986
H	2.91867448	1.62798842	0.37559895
H	1.90084181	1.73087766	-1.06692439
H	1.04453012	2.18669563	1.82819775
H	0.69525812	3.19695365	0.41413825
C	-1.66258580	1.73343093	0.61075461
C	-0.63464158	-1.00912265	1.05448687
O	-2.56646581	0.94488593	0.36406849
O	-0.66383987	-0.86447565	2.24997421
C	-1.92683546	3.15033913	1.07216321
H	-1.56139737	3.87639556	0.34135316
H	-3.00018118	3.27403809	1.19111871
H	-1.42861974	3.35411317	2.02285794
N	-0.36021136	1.36513293	0.47478747
O	-1.05204777	-2.10970883	0.41153860
H	-2.51585658	-2.72917242	1.75043120
H	-1.91183906	-3.93271953	0.56977936
H	-0.91678359	-3.47101709	1.98698033
C	-1.63656921	-3.12662795	1.24469902



### Proline 2, *endo*

C	-0.00230523	-0.00997116	-0.07817482
H	1.08198146	-0.09051382	-0.11302520
C	-1.48926353	1.91548057	0.01058729
H	-2.34156465	2.13851266	-0.63046534
H	-1.09620447	2.85982488	0.40098881
C	-1.84725729	0.94514123	1.13877567
H	-2.64639203	0.27974496	0.81077788
H	-2.17855304	1.46528453	2.03756069
C	-0.55505250	0.14833344	1.34944868
H	0.16135516	0.71959512	1.94413755
H	-0.71134554	-0.81092855	1.84150039
N	-0.44109364	1.20938081	-0.74701146
C	0.03218400	1.57578430	-1.94751358
S	1.15413288	0.66997017	-2.78621506
C	-0.52109727	2.85940574	-2.50830010
H	-1.58055587	2.73717589	-2.75425656
H	-0.44262433	3.67827872	-1.78743538
H	0.01706386	3.12267540	-3.41308604
C	-0.59965201	-1.23812837	-0.75902063
O	0.19204420	-2.30599121	-0.58835140
C	-0.28130798	-3.52978105	-1.17956380
H	-0.39665000	-3.40056521	-2.25506865
H	0.48144656	-4.27196109	-0.96004708
H	-1.23821093	-3.81650072	-0.74397653
O	-1.67442906	-1.26368993	-1.30400007

### Proline 2, *exo*

C	-0.08132024	0.00422931	0.08738154
C	1.46312962	-0.04995729	0.09956095
C	1.88943489	1.41923072	0.00662183
C	0.81179674	2.13991651	0.81225392
H	-0.49929565	-0.18566790	-0.90156258
H	1.80741932	-0.47645560	1.04382334
H	1.84702980	-0.66611736	-0.71175703
H	2.89112578	1.59599243	0.39890642
H	1.86359852	1.76110973	-1.03083714
H	1.01933641	2.09358769	1.88698464
H	0.69385700	3.18301124	0.52769997
C	-1.66150610	1.82000730	0.57076836
C	-0.65741505	-1.01252534	1.06449693
S	-2.97104177	0.87326213	0.15910211
O	-0.70720248	-0.85215727	2.25729064
C	-1.83771978	3.24045494	1.04219408
H	-1.38536562	3.94463064	0.33712063
H	-2.89639747	3.46361454	1.12521569
H	-1.36095078	3.39165509	2.01492543
N	-0.40002115	1.37051635	0.50214906
O	-0.98958476	-2.14625959	0.43128776
H	-2.46133187	-2.82557507	1.72979085
H	-1.73984104	-4.01570823	0.60254658
H	-0.82935089	-3.46083109	2.04353379
C	-1.54045183	-3.17945685	1.26721861

### Proline 3, *endo*

C	0.05622775	0.46173389	0.73133664
H	-0.19941277	-0.11169032	1.61702959
C	2.26094855	0.94941434	-0.21350006
H	2.57496363	0.85038964	-1.25347493
H	3.14892852	0.86052923	0.42166207
C	1.51927411	2.26737576	0.03772291
H	1.02512768	2.58895676	-0.87652109
H	2.19396234	3.05537231	0.37425661
C	0.46158859	1.90348621	1.08890175
H	0.89597896	1.90716172	2.09173674
H	-0.38840917	2.58489985	1.08351704
N	1.28046155	-0.08381053	0.14223987
C	1.43293531	-1.42220951	-0.00422921
O	0.56131027	-2.21191309	0.35294199
C	2.72937416	-1.89076933	-0.62930782
H	2.81259808	-1.53112538	-1.65786514
H	3.59561323	-1.51666388	-0.07845765
H	2.73783737	-2.97768008	-0.62642954
C	-1.08192510	0.46245600	-0.30266619
N	-2.24080300	-0.17110238	0.01201506
C	-3.36904659	-0.05699162	-0.90149003
H	-3.51656228	-0.99022710	-1.45442826
H	-4.27824553	0.16115207	-0.33578193
H	-3.17253999	0.74352653	-1.60848207
C	-2.40517602	-1.09200812	1.13423346
H	-3.18280502	-1.80952371	0.87123743
H	-1.48904704	-1.65173958	1.30692017
H	-2.71843876	-0.57326790	2.04616383
O	-0.93051882	1.08536822	-1.34988122

### Proline 3, *exo*

C	0.09970946	-0.68065021	-0.51819724
C	0.57704643	-2.14137391	-0.38324110
C	2.10808674	-2.04874625	-0.42324759
C	2.38949241	-0.73655369	0.30845078
H	-0.14513370	-0.43634662	-1.54972729
H	0.25411784	-2.52675571	0.58425790
H	0.16370872	-2.77574177	-1.16729184
H	2.59588866	-2.90238385	0.04830388
H	2.46391590	-1.97870560	-1.45448009
H	2.37606654	-0.88117957	1.39433617
H	3.34306385	-0.29065728	0.02765116
C	1.19717073	1.45797099	-0.07305435
C	-1.07289224	-0.40683441	0.43762760
O	0.18586468	2.05002393	-0.44269464
O	-0.89914210	-0.57887465	1.63850826
C	2.41549949	2.19621006	0.43852018
H	3.27081643	2.04617547	-0.22549976
H	2.17865741	3.25634266	0.47950215
H	2.69963058	1.84597633	1.43336175
C	-3.37319680	0.23209991	0.80709340
H	-3.16538970	-0.22685653	1.76917161
H	-3.49168952	1.31143297	0.94997319
H	-4.29903313	-0.17397823	0.39455514
N	1.27064480	0.10614637	-0.11282347
N	-2.26816323	-0.05159830	-0.09879163
C	-2.41799465	0.40169041	-1.48154443
H	-2.26423818	-0.41279562	-2.19285640
H	-3.43740278	0.76114593	-1.61061632
H	-1.72780464	1.21881718	-1.69614702

### Proline 4, *endo*

C	0.08419572	0.59225115	-0.69349426
H	0.26338618	-0.04908266	-1.55043388
C	-2.00910679	1.51737258	0.14643924
H	-2.38960298	1.47637985	1.16653433
H	-2.86042963	1.60916424	-0.53601318
C	-1.00021551	2.65155624	-0.05091213
H	-0.49153255	2.85414900	0.89030743
H	-1.47952287	3.56799354	-0.39627269
C	-0.00361119	2.08161674	-1.06897823
H	-0.39216967	2.17394274	-2.08621277
H	0.96850833	2.57304468	-1.03163435
N	-1.24809372	0.29744747	-0.17053930
C	-1.66120014	-0.95341820	0.05213522
C	-3.04759307	-1.10089089	0.62116597
H	-3.07740843	-0.70717632	1.64173447
H	-3.78263581	-0.54516065	0.03201646
H	-3.32281189	-2.15037853	0.64389272
C	1.12828660	0.36524522	0.41369983
N	2.34328688	-0.11675198	0.04017266
C	3.31729708	-0.42064575	1.08019901
H	3.37067639	-1.50056789	1.25348195
H	4.30429620	-0.06146650	0.78078135
H	3.01131093	0.06908976	1.99976159
C	2.61022619	-0.67266105	-1.28237036
H	3.67665293	-0.88165119	-1.35381419
H	2.05499237	-1.60096303	-1.44585206
H	2.36473004	0.03795544	-2.07165052
O	0.86103956	0.69766161	1.56192211
S	-0.70795115	-2.29215566	-0.26226642

### Proline 4, *exo*

C	0.00705592	0.75750680	-0.50793317
C	-0.23288441	2.28342281	-0.52742121
C	-1.75923686	2.43617859	-0.49577024
C	-2.20632809	1.24739462	0.35042661
H	0.21078631	0.35618510	-1.49772727
H	0.20273080	2.72845990	0.36794371
H	0.22497968	2.75059707	-1.39903181
H	-2.07989283	3.38952025	-0.07513534
H	-2.17683867	2.34910926	-1.50193149
H	-2.09369205	1.45431979	1.41976444
H	-3.23351981	0.94744471	0.15616283
C	-1.47823816	-1.12297877	0.02143132
C	1.11403816	0.40677831	0.50082754
O	0.86217418	0.49194283	1.69564365
C	-2.80870819	-1.56009830	0.57792325
H	-3.62787666	-1.23292280	-0.06976896
H	-2.83266156	-2.64263376	0.64894149
H	-2.97495156	-1.12937202	1.56924171
C	3.37608329	-0.30694332	0.95629417
H	3.08335338	-0.00090855	1.95612826
H	3.48383292	-1.39676153	0.93670945
H	4.33312744	0.14854517	0.69438556
N	-1.26700319	0.19386234	-0.04904863
N	2.35113480	0.12329439	0.01424389
C	2.60815069	-0.15725229	-1.39394663
H	2.27030131	0.65922339	-2.03234532
H	3.68443158	-0.25182519	-1.53056666
H	2.12517486	-1.08707074	-1.70833176
S	-0.34492327	-2.24711803	-0.47890941

### Proline 5, *endo*

C	-0.14799602	-0.24474111	0.90202899
H	0.05785554	0.45566921	1.70534740
C	-2.34974882	-0.93819827	0.08171079
H	-2.64284687	-1.03703458	-0.96422457
H	-3.24939889	-0.74589243	0.67553799
C	-1.59984019	-2.18270197	0.57584828
H	-1.16364468	-2.70545880	-0.27194412
H	-2.26043784	-2.86795571	1.10853236
C	-0.48399799	-1.63477531	1.47900652
H	-0.84625728	-1.50509384	2.50163194
H	0.38780535	-2.28683706	1.50790839
N	-1.39013650	0.15754558	0.25285085
C	-1.51623653	1.42619863	-0.20640265
C	-2.79200224	1.75747191	-0.94661736
H	-2.81806703	1.22443005	-1.90070888
H	-3.67808954	1.46479874	-0.37921690
H	-2.81305920	2.82783782	-1.13502515
C	1.02308513	-0.27512050	-0.08546202
N	2.14351964	0.36506714	0.27726521
C	3.32288957	0.29945682	-0.58187099
H	3.20037529	0.94386351	-1.45721427
H	4.19177127	0.61832046	-0.00922147
H	3.46226953	-0.71918054	-0.93715524
C	2.18787927	1.33442674	1.38121188
H	3.11781067	1.89170673	1.30457872
H	1.35575717	2.03325217	1.29928981
H	2.17053954	0.83755993	2.35406352
S	0.87694052	-1.12660924	-1.51839299
O	-0.62723889	2.25709396	-0.03095603

### Proline 5, *exo*

C	0.17829230	-0.45890184	-0.76795826
C	0.58609692	-1.93493702	-0.98712277
C	2.11790579	-1.93407041	-0.87750694
C	2.39251360	-0.84134639	0.15602409
H	0.00654197	0.03178444	-1.72282049
H	0.15596964	-2.54368472	-0.19343349
H	0.22732441	-2.30799082	-1.94671938
H	2.51579280	-2.90333511	-0.57548422
H	2.57432304	-1.66018738	-1.83212079
H	2.26411179	-1.22007906	1.17510261
H	3.38748477	-0.40899469	0.06105629
C	1.38121054	1.47618451	0.10454138
C	-1.04974162	-0.32530986	0.13817131
C	2.59501731	2.01727570	0.82736765
H	3.49636500	1.90513945	0.21930834
H	2.42907589	3.07294891	1.02654623
H	2.75813551	1.48757744	1.76853582
C	-3.37192836	0.29786886	0.41069036
H	-3.50681012	-0.62413769	0.97215723
H	-3.30172949	1.11926588	1.12960562
H	-4.21987574	0.46090040	-0.25207015
N	1.36139977	0.14699943	-0.15331754
N	-2.15620817	0.20923083	-0.39345781
C	-2.15937805	0.92571546	-1.67612533
H	-2.06267740	0.23856994	-2.51982950
H	-3.10904026	1.44540321	-1.77213130
H	-1.35477694	1.66031427	-1.69199764
S	-0.95569310	-0.88427205	1.71224117
O	0.45139821	2.20316829	-0.23835250

### Proline 6, *endo*

C	-0.00225593	0.40291628	-0.86066791
H	0.10168729	-0.35541442	-1.63003343
C	-2.03685685	1.51966818	-0.10653942
H	-2.33018009	1.66300385	0.93334399
H	-2.93907519	1.51422447	-0.72554882
C	-1.03459639	2.58284694	-0.56790337
H	-0.50945343	2.98568265	0.29553475
H	-1.52594839	3.40224651	-1.09340779
C	-0.05212169	1.81894527	-1.46602993
H	-0.43451602	1.74959887	-2.48719095
H	0.93260949	2.28368667	-1.50299130
N	-1.32298316	0.24170169	-0.26465398
C	-1.78394586	-0.95505463	0.11165152
C	-3.14273161	-0.96372393	0.75813788
H	-3.10544089	-0.42323225	1.70902342
H	-3.88749849	-0.46983557	0.12747411
H	-3.45269881	-1.98648142	0.94620112
C	1.11020035	0.25537891	0.18049579
N	2.24533566	-0.32435747	-0.23506492
C	3.36118075	-0.45689951	0.69888677
H	3.10551187	-1.14703596	1.50701806
H	4.23050190	-0.82516156	0.15894066
H	3.58441445	0.50916448	1.15002080
C	2.34976559	-1.01872516	-1.52285244
H	3.34135261	-1.45560269	-1.59991717
H	1.60733633	-1.81802450	-1.58518244
H	2.21934539	-0.33023649	-2.35961560
S	-0.91294240	-2.36933667	-0.09138533
S	0.91050350	0.88405744	1.71565594

### Proline 6, *exo*

C	0.05546977	-0.61412938	-0.71667258
C	0.22574025	-2.13395527	-0.95012281
C	1.73970486	-2.37101764	-0.87086183
C	2.20019517	-1.33381710	0.15029368
H	-0.06674733	-0.08118232	-1.65644422
H	-0.27919685	-2.67732277	-0.15222316
H	-0.20583176	-2.43929330	-1.90340861
H	1.98928328	-3.38848772	-0.56915061
H	2.21398671	-2.17445499	-1.83545570
H	2.01678945	-1.67366784	1.17419153
H	3.24875209	-1.06653448	0.04396521
C	1.61815592	1.09997595	0.07987272
C	-1.11105413	-0.32622038	0.23085637
C	2.93378631	1.38678818	0.75488004
H	3.77248813	1.07936348	0.12291708
H	3.01653024	2.45102687	0.94986940
H	3.00704592	0.83869180	1.69835532
C	-3.40281559	0.36802509	0.54364719
H	-3.57680211	-0.48388784	1.19937933
H	-3.21300112	1.23966911	1.17553711
H	-4.27761025	0.54556944	-0.07776870
N	1.33469414	-0.18582513	-0.14316804
N	-2.25436002	0.10232782	-0.31917234
C	-2.34645683	0.52351841	-1.71996667
H	-2.13575390	-0.30459302	-2.39884883
H	-3.35981156	0.86459422	-1.91226653
H	-1.65329944	1.34572388	-1.91396789
S	0.58234435	2.34221191	-0.34633146
S	-0.93522566	-0.66709698	1.85726500

## Set $\omega$ B97X-D4/6-311+G(2d,p)

### Proline 1, *endo*

C	0.03372990	0.01106943	-0.03564318
H	1.12054779	-0.08812895	-0.05210496
C	-1.46547080	1.92835009	0.04966935
H	-2.31242766	2.13754726	-0.60934461
H	-1.10659833	2.87855430	0.46599269
C	-1.83632461	0.93498847	1.15808216
H	-2.62303228	0.26534673	0.80008443
H	-2.19227228	1.43640464	2.06105242
C	-0.54139640	0.14502995	1.38353686
H	0.16123997	0.71897612	1.99649761
H	-0.69906046	-0.82321332	1.86470159
N	-0.38862881	1.24456267	-0.67358064
C	0.04194475	1.50965145	-1.93827765
O	0.83582087	0.76546112	-2.49623449
C	-0.50607644	2.75520763	-2.59733702
H	-1.55126794	2.59303646	-2.88148852
H	-0.46659457	3.61966701	-1.92815160
H	0.07816724	2.95228725	-3.49537349
C	-0.56919724	-1.19393159	-0.75023947
O	0.20456131	-2.27712674	-0.60630431
C	-0.29421278	-3.46371766	-1.24050259
H	-0.41649371	-3.29011552	-2.31123900
H	0.45625986	-4.23138712	-1.05693905
H	-1.25532266	-3.74970938	-0.80783502
O	-1.63124601	-1.19225301	-1.32075630

### Proline 1, *exo*

C	-0.01607159	-0.00389190	0.05628326
C	1.52397586	-0.03497666	0.13076302
C	1.92990635	1.43589199	-0.01944054
C	0.82660874	2.17153012	0.74148174
H	-0.39211548	-0.22147393	-0.94787073
H	1.82903575	-0.40256689	1.11621192
H	1.95656177	-0.68749389	-0.63018370
H	2.92553412	1.64478190	0.37898850
H	1.91144376	1.73190169	-1.07380683
H	1.03157146	2.18382659	1.82076572
H	0.69165448	3.20075095	0.40043327
C	-1.65624111	1.70267537	0.61069065
C	-0.62592640	-1.00379090	1.02976441
O	-2.54704655	0.89905402	0.37182333
O	-0.64595498	-0.85456981	2.22507424
C	-1.93602543	3.10880043	1.09288357
H	-1.60421434	3.84534439	0.35393971
H	-3.01009556	3.20868883	1.24316906
H	-1.41212503	3.31123292	2.03208658
N	-0.35073108	1.35959609	0.44394265
O	-1.06557087	-2.09668537	0.39691619
H	-2.52966313	-2.65637295	1.75769829
H	-1.96272823	-3.89751413	0.59176252
H	-0.94129056	-3.43063344	1.99308513
C	-1.66256040	-3.08359838	1.25025442

### Proline 2, *endo*

C	0.00947181	-0.00084354	-0.06366532
H	1.09555571	-0.07926075	-0.09633463
C	-1.48382758	1.91529309	0.01722299
H	-2.33307848	2.14061591	-0.62940823
H	-1.09233240	2.85696955	0.41843200
C	-1.84829794	0.93579588	1.13503667
H	-2.63591508	0.26279243	0.79040040
H	-2.19726370	1.44870252	2.03288049
C	-0.55062592	0.15372046	1.35778603
H	0.15560196	0.73627438	1.95609916
H	-0.69941152	-0.80782245	1.85133787
N	-0.43380027	1.21152678	-0.73314615
C	0.02645539	1.55604039	-1.94090792
S	1.12728392	0.63162751	-2.76713641
C	-0.52319948	2.83358777	-2.51808375
H	-1.57729559	2.69691489	-2.78111544
H	-0.46079279	3.65542568	-1.79848152
H	0.03025272	3.09153778	-3.41697102
C	-0.58749325	-1.22446444	-0.74790342
O	0.19403222	-2.29564597	-0.58126386
C	-0.28997857	-3.50001152	-1.19259280
H	-0.41389193	-3.34723777	-2.26549878
H	0.47019438	-4.25380867	-0.99609383
H	-1.24594173	-3.79118793	-0.75418133
O	-1.65905318	-1.23998470	-1.29814599

### Proline 2, *exo*

C	-0.06883405	0.00600774	0.06591486
C	1.47175226	-0.04730213	0.10318482
C	1.89592140	1.42087483	0.00684913
C	0.81049273	2.14049944	0.80262460
H	-0.47707297	-0.18572942	-0.92834764
H	1.79947161	-0.46397970	1.05957101
H	1.87265046	-0.67035247	-0.69661219
H	2.89514551	1.60209049	0.40672552
H	1.87551860	1.75903302	-1.03333173
H	1.00938763	2.09691727	1.87995157
H	0.69150493	3.18346230	0.51089489
C	-1.65462766	1.79579088	0.56937614
C	-0.65402708	-1.00430782	1.04239780
S	-2.94361397	0.83869474	0.15958732
O	-0.70917800	-0.83273981	2.23256305
C	-1.84467053	3.20754622	1.06086632
H	-1.42603947	3.92250266	0.34523250
H	-2.90675718	3.40698950	1.17455606
H	-1.34128421	3.35563906	2.02090274
N	-0.39131298	1.36548655	0.48300184
O	-0.99237511	-2.13771735	0.42037683
H	-2.47154561	-2.76828584	1.73105868
H	-1.77001711	-3.99196577	0.62356751
H	-0.84662180	-3.42386958	2.05331730
C	-1.55593581	-3.14477777	1.27248749

### Proline 3, *endo*

C	0.07270827	0.44560956	0.79661472
H	-0.20266526	-0.12020550	1.68334375
C	2.29629608	0.96576987	-0.06708237
H	2.67051846	0.85033780	-1.08587010
H	3.14809759	0.91754153	0.62214926
C	1.50563231	2.26666545	0.10564576
H	1.03765559	2.53578696	-0.84105383
H	2.14063773	3.09111953	0.43638226
C	0.42335468	1.90430719	1.12997393
H	0.82458733	1.95043477	2.14701799
H	-0.44731513	2.56025526	1.07784303
N	1.32146547	-0.07794747	0.25728370
C	1.36754212	-1.37608774	-0.12684671
O	0.41563942	-2.12381895	0.07209922
C	2.63260902	-1.84484122	-0.80988071
H	2.67058019	-1.44372954	-1.82703868
H	3.52866084	-1.51050517	-0.28152267
H	2.61372041	-2.93216326	-0.85864743
C	-1.01331261	0.37491953	-0.28572225
N	-2.23068828	-0.11733349	0.05991219
C	-3.23178939	-0.24125630	-0.99016597
H	-3.20193305	-1.23813897	-1.44530143
H	-4.22449234	-0.07164792	-0.56650262
H	-3.03079670	0.49858782	-1.76155884
C	-2.44384290	-0.91629184	1.26455155
H	-3.47209647	-1.27855594	1.25068318
H	-1.76831214	-1.77512970	1.29334441
H	-2.32097737	-0.31846147	2.17094652
O	-0.76728388	0.81587922	-1.40119786

### Proline 3, *exo*

C	0.11004522	-0.68177199	-0.54879226
C	0.57609605	-2.14111394	-0.38976363
C	2.10601494	-2.05555211	-0.43573367
C	2.39233037	-0.73869584	0.28439782
H	-0.13840941	-0.44823070	-1.58328955
H	0.25548953	-2.50899425	0.58715696
H	0.15708176	-2.78892107	-1.16179631
H	2.59280246	-2.90789745	0.04202081
H	2.45898913	-1.99386370	-1.46985062
H	2.37154422	-0.87224587	1.37270997
H	3.35063940	-0.30011609	0.00122661
C	1.17611314	1.44536629	-0.05264770
C	-1.04918710	-0.38263281	0.41204290
O	0.14857578	2.02337917	-0.39132249
O	-0.84704569	-0.48921730	1.61337694
C	2.37945125	2.18651973	0.48601374
H	3.24586774	2.05040473	-0.16722936
H	2.13200945	3.24488388	0.54136336
H	2.64477890	1.81888098	1.48083002
C	-3.32441998	0.28517530	0.81639493
H	-3.13633675	-0.19079149	1.77591111
H	-3.35519767	1.37113925	0.96358221
H	-4.28614423	-0.04965996	0.42045883
N	1.28056000	0.09944859	-0.15412083
N	-2.26547608	-0.08363685	-0.11266275
C	-2.43765221	0.35201066	-1.49591274
H	-2.17596769	-0.43992958	-2.20103262
H	-3.49220319	0.58476079	-1.64690134
H	-1.84304933	1.24530164	-1.70533033



### Proline 4, *endo*

C	0.07929850	0.59581809	-0.71529799
H	0.26301421	-0.03815514	-1.57911647
C	-2.01136322	1.51543945	0.12739824
H	-2.39866596	1.46331903	1.14581134
H	-2.85635721	1.61839100	-0.56294838
C	-0.99624562	2.64711903	-0.04711822
H	-0.48926716	2.83135497	0.90041202
H	-1.47042645	3.57227921	-0.38027921
C	-0.00040062	2.08807718	-1.07011038
H	-0.38812832	2.19625713	-2.08755450
H	0.97581296	2.57411412	-1.02353419
N	-1.24990432	0.30205773	-0.19656388
C	-1.63905948	-0.94658380	0.05537849
C	-3.01688375	-1.10673384	0.64035641
H	-3.02362832	-0.72736612	1.66731939
H	-3.76120008	-0.54375065	0.06959773
H	-3.28555891	-2.15963871	0.65370213
C	1.10959444	0.35814193	0.39796444
N	2.33203037	-0.10563397	0.03345488
C	3.28845188	-0.42110818	1.08439263
H	3.30318532	-1.49888759	1.28309182
H	4.28862065	-0.10093989	0.78082010
H	2.99705484	0.09966842	1.99334325
C	2.60079913	-0.66926474	-1.28406433
H	3.66150016	-0.91730930	-1.33576255
H	2.01562699	-1.57786247	-1.45809480
H	2.39663572	0.05290292	-2.07741957
O	0.82451263	0.67239070	1.54488728
S	-0.66404838	-2.26219652	-0.23626568

### Proline 4, *exo*

C	0.00105511	0.76002756	-0.52711773
C	-0.23134838	2.28386434	-0.52509945
C	-1.75602256	2.43768443	-0.51321494
C	-2.21159790	1.24794541	0.32629944
H	0.20734805	0.36694320	-1.52153779
H	0.19095664	2.71125481	0.38719270
H	0.24139610	2.76676926	-1.38196283
H	-2.08325606	3.39159140	-0.09575895
H	-2.16064681	2.34860441	-1.52602811
H	-2.10691527	1.45128746	1.39811206
H	-3.23860076	0.94897576	0.11870497
C	-1.45724349	-1.11350271	0.03628823
C	1.09642554	0.39588134	0.48590399
O	0.82764826	0.45805739	1.67631115
C	-2.77445170	-1.55735134	0.61791908
H	-3.60178579	-1.26680916	-0.03742953
H	-2.77390789	-2.63876321	0.72459121
H	-2.93722639	-1.09400673	1.59554862
C	3.34191940	-0.34522972	0.95482797
H	3.04105570	-0.06023002	1.96010668
H	3.43006934	-1.43686257	0.90666312
H	4.31103104	0.10222292	0.71933276
N	-1.26945623	0.20060978	-0.07136119
N	2.33951135	0.12836001	0.01137111
C	2.60813957	-0.12443629	-1.39793649
H	2.28078301	0.70940108	-2.02190161
H	3.68735432	-0.21918417	-1.52513627
H	2.12732393	-1.04734407	-1.73827874
S	-0.30895814	-2.21786059	-0.43820948

### Proline 5, *endo*

C	-0.16217581	-0.22435164	0.93585695
H	0.04827783	0.47382915	1.74199962
C	-2.34086161	-0.93881132	0.08643290
H	-2.59937525	-1.03272411	-0.97048636
H	-3.26079336	-0.76781118	0.65695035
C	-1.58381577	-2.17650484	0.58739591
H	-1.14190038	-2.70108174	-0.25779650
H	-2.24335701	-2.86458272	1.12056102
C	-0.47767893	-1.62151266	1.49656229
H	-0.84516688	-1.50715465	2.52059858
H	0.40472485	-2.26251174	1.52127537
N	-1.40627367	0.16774978	0.29752391
C	-1.50462947	1.41932848	-0.21106716
C	-2.76125387	1.74368631	-0.98433797
H	-2.74535315	1.21569911	-1.94242969
H	-3.65998842	1.43536207	-0.44463460
H	-2.78685253	2.81629813	-1.16758262
C	0.99124474	-0.24214504	-0.06973476
N	2.12457111	0.36944613	0.28294199
C	3.26868207	0.32031428	-0.62142214
H	3.08097006	0.92609078	-1.51317421
H	4.14822861	0.69305744	-0.09730151
H	3.43762737	-0.70604020	-0.94672087
C	2.20572617	1.29341683	1.41952098
H	3.16107819	1.81222471	1.36848889
H	1.40516914	2.03275424	1.36042159
H	2.16087390	0.76190677	2.37378731
S	0.80551047	-1.04717673	-1.51307940
O	-0.60370845	2.23634437	-0.04814990

### Proline 5, *exo*

C	0.19084728	-0.44768470	-0.79989052
C	0.58127469	-1.92802372	-0.99718942
C	2.11183376	-1.93928074	-0.88635545
C	2.39423223	-0.83828615	0.13538348
H	0.01639571	0.03710053	-1.75901626
H	0.14549220	-2.52232876	-0.19357761
H	0.22011338	-2.31302234	-1.95283518
H	2.50133281	-2.90955306	-0.57258474
H	2.57156178	-1.67843116	-1.84458156
H	2.25940480	-1.20383425	1.15955602
H	3.39440049	-0.41439035	0.03461401
C	1.36333947	1.46799667	0.11733641
C	-1.02470229	-0.29748622	0.11779762
C	2.55792123	2.00393206	0.87302946
H	3.47090536	1.90876626	0.27857910
H	2.37882058	3.05479888	1.09237031
H	2.70078233	1.45129938	1.80533977
C	-3.32631221	0.33403728	0.43959520
H	-3.47735887	-0.59141767	0.99449287
H	-3.20144805	1.14353565	1.16533013
H	-4.19043849	0.53274326	-0.19398474
N	1.37326219	0.15063574	-0.19198672
N	-2.14131879	0.21243187	-0.40288151
C	-2.17218143	0.88304266	-1.70669317
H	-2.03834311	0.17217529	-2.52607589
H	-3.14713104	1.35207767	-1.82532050
H	-1.40373326	1.65693674	-1.74674898
S	-0.89808803	-0.80894821	1.69526110
O	0.42023528	2.18227738	-0.20806323

### Proline 6, *endo*

C	-0.01192970	0.39724909	-0.89237056
H	0.09387329	-0.35903276	-1.66597001
C	-2.03150823	1.51698495	-0.11573889
H	-2.30611979	1.64985670	0.93199632
H	-2.94236667	1.52480370	-0.72360253
C	-1.02797307	2.57876570	-0.57737362
H	-0.50139520	2.98250748	0.28630261
H	-1.52043713	3.39936758	-1.10272363
C	-0.04934445	1.81698335	-1.48013097
H	-0.43079024	1.76244433	-2.50390749
H	0.94063600	2.27528701	-1.50917056
N	-1.32769167	0.24094466	-0.29760518
C	-1.76519131	-0.94995928	0.10983150
C	-3.10808221	-0.96371045	0.78765505
H	-3.02740075	-0.45494878	1.75400985
H	-3.86272782	-0.43961411	0.19415495
H	-3.42171295	-1.99077174	0.95391300
C	1.08655033	0.24506586	0.15831726
N	2.22542900	-0.32698520	-0.23854636
C	3.31186397	-0.47415680	0.72465341
H	3.00658242	-1.13035843	1.54453502
H	4.18053965	-0.89190288	0.21740222
H	3.56351362	0.49692145	1.15356875
C	2.35617110	-0.99569884	-1.53466357
H	3.36317102	-1.40003641	-1.61506766
H	1.63892186	-1.81729506	-1.61511618
H	2.20992355	-0.29505408	-2.36002782
S	-0.87592113	-2.34311930	-0.07540671
S	0.85991650	0.85946229	1.68448180

### Proline 6, *exo*

C	0.06442536	-0.60865592	-0.74283963
C	0.22394078	-2.12890660	-0.96075300
C	1.73457843	-2.37501681	-0.86775460
C	2.19384380	-1.33211726	0.14707479
H	-0.05882461	-0.07619537	-1.68470601
H	-0.29040114	-2.66190864	-0.15969817
H	-0.20163459	-2.44263838	-1.91576737
H	1.97532976	-3.39241636	-0.55448339
H	2.21793776	-2.18937932	-1.83159834
H	2.00237057	-1.66033162	1.17412093
H	3.24602423	-1.07102969	0.04065973
C	1.60193909	1.09443541	0.08130504
C	-1.09267706	-0.31695759	0.21029084
C	2.90663526	1.38640611	0.77399414
H	3.75369020	1.09388344	0.14552267
H	2.97323575	2.45096601	0.98139017
H	2.96980853	0.82655617	1.71203818
C	-3.36478412	0.38497365	0.56024129
H	-3.55931434	-0.48038184	1.19485458
H	-3.13556461	1.23251595	1.21251859
H	-4.24314345	0.60742205	-0.04427904
N	1.33668312	-0.18710641	-0.16590323
N	-2.23800831	0.10690848	-0.32426851
C	-2.35113641	0.50446776	-1.72813721
H	-2.13173280	-0.33204159	-2.39577164
H	-3.37499293	0.82139183	-1.91604926
H	-1.67670396	1.33794911	-1.94316204
S	0.55453310	2.31766285	-0.33156691
S	-0.89905739	-0.64445540	1.82792739

## Set $\omega$ B97X-V /6-311+G(2d,p)

### Proline 1, *endo*

C	0.03372990	0.01106943	-0.03564318
H	1.12054779	-0.08812895	-0.05210496
C	-1.46547080	1.92835009	0.04966935
H	-2.31242766	2.13754726	-0.60934461
H	-1.10659833	2.87855430	0.46599269
C	-1.83632461	0.93498847	1.15808216
H	-2.62303228	0.26534673	0.80008443
H	-2.19227228	1.43640464	2.06105242
C	-0.54139640	0.14502995	1.38353686
H	0.16123997	0.71897612	1.99649761
H	-0.69906046	-0.82321332	1.86470159
N	-0.38862881	1.24456267	-0.67358064
C	0.04194475	1.50965145	-1.93827765
O	0.83582087	0.76546112	-2.49623449
C	-0.50607644	2.75520763	-2.59733702
H	-1.55126794	2.59303646	-2.88148852
H	-0.46659457	3.61966701	-1.92815160
H	0.07816724	2.95228725	-3.49537349
C	-0.56919724	-1.19393159	-0.75023947
O	0.20456131	-2.27712674	-0.60630431
C	-0.29421278	-3.46371766	-1.24050259
H	-0.41649371	-3.29011552	-2.31123900
H	0.45625986	-4.23138712	-1.05693905
H	-1.25532266	-3.74970938	-0.80783502
O	-1.63124601	-1.19225301	-1.32075630

### Proline 1, *exo*

C	-0.01607159	-0.00389190	0.05628326
C	1.52397586	-0.03497666	0.13076302
C	1.92990635	1.43589199	-0.01944054
C	0.82660874	2.17153012	0.74148174
H	-0.39211548	-0.22147393	-0.94787073
H	1.82903575	-0.40256689	1.11621192
H	1.95656177	-0.68749389	-0.63018370
H	2.92553412	1.64478190	0.37898850
H	1.91144376	1.73190169	-1.07380683
H	1.03157146	2.18382659	1.82076572
H	0.69165448	3.20075095	0.40043327
C	-1.65624111	1.70267537	0.61069065
C	-0.62592640	-1.00379090	1.02976441
O	-2.54704655	0.89905402	0.37182333
O	-0.64595498	-0.85456981	2.22507424
C	-1.93602543	3.10880043	1.09288357
H	-1.60421434	3.84534439	0.35393971
H	-3.01009556	3.20868883	1.24316906
H	-1.41212503	3.31123292	2.03208658
N	-0.35073108	1.35959609	0.44394265
O	-1.06557087	-2.09668537	0.39691619
H	-2.52966313	-2.65637295	1.75769829
H	-1.96272823	-3.89751413	0.59176252
H	-0.94129056	-3.43063344	1.99308513
C	-1.66256040	-3.08359838	1.25025442

### Proline 2, *endo*

C	0.01125632	-0.00439050	-0.07360662
H	1.09894331	-0.08377832	-0.11214481
C	-1.49048623	1.90718711	0.00792777
H	-2.34364590	2.12498393	-0.63875298
H	-1.10418290	2.85368100	0.40664939
C	-1.84604969	0.92809819	1.12962890
H	-2.63087321	0.24794563	0.78795515
H	-2.19692450	1.44155311	2.02764746
C	-0.54220390	0.15477843	1.35104061
H	0.16464225	0.74623870	1.94223028
H	-0.68248594	-0.80606571	1.85145551
N	-0.43514408	1.20861059	-0.74335226
C	0.03787851	1.57178191	-1.94306719
S	1.16195134	0.67244201	-2.76929037
C	-0.52234699	2.85068438	-2.51040466
H	-1.57544650	2.70649933	-2.77838681
H	-0.47012812	3.66662266	-1.78149927
H	0.03247098	3.12320583	-3.40534345
C	-0.58981914	-1.23205313	-0.75021777
O	0.18860791	-2.30434663	-0.57484052
C	-0.30115585	-3.51126138	-1.17746318
H	-0.42621895	-3.36437646	-2.25192615
H	0.45688530	-4.26691612	-0.97650417
H	-1.25861758	-3.79480177	-0.73533728
O	-1.66025776	-1.24976549	-1.30413236

### Proline 2, *exo*

C	-0.07838646	0.00547405	0.06476855
C	1.46384260	-0.04987035	0.09577983
C	1.89019422	1.41877590	0.01053857
C	0.80808420	2.13235572	0.81653292
H	-0.49203207	-0.18576573	-0.92941178
H	1.79487539	-0.47525209	1.04900673
H	1.86114999	-0.66764862	-0.71150163
H	2.89193850	1.59516809	0.40906190
H	1.86598156	1.76629707	-1.02774584
H	1.00654859	2.07048866	1.89465715
H	0.69360119	3.18129670	0.54027033
C	-1.66009101	1.81008187	0.55674780
C	-0.65792345	-1.00815065	1.04335926
S	-2.95793448	0.87049307	0.12610082
O	-0.71488125	-0.83627689	2.23412543
C	-1.83974445	3.22280202	1.05339905
H	-1.40778418	3.93737841	0.34351744
H	-2.90175032	3.43246476	1.15894703
H	-1.34264967	3.36152494	2.01947284
N	-0.39833269	1.36663292	0.48445926
O	-0.98929108	-2.14423686	0.42279505
H	-2.45659657	-2.78586953	1.74267650
H	-1.74895326	-4.00578663	0.63213003
H	-0.82247933	-3.42631989	2.05744012
C	-1.53945441	-3.15554993	1.27958905

### Proline 3, *endo*

C	0.07197830	0.44694218	0.79207817
H	-0.20219529	-0.12119369	1.68031735
C	2.30003818	0.96756679	-0.06659845
H	2.68262658	0.85232857	-1.08392745
H	3.14713949	0.91887908	0.63066822
C	1.50730765	2.26824387	0.10169107
H	1.03762495	2.53284469	-0.84711823
H	2.14140919	3.09577605	0.42991144
C	0.42552162	1.90607141	1.12747396
H	0.82939163	1.94958563	2.14502695
H	-0.44533602	2.56432886	1.07791498
N	1.32100803	-0.07635793	0.24960982
C	1.37173859	-1.37806749	-0.12525883
O	0.42083417	-2.12677007	0.07880964
C	2.63791959	-1.84880986	-0.80505120
H	2.67375804	-1.45495082	-1.82630181
H	3.53429785	-1.50787724	-0.27925460
H	2.62079585	-2.93734924	-0.84531608
C	-1.01919125	0.37877701	-0.28766631
N	-2.23489061	-0.11805797	0.06002956
C	-3.24112596	-0.23381056	-0.98672228
H	-3.21699255	-1.23015272	-1.44578481
H	-4.23211031	-0.06119452	-0.55790067
H	-3.03866945	0.50882717	-1.75653250
C	-2.44336600	-0.92506459	1.26137832
H	-3.46744089	-1.30147536	1.23955724
H	-1.75575795	-1.77598913	1.28886049
H	-2.33309795	-0.32889841	2.17202794
O	-0.77901548	0.82694831	-1.40252192

### Proline 3, *exo*

C	0.10930738	-0.68227516	-0.54135503
C	0.57730591	-2.14225470	-0.38376148
C	2.10723223	-2.05497431	-0.43768653
C	2.39503588	-0.74166849	0.28942477
H	-0.13625558	-0.44576702	-1.57819459
H	0.26171667	-2.50826540	0.59732384
H	0.15361022	-2.79203622	-1.15333526
H	2.59774873	-2.91037988	0.03304857
H	2.45508412	-1.98622467	-1.47432779
H	2.37774179	-0.88189495	1.37845232
H	3.35277724	-0.29929197	0.00516205
C	1.18105031	1.44654398	-0.05174208
C	-1.05605396	-0.38673034	0.41568319
O	0.15432747	2.02468350	-0.39529413
O	-0.86070321	-0.49900801	1.61827450
C	2.38701791	2.18977445	0.47837105
H	3.24867381	2.05705762	-0.18364083
H	2.13606812	3.24806098	0.53600442
H	2.66303847	1.82209158	1.47139490
C	-3.33383466	0.27895096	0.81295932
H	-3.14697864	-0.19988721	1.77244686
H	-3.36658225	1.36551898	0.96303774
H	-4.29429564	-0.05668154	0.41226063
N	1.27969225	0.09831347	-0.14084540
N	-2.27076249	-0.08537980	-0.11400452
C	-2.43761253	0.35875716	-1.49620004
H	-2.17638690	-0.43094249	-2.20584769
H	-3.49212814	0.59561308	-1.64791581
H	-1.83853453	1.25229641	-1.69859299

### Proline 4, *endo*

C	0.07863133	0.58426401	-0.71162139
H	0.26048400	-0.05746154	-1.57290832
C	-2.00675230	1.51367928	0.13855140
H	-2.38683147	1.46692685	1.16160355
H	-2.85783276	1.61678627	-0.54659189
C	-0.98960512	2.64207065	-0.04931138
H	-0.47370757	2.82924362	0.89458505
H	-1.46418674	3.56784799	-0.38364867
C	-0.00313268	2.07496719	-1.07783249
H	-0.40074882	2.17538720	-2.09376078
H	0.97497783	2.56181317	-1.04367611
N	-1.25175538	0.29473989	-0.18860049
C	-1.65820455	-0.95329376	0.05001414
C	-3.03728041	-1.09638294	0.63987125
H	-3.03966893	-0.71171825	1.66613018
H	-3.77679002	-0.52735415	0.06629233
H	-3.31774178	-2.14722128	0.65736141
C	1.11399098	0.35573855	0.40144941
N	2.33958656	-0.10215055	0.03628873
C	3.29709861	-0.41756525	1.08717275
H	3.33423792	-1.49983941	1.26253757
H	4.29281735	-0.06874226	0.79698123
H	2.98702445	0.07861221	2.00499533
C	2.61757546	-0.65667695	-1.28396260
H	3.68645355	-0.87131502	-1.34149192
H	2.05969011	-1.58439157	-1.45644063
H	2.38647564	0.06025746	-2.07606542
O	0.82880835	0.66905953	1.54946169
S	-0.70861361	-2.28538094	-0.26358393

### Proline 4, *exo*

C	0.00148212	0.74796077	-0.52717141
C	-0.22963552	2.27405432	-0.53749021
C	-1.75440351	2.43117507	-0.50794998
C	-2.20162824	1.24758470	0.34524605
H	0.20692444	0.34397896	-1.51971963
H	0.20502384	2.71043425	0.36661726
H	0.23365793	2.74853444	-1.40579936
H	-2.07439763	3.38942592	-0.09218195
H	-2.17212619	2.33552061	-1.51608571
H	-2.07493338	1.45533978	1.41542736
H	-3.23471559	0.95241485	0.15741301
C	-1.47624822	-1.12234922	0.02458796
C	1.10091502	0.39424999	0.48863404
O	0.83198793	0.45786087	1.67978856
C	-2.79873942	-1.55385988	0.60770031
H	-3.62451886	-1.24819482	-0.04469689
H	-2.81115659	-2.63695901	0.70595825
H	-2.95324293	-1.09512593	1.59008668
C	3.35339635	-0.32875546	0.96062700
H	3.04502977	-0.04741107	1.96583064
H	3.45619804	-1.42008747	0.91223711
H	4.31765967	0.13214553	0.72709352
N	-1.27055960	0.19275745	-0.06464613
N	2.34613959	0.13142616	0.01481714
C	2.61866142	-0.12012464	-1.39511198
H	2.28249054	0.71051411	-2.02082708
H	3.70002034	-0.20326660	-1.52062168
H	2.14796996	-1.04981962	-1.73570576
S	-0.35065126	-2.24152406	-0.47585714

### Proline 5, *endo*

C	-0.15593180	-0.23529515	0.91668558
H	0.05224011	0.46635385	1.72332089
C	-2.35292496	-0.93727268	0.09347101
H	-2.64565951	-1.03178154	-0.95608717
H	-3.25435142	-0.75380002	0.69215164
C	-1.59399672	-2.17989938	0.57897477
H	-1.15562620	-2.69748830	-0.27443703
H	-2.25092803	-2.87295469	1.11100871
C	-0.48160741	-1.62973803	1.48451047
H	-0.84761941	-1.50761664	2.50968569
H	0.39675690	-2.27867633	1.51087515
N	-1.39831557	0.15960033	0.27219197
C	-1.50730444	1.41945032	-0.21572798
C	-2.77389883	1.75216775	-0.96955345
H	-2.77546350	1.22822851	-1.93122862
H	-3.66654698	1.44514784	-0.41682335
H	-2.79676869	2.82670502	-1.14676267
C	1.01045174	-0.25798275	-0.07943736
N	2.13461487	0.36972320	0.28070866
C	3.29514902	0.31455690	-0.60365756
H	3.12081665	0.91088004	-1.50595204
H	4.16459457	0.69649115	-0.06746816
H	3.47297111	-0.71582096	-0.91501374
C	2.19616162	1.31078968	1.40620300
H	3.14363662	1.84533099	1.34920836
H	1.38267377	2.03666137	1.33419108
H	2.15837437	0.79084743	2.36859379
S	0.85440665	-1.08669829	-1.51648773
O	-0.60640455	2.23719036	-0.05074388

### Proline 5, *exo*

C	0.18619768	-0.45155796	-0.77826706
C	0.58121197	-1.93098198	-0.98277800
C	2.11355129	-1.93276658	-0.89380653
C	2.40020023	-0.84273820	0.13942128
H	0.01549473	0.03812610	-1.73813079
H	0.16052283	-2.52810598	-0.17071979
H	0.20684115	-2.31832175	-1.93389753
H	2.51498444	-2.90509136	-0.59819874
H	2.55854163	-1.65432811	-1.85549492
H	2.27788375	-1.22283275	1.16168558
H	3.39781279	-0.41043857	0.03443270
C	1.37238063	1.46852753	0.12186701
C	-1.03965343	-0.30548359	0.13223410
C	2.57647895	2.00925045	0.85942239
H	3.47998471	1.92096051	0.24750541
H	2.39432919	3.05978577	1.08221182
H	2.74000234	1.45626321	1.78934762
C	-3.34946546	0.32506840	0.42343251
H	-3.50062811	-0.60068710	0.97992144
H	-3.24329781	1.13966167	1.14833676
H	-4.20569935	0.51385304	-0.22547934
N	1.36894814	0.14503250	-0.16532195
N	-2.14988184	0.21081080	-0.40066059
C	-2.16520806	0.89233220	-1.70073710
H	-2.03482913	0.18582267	-2.52614813
H	-3.13530326	1.37350713	-1.82002497
H	-1.38739846	1.65928376	-1.72957052
S	-0.93512377	-0.82869403	1.71052124
O	0.43222222	2.18484221	-0.21020388



### Proline 6, *endo*

C	-0.00874320	0.38645952	-0.87061550
H	0.09516403	-0.38007198	-1.63749422
C	-2.03113412	1.51531573	-0.10657551
H	-2.31120491	1.65878176	0.94013620
H	-2.94043520	1.51789941	-0.71951373
C	-1.02505441	2.57201221	-0.57606872
H	-0.49424201	2.97971000	0.28523808
H	-1.51649996	3.39198857	-1.10563111
C	-0.05088954	1.80050414	-1.47650997
H	-0.44050868	1.73213902	-2.49796799
H	0.93961944	2.26068935	-1.51862283
N	-1.32699908	0.23497328	-0.27459894
C	-1.78878003	-0.95746280	0.10877612
C	-3.13977679	-0.95512443	0.77382919
H	-3.06453152	-0.44608813	1.74193622
H	-3.88244784	-0.42173749	0.17116595
H	-3.46792563	-1.97934619	0.93622735
C	1.10020626	0.24477019	0.17587772
N	2.23901979	-0.32262256	-0.23398463
C	3.33941854	-0.46233213	0.71597404
H	3.04717330	-1.11770310	1.54283736
H	4.20341878	-0.87891114	0.19783101
H	3.59332268	0.51219936	1.13898086
C	2.36397981	-0.98544658	-1.53546101
H	3.37526470	-1.37945144	-1.62617766
H	1.65372429	-1.81519781	-1.61376190
H	2.20335722	-0.28220050	-2.35774507
S	-0.92729521	-2.36860104	-0.09264170
S	0.88929930	0.85885476	1.70796038

### Proline 6, *exo*

C	0.06052227	-0.60074220	-0.72504671
C	0.22191366	-2.12099609	-0.95364126
C	1.73414511	-2.36359934	-0.87152043
C	2.19236445	-1.33271451	0.15674660
H	-0.06131392	-0.06156745	-1.66588116
H	-0.28567428	-2.66084400	-0.15032955
H	-0.21030870	-2.43093795	-1.90854041
H	1.98025738	-3.38546943	-0.57358548
H	2.21288928	-2.16092926	-1.83569982
H	1.99646809	-1.67350864	1.18074307
H	3.24633791	-1.07128785	0.05675131
C	1.62172805	1.10211676	0.07927835
C	-1.10608963	-0.31700923	0.22560234
C	2.93635997	1.38107399	0.76285271
H	3.77453849	1.08835845	0.12048506
H	3.01162425	2.44502705	0.97584224
H	3.00746569	0.81373336	1.69709830
C	-3.39035427	0.37030797	0.55086788
H	-3.57722504	-0.49496223	1.18984838
H	-3.18169883	1.22708581	1.20016573
H	-4.26632267	0.57451785	-0.06522219
N	1.33579500	-0.18167424	-0.14641422
N	-2.24934138	0.10416421	-0.32063689
C	-2.35309702	0.50175220	-1.72702089
H	-2.13374628	-0.33704058	-2.39401143
H	-3.37550977	0.82405149	-1.91964562
H	-1.67438183	1.33417129	-1.93915758
S	0.59770969	2.34162374	-0.35162332
S	-0.92805568	-0.64870116	1.84689497

## Set M06-2X/6-311+G(2d,p)

### Proline 1, *endo*

C	0.04904241	0.02001494	0.00206103
H	1.13148394	-0.09268045	-0.00197780
C	-1.44279374	1.93865455	0.06353648
H	-2.27013400	2.15295061	-0.61302151
H	-1.08965189	2.88142448	0.49217779
C	-1.83996661	0.93922876	1.15477535
H	-2.60745565	0.26856764	0.76874468
H	-2.22147361	1.43151983	2.04777818
C	-0.54874248	0.15487842	1.40878318
H	0.13858834	0.73309100	2.02878615
H	-0.71150936	-0.81051864	1.88620480
N	-0.35284148	1.25726522	-0.63931120
C	0.04448648	1.47139022	-1.92336436
O	0.81331736	0.70205459	-2.47076422
C	-0.51677957	2.69154413	-2.61108973
H	-1.55051902	2.49539590	-2.90461717
H	-0.50930114	3.56594684	-1.95966583
H	0.07196748	2.88341651	-3.50349812
C	-0.56421413	-1.16935135	-0.72496659
O	0.20882604	-2.25201448	-0.62755934
C	-0.29449078	-3.41483388	-1.28742061
H	-0.44065013	-3.20479511	-2.34566329
H	0.45943212	-4.18357352	-1.14764473
H	-1.24345794	-3.71915117	-0.84818744
O	-1.63651393	-1.15386777	-1.26583047

### Proline 1, *exo*

C	-0.02148377	-0.00323067	0.05990996
C	1.51638643	-0.03435839	0.13838963
C	1.91915022	1.43418556	-0.02408983
C	0.82198184	2.16735875	0.74429964
H	-0.39568768	-0.21679565	-0.94262018
H	1.81438426	-0.38678159	1.12802991
H	1.95056947	-0.69374725	-0.61036581
H	2.91488421	1.64544940	0.36275859
H	1.88633208	1.72349182	-1.07620430
H	1.03291441	2.17317260	1.81929065
H	0.68284569	3.19456792	0.40929254
C	-1.65723380	1.70199672	0.62269269
C	-0.62908501	-1.00469418	1.02807350
O	-2.54991605	0.90489941	0.39635586
O	-0.65826395	-0.85426455	2.21764947
C	-1.92311184	3.11291700	1.09008405
H	-1.60096938	3.83265673	0.33525170
H	-2.99109620	3.21878419	1.25568843
H	-1.38193626	3.32651918	2.01297507
N	-0.35438715	1.35674100	0.45126797
O	-1.05381177	-2.09933333	0.39604140
H	-2.52585569	-2.66181255	1.73328445
H	-1.93665356	-3.90226534	0.58562713
H	-0.94022236	-3.42067915	1.99270511
C	-1.65180260	-3.08427059	1.24032876

### Proline 2, *endo*

C	0.02136743	0.00006784	-0.05398604
H	1.10552211	-0.08783833	-0.08587584
C	-1.47355998	1.91230560	0.01497669
H	-2.31266130	2.14036192	-0.64099883
H	-1.08575991	2.84970311	0.42516698
C	-1.84727226	0.92699106	1.12177769
H	-2.61466420	0.24428455	0.75709710
H	-2.21905891	1.43070305	2.01244373
C	-0.54408847	0.16215924	1.36339410
H	0.15084938	0.75973371	1.95597801
H	-0.68470482	-0.79533016	1.86270518
N	-0.41461448	1.21267271	-0.72810286
C	0.03797848	1.55125360	-1.94108877
S	1.13315787	0.62703229	-2.77868002
C	-0.52857946	2.82165303	-2.51438152
H	-1.56842375	2.65461032	-2.80870248
H	-0.51402367	3.63174107	-1.78221834
H	0.03975175	3.10794113	-3.39278536
C	-0.58892191	-1.22040734	-0.73006655
O	0.18632222	-2.29363475	-0.57735172
C	-0.30210532	-3.48437739	-1.19756124
H	-0.44609743	-3.31098538	-2.26275969
H	0.46033241	-4.23900302	-1.02986082
H	-1.24856968	-3.78382374	-0.74981100
O	-1.66552741	-1.23125681	-1.26104318

### Proline 2, *exo*

C	-0.06071980	0.00161492	0.06479346
C	1.47872853	-0.04222267	0.11053338
C	1.89107663	1.42687570	0.00176160
C	0.80715216	2.13588641	0.80540186
H	-0.46578164	-0.19196707	-0.92946576
H	1.80003568	-0.44133489	1.07470101
H	1.88766694	-0.67111332	-0.67731579
H	2.88989793	1.61709519	0.39150451
H	1.85419597	1.75900617	-1.03725999
H	1.00867364	2.07740883	1.88023135
H	0.68230248	3.17972195	0.52671041
C	-1.65667732	1.78730355	0.57024777
C	-0.64206395	-1.01089983	1.03932490
S	-2.95248263	0.83346487	0.16254448
O	-0.68979592	-0.84125042	2.22565497
C	-1.83945649	3.19966660	1.06005517
H	-1.44664515	3.90987785	0.32797628
H	-2.89664197	3.39414918	1.20379501
H	-1.30750028	3.35539101	2.00117557
N	-0.39247920	1.35881549	0.48212764
O	-0.98833689	-2.13833893	0.42016182
H	-2.48356118	-2.74628509	1.70768696
H	-1.77427883	-3.98369636	0.62620088
H	-0.87015780	-3.40541452	2.06041089
C	-1.56521937	-3.13324758	1.26775805

### Proline 3, *endo*

C	0.07150996	0.43476094	0.79431581
H	-0.20740105	-0.13158845	1.67846407
C	2.23529118	0.95413702	-0.20634145
H	2.45371523	0.84353137	-1.26919607
H	3.17456647	0.89551196	0.35057880
C	1.48873275	2.26486469	0.07793824
H	0.99395503	2.60648306	-0.82762116
H	2.16338840	3.04430001	0.42952701
C	0.43986187	1.88658988	1.13129285
H	0.87578760	1.91019949	2.13180112
H	-0.42735233	2.54584833	1.11846147
N	1.31513684	-0.08995295	0.24980619
C	1.42896277	-1.41734078	0.00630460
O	0.55131177	-2.20147067	0.33599673
C	2.68771467	-1.86434818	-0.69729810
H	2.66257363	-1.52944320	-1.73630017
H	3.57941292	-1.44335213	-0.23185743
H	2.72837763	-2.94935638	-0.67058243
C	-1.01617153	0.39802368	-0.28656191
N	-2.20768687	-0.16715915	0.01781376
C	-3.27936143	-0.10119653	-0.96146382
H	-3.40459005	-1.06476047	-1.46251601
H	-4.21320523	0.15911502	-0.46023406
H	-3.03606897	0.65403598	-1.70225825
C	-2.43163676	-1.02051011	1.17928538
H	-3.29394908	-1.65054980	0.96626529
H	-1.57597438	-1.67211756	1.34745178
H	-2.65191174	-0.43800837	2.07723781
O	-0.79078927	0.93485329	-1.36091003

### Proline 3, *exo*

C	0.10689773	-0.69281636	-0.54317139
C	0.58374115	-2.14668552	-0.37500290
C	2.11117149	-2.04949705	-0.43837158
C	2.38930221	-0.73566362	0.28711506
H	-0.14070403	-0.46322313	-1.57807173
H	0.27915886	-2.50064667	0.61045530
H	0.16078602	-2.80532506	-1.13194658
H	2.60845906	-2.89802218	0.02889997
H	2.45039486	-1.97526413	-1.47358447
H	2.36467551	-0.87561179	1.37303922
H	3.34231557	-0.28758158	0.00814507
C	1.16058310	1.43960381	-0.04637937
C	-1.05472223	-0.39387477	0.41527743
O	0.13073519	2.01076218	-0.37445155
O	-0.85869283	-0.51002379	1.61215742
C	2.36834103	2.18093276	0.47441413
H	3.21148024	2.06787568	-0.20957721
H	2.11094167	3.23250822	0.56016142
H	2.66955033	1.79253444	1.44854722
C	-3.32674285	0.28274788	0.80749695
H	-3.13976571	-0.19062917	1.76628354
H	-3.36197493	1.36688933	0.95071287
H	-4.28211350	-0.05665871	0.40699321
N	1.27258822	0.09518721	-0.14872426
N	-2.26261871	-0.07939582	-0.11506754
C	-2.42046385	0.36920614	-1.49482038
H	-2.20538513	-0.43148387	-2.20299772
H	-3.45989724	0.65880247	-1.63544974
H	-1.78074123	1.22935312	-1.70098240

### Proline 4, *endo*

C	0.07860627	0.59378251	-0.73623926
H	0.26770606	-0.04589848	-1.59370220
C	-2.00579364	1.51111747	0.11869081
H	-2.38324640	1.45414084	1.13877984
H	-2.85463452	1.61540115	-0.56375153
C	-0.99237762	2.64171508	-0.06186255
H	-0.47782078	2.82043747	0.88044617
H	-1.46693898	3.56543958	-0.38965980
C	-0.00732035	2.08320813	-1.09479429
H	-0.40803352	2.18728005	-2.10514319
H	0.96719069	2.56970150	-1.05847489
N	-1.24931299	0.29696282	-0.21561132
C	-1.63224912	-0.94890357	0.05938815
C	-2.99858063	-1.09374794	0.67149942
H	-2.97317424	-0.72597378	1.70065188
H	-3.74342880	-0.51065540	0.12570698
H	-3.28408674	-2.14015168	0.68036443
C	1.10044863	0.36478379	0.38757415
N	2.32401143	-0.10347244	0.03895772
C	3.25669623	-0.45251986	1.09803728
H	3.29033504	-1.53776866	1.23022359
H	4.25518833	-0.09425090	0.84407437
H	2.92458007	0.00785623	2.02316068
C	2.61797614	-0.63665132	-1.28325060
H	3.68445123	-0.85039441	-1.32945040
H	2.06277186	-1.55878484	-1.47628462
H	2.39678372	0.09221882	-2.06264950
O	0.80059945	0.68194778	1.52544760
S	-0.66534682	-2.27491996	-0.22832893

### Proline 4, *exo*

C	0.00564439	0.76514840	-0.52120072
C	-0.23642176	2.28633078	-0.51502575
C	-1.76096781	2.42551182	-0.52551294
C	-2.20679338	1.24623382	0.33045971
H	0.20961043	0.37088504	-1.51496969
H	0.16319087	2.70511933	0.40978901
H	0.24773209	2.77774700	-1.35736141
H	-2.10323790	3.38065646	-0.13052787
H	-2.15087521	2.30777393	-1.53859818
H	-2.09022965	1.46219140	1.39732408
H	-3.23170713	0.93912955	0.13543150
C	-1.45345304	-1.11470632	0.04171622
C	1.10477488	0.40693125	0.49060007
O	0.83882548	0.47124012	1.67689286
C	-2.77644853	-1.54826358	0.61598951
H	-3.59167688	-1.27647355	-0.05930869
H	-2.77473586	-2.62471869	0.74809098
H	-2.95538047	-1.06077103	1.57694675
C	3.34287437	-0.35356658	0.94766800
H	3.04282797	-0.08364583	1.95509298
H	3.42343318	-1.44253024	0.87829299
H	4.31209867	0.09110825	0.71940926
N	-1.26175835	0.19916387	-0.06200752
N	2.34466804	0.13776414	0.01131854
C	2.60716452	-0.11587065	-1.39759574
H	2.28726892	0.72141555	-2.01737051
H	3.68297391	-0.22246325	-1.52457925
H	2.11557889	-1.03244761	-1.73514219
S	-0.31438062	-2.23099338	-0.43762200

### Proline 5, *endo*

C	-0.15912703	-0.23899326	0.94243942
H	0.05538253	0.45066617	1.75386746
C	-2.34786853	-0.92985315	0.09826081
H	-2.60671827	-1.01294642	-0.95816539
H	-3.26360312	-0.75556455	0.67005480
C	-1.60105341	-2.17730070	0.58806718
H	-1.17316964	-2.70355431	-0.26082220
H	-2.26253632	-2.85649171	1.12470147
C	-0.48178772	-1.63910226	1.49138179
H	-0.83863999	-1.53294311	2.51742672
H	0.39470241	-2.28558822	1.49828132
N	-1.40489349	0.16699922	0.31562101
C	-1.48316642	1.41408405	-0.20646037
C	-2.73181001	1.74144556	-0.98557564
H	-2.70983165	1.20708806	-1.93812271
H	-3.63185871	1.43746284	-0.44987595
H	-2.75102869	2.81086981	-1.17443091
C	0.99248497	-0.24727322	-0.06932170
N	2.12021108	0.37480379	0.28279351
C	3.26141059	0.33672540	-0.62451589
H	3.04075344	0.89816585	-1.53513740
H	4.12496412	0.76398151	-0.12222247
H	3.46924433	-0.69243903	-0.91132990
C	2.19296353	1.30189018	1.41711939
H	3.14250889	1.82613214	1.36668123
H	1.38575353	2.03141841	1.35177162
H	2.14905234	0.77187067	2.36974104
S	0.81086571	-1.05305827	-1.51818415
O	-0.57370446	2.21660454	-0.05164410

### Proline 5, *exo*

C	0.18391875	-0.45600243	-0.77376418
C	0.58398080	-1.93361074	-0.97242572
C	2.11512062	-1.92406890	-0.89344443
C	2.39335397	-0.84070146	0.14629165
H	0.01854298	0.02917618	-1.73346574
H	0.17593148	-2.52566262	-0.15451930
H	0.20590583	-2.32694047	-1.91531865
H	2.52477333	-2.89212334	-0.60884100
H	2.54929360	-1.63086749	-1.85149106
H	2.26196236	-1.22740307	1.16198027
H	3.38668665	-0.40455535	0.05174875
C	1.36686339	1.46690694	0.11502794
C	-1.04221057	-0.30367159	0.13399768
C	2.57149101	2.00554368	0.84765021
H	3.46442288	1.93471389	0.22368737
H	2.38220463	3.04778661	1.08727125
H	2.75060493	1.43902296	1.76248989
C	-3.34640002	0.32664528	0.42242646
H	-3.52992776	-0.62352970	0.92030902
H	-3.21577892	1.08792767	1.19489745
H	-4.18889604	0.58123868	-0.21517194
N	1.36312269	0.14312125	-0.16071180
N	-2.14534327	0.22342201	-0.39817380
C	-2.15814492	0.89384245	-1.70189024
H	-2.02966148	0.18009156	-2.51708208
H	-3.12256981	1.37734507	-1.82535617
H	-1.37621850	1.65208580	-1.73573993
S	-0.94476392	-0.82900042	1.71285755
O	0.43283531	2.18036755	-0.22233944

### Proline 6, *endo*

C	-0.00909093	0.38883452	-0.88878717	H	1.98811273	-1.66495988	1.16560325
H	0.10036866	-0.37213398	-1.65580872	H	3.24175624	-1.06281746	0.05141046
C	-2.02095143	1.50884751	-0.09897208	C	1.60611834	1.10092388	0.07838547
H	-2.26755596	1.63878360	0.95509363	C	-1.10007828	-0.31982627	0.21887781
H	-2.94342758	1.51963724	-0.68494099	C	2.90899455	1.37503989	0.78017792
C	-1.02682954	2.56956410	-0.58232728	H	3.75527470	1.09997114	0.14589690
H	-0.49382678	2.98427763	0.26977271	H	2.97493334	2.43134245	1.01668379
H	-1.52755454	3.37941063	-1.11092982	H	2.96835415	0.78753386	1.69972506
C	-0.05476714	1.80325843	-1.48769043	C	-3.36344586	0.40972703	0.56180073
H	-0.44831795	1.73637875	-2.50368889	H	-3.60288356	-0.46265622	1.16856521
H	0.93216727	2.26292993	-1.53072213	H	-3.09668751	1.22328996	1.23938741
N	-1.32658362	0.22953278	-0.29875108	H	-4.22232822	0.69128921	-0.04079489
C	-1.77873934	-0.96272306	0.09225370	N	1.33403037	-0.18086801	-0.16538830
C	-3.11711170	-0.95487372	0.77758223	N	-2.24170304	0.10828167	-0.32006854
H	-3.01106473	-0.47130668	1.75306017	C	-2.35909272	0.47102401	-1.73221397
H	-3.85778939	-0.39294630	0.20510774	H	-2.09825166	-0.36973444	-2.37551603
H	-3.45978322	-1.97355627	0.92312771	H	-3.39162911	0.73768851	-1.93598838
C	1.09073486	0.24739296	0.16693977	H	-1.71607368	1.32436129	-1.96104000
N	2.22818516	-0.32735746	-0.22936709	S	0.57636733	2.34001120	-0.34285832
C	3.31653963	-0.46975781	0.73082102	S	-0.91083909	-0.64080499	1.84147568
H	2.99045225	-1.07342180	1.57981226				
H	4.16254313	-0.94172884	0.23952564				
H	3.60507139	0.50897734	1.11346027				
C	2.36389617	-0.97801275	-1.53333719				
H	3.37551485	-1.36100859	-1.62539256				
H	1.65993512	-1.80915218	-1.61866123				
H	2.19691490	-0.26968206	-2.34552206				
S	-0.91849579	-2.37469044	-0.11373944				
S	0.86606624	0.86852650	1.69548129				

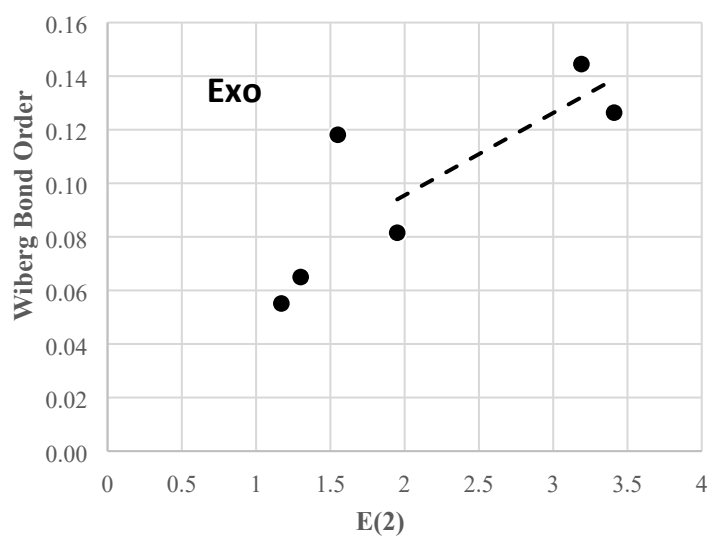
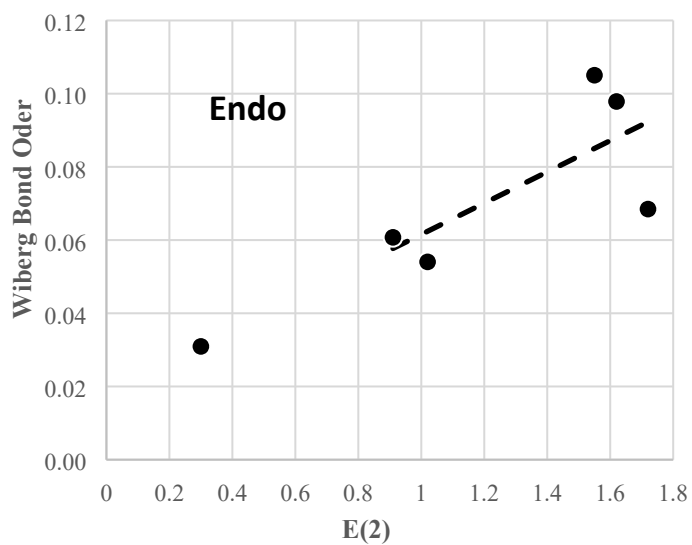
### Proline 6, *exo*

C	0.06009705	-0.60852436	-0.73815176
C	0.22834706	-2.12733419	-0.95886694
C	1.74074868	-2.36012680	-0.88167345
C	2.19123665	-1.32702735	0.14477177
H	-0.06577078	-0.07401016	-1.67757925
H	-0.27021428	-2.66304238	-0.15157974
H	-0.20478739	-2.44366940	-1.90711028
H	1.99279429	-3.37712888	-0.58552866
H	2.21361970	-2.15195332	-1.84320293

**Table S1.** Energy gap (Hartree) and overlap integrals between the  $n$  and  $\pi^*$  orbitals.

Com- pound	B3LYP		B3LYP-D3		M06-2X		WB97X-D4		Wb97X-V		
	$E_j - E_i$	Orbital Overlap	$E_j - E_i$	Orbital Overlap	$E_j - E_i$	Orbital Overlap	$E_j - E_i$	Orbital Overlap	$E_j - E_i$	Orbital Overlap	
<b>Endo</b>	1	0.25	0.0716260	0.25	0.079814417	0.38	0.09333792	0.44	0.0849891	0.44	0.084989155
	2	0.19	0.0951706	0.19	0.108083632	0.30	0.11464861	0.37	0.1091156	0.37	0.109115583
	3	0.30	0.0608885	0.28	0.059112956	0.48	0.07403054	0.55	0.1035855	0.54	0.10358516
	4	0.23	0.0929806	0.24	0.111600343	0.34	0.12211548	0.47	0.1158169	0.45	0.115816915
	5	0.20	0.0669084	0.20	0.082894732	0.30	0.09877218	0.36	0.0947762	0.36	0.094776247
	6	0.14	0.0926631	0.15	0.10611385	0.22	0.11099934	0.29	0.1130633	0.29	0.113063267
<b>Exo</b>	1	0.26	0.1019014	0.26	0.110525689	0.38	0.11831056	0.44	0.1191303	0.44	0.11913026
	2	0.20	0.1248155	0.20	0.137930875	0.30	0.14451327	0.37	0.1383152	0.38	0.138315211
	3	0.34	0.0938591	0.33	0.108098041	0.51	0.12196114	0.62	0.1177023	0.60	0.117702274
	4	0.33	0.1182367	0.33	0.131918668	0.47	0.14121346	0.63	0.1342440	0.61	0.134244044
	5	0.20	0.0848112	0.20	0.095470172	0.30	0.10461177	0.36	0.1068199	0.36	0.106819906
	6	0.14	0.1092094	0.15	0.124763945	0.29	0.13578751	0.29	0.1316176	0.29	0.131617784





**Figure S1.** Correlation between  $E(2)$  and the WBI in endo and exo pucker.