Supporting Information Belonging to the paper:

The Radical Mechanism of Cobalt(II) Porphyrin-Catalyzed Olefin Aziridination and the Importance of Cooperative H-Bonding

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Contents

Energies

Table S1. Co(Por) species: (Free) energies, enthalpies and entropies, ZPE and thermal corrections and S^2 values.

	SCF energy (a.u.)	negative eigenvalues (cm^{-1})	G gasphase (a.u.)	ZPE (a.u.)	RT+TRV (a.u.)	E+ZPE=E0 (a.u.)	H (a.u.)	S (a.u.)	S^2
$PhSO_2N_3$	-944.70085	-	-944.62795	0.11022	0.12177	-944.59063	-944.57908	0.000164	0
Styrene	-309.75	-	-309.65306	0.13082	0.13809	-309.62289	-309.61562	0.000126	0
N_2	-109.58	-	-109.58937	0.00543	0.00873	-109.57026	-109.56696	7.52E-05	0
Aziridine_product_cis	-1144.94	-	-1144.74795	0.23458	0.251	-1144.704	-1144.6876	0.000203	0
Aziridine_product_trans	-1144.95	-	-1144.75574	0.23472	0.25109	-1144.7119	-1144.6956	0.000202	0
A	-2371.87043	-	-2371.64075	0.27028	0.2881	-2371.6002	-2371.5823	0.000196	0.7616
B	-3316.57397	-	-3316.25295	0.37972	0.4103	-3316.1943	-3316.1637	0.0003	0.764
TS1	-3316.54711	-565.39 cm-1	-3316.22849	0.37628	0.40662	-3316.1708	-3316.1405	0.000295	0.7794
C	-3207.02472	-	-3206.71011	0.37005	0.39822	-3206.6547	-3206.6265	0.000281	0.7567
TS2	-3516.75757	-246.12 cm-1	-3516.32073	0.50073	0.53626	-3516.2568	-3516.2213	0.000334	0.782
D	-3516.78328	-	-3516.34538	0.50242	0.53817	-3516.2809	-3516.2451	0.000336	1.3428
TS3	-3516.7839	-37.76 cm-1	-3516.34468	0.50234	0.53741	-3516.2816	-3516.2465	0.000329	0.8779
E	-3516.80769	-	-3516.36434	0.50577	0.5407	-3516.3019	-3516.267	0.000327	0.7642
^{4}A	-2371.83727	-	-2371.61169	0.26747	0.28602	-2371.5698	-2371.5513	0.000203	3.7618
^{4}B	-3316.53995	-	-3316.22317	0.37712	0.40847	-3316.1628	-3316.1315	0.000308	3.7771
^{4}TS1	-3316.52362	-489.48 cm-1	-3316.20465	0.37645	0.40677	-3316.1472	-3316.1169	0.000295	3.7754
^{4}C	-3207.00711	-	-3206.69415	0.36959	0.39808	-3206.6375	-3206.609	0.000286	3.7783
^{4}TS2	-3516.74537	-225.24 cm-1	-3516.3094	0.50045	0.53625	-3516.2449	-3516.2091	0.000337	3.7832
^{4}D	-3516.78153	-	-3516.34204	0.50286	0.53825	-3516.2787	-3516.2433	0.000331	3.785

Table S2. Co(PorAmide) species: (Free) energies, enthalpies and entropies, ZPE and thermal corrections and S^2 values.

	SCF energy (a.u.)	negative eigenvalues (cm^{-1})	G_gasphase (a.u.)	ZPE (a.u.)	RT+TRV (a.u.)	E+ZPE=E0 (a.u.)	H (a.u.)	S (a.u.)	S^2
$PhSO_2N_3$	-944.70085	-	-944.62795	0.11022	0.12177	-944.591	-944.579	0.000164	0
Styrene	-309.75	-	-309.65306	0.13082	0.13809	-309.623	-309.616	0.000126	0
N_2	-109.58	-	-109.58937	0.00543	0.00873	-109.57	-109.567	7.52E-05	0
Aziridine_product_cis	-1144.94	-	-1144.74795	0.23458	0.251	-1144.7	-1144.69	0.000203	0
Aziridine_product_trans	-1144.95	-	-1144.75574	0.23472	0.25109	-1144.71	-1144.7	0.000202	0
A	-2811.1075	-	-2810.76023	0.40144	0.42887	-2810.71	-2810.68	0.000274	0.7618
B	-3755.81406	-	-3755.37118	0.37972	0.51194	-3755.43	-3755.3	0.000232	0.7645
TS1	-3755.79093	-565.39 cm-1	-3755.35109	0.37628	0.5083	-3755.41	-3755.28	0.00023	0.7795
C	-3646.2699	-	-3645.83349	0.37005	0.50229	-3645.9	-3645.77	0.000221	0.7566
TS2	-3956.00	-246.12 cm-1	-3955.44622	0.50073	0.63274	-3955.5	-3955.37	0.000252	0.7817
D	-3956.03	-	-3955.46813	0.5028	0.63408	-3955.52	-3955.39	0.000256	1.2647
TS3	-3956.03	-37.76 cm-1	-3955.46716	0.50234	0.63496	-3955.53	-3955.39	0.000247	0.8076
E	-3956.05	-	-3955.4846	0.50577	0.63765	-3955.54	-3955.41	0.000245	0.7641
^{4}C	-3646.25	-	-3645.81602	0.50158	0.53929	-3645.75	-3645.71	0.000351	3.7786
^{4}TS2	-3955.99047	-221.88 cm-1	-3955.43317	0.63251	0.67757	-3955.36	-3955.31	0.000404	3.7827
^{4}D	-3956.018	-	-3955.45624	0.63539	0.63539	-3955.38	-3955.38	0.000247	3.786

Table S3. Co(Por) species: Relative free energies, enthalpies and entropies.

	a.u	*ΔG 298K kcal mol^{-1}*	*ΔG 298K solution kcal mol^{-1}*	Barriers
A + $PhSO_2N_3$ + Styrene	-3625.92176	0	0	
B + Styrene	-3625.90601	9.8832825	7.3992225	
TS1 + Styrene	-3625.88155	25.2321771	22.7481171	**22.74812**
C + Styrene + N_2	-3625.95254	-19.3147578	-21.7988178	
TS2 + N_2	-3625.9101	7.3167666	2.3486466	**24.14746**
D + N_2	-3625.93475	-8.1513549	-13.1194749	
TS3 + N_2	-3625.93405	-7.7120979	-12.6802179	**0.439257**
E + N_2	-3625.95371	-20.0489445	-25.0170645	
A + Aziridine_product_cis + N_2	-3625.98	-35.3350881	-37.8191481	
A + Aziridine_product_trans + N_2	-3625.99	-40.223391	-42.707451	
^{4}A + $PhSO_2N_3$ + Styrene	-3625.89	18.2354406	18.2354406	
^{4}B + Styrene	-3625.88	28.5705303	26.0864703	
^{4}TS1 + Styrene	-3625.86	40.1920155	37.7079555	**19.47251**
^{4}C + Styrene + N_2	-3625.93658	-9.2996982	-11.7837582	
^{4}TS2 + N_2	-3625.89877	14.4264549	11.9423949	**23.72615**
^{4}D + N_2	-3625.93141	-6.0554715	-11.0235915	
			ΔH kcal mol^{-1}	
A + $PhSO_2N_3$ + Styrene	-3625.77703		0	
B + Styrene	-3625.77929		-1.4181726	
TS1 + Styrene	-3625.75611		13.1275092	
C + Styrene + N_2	-3625.80908		-20.1116955	
TS2 + N_2	-3625.78827		-7.0532124	
D + N_2	-3625.81207		-21.9879504	
TS3 + N_2	-3625.81345		-22.8539142	
E + N_2	-3625.83395		-35.7178692	
A + Aziridine_product_cis + N_2	-3625.83684		-37.5313731	
A + Aziridine_product_trans + N_2	-3625.84484		-42.5514531	
^{4}A + $PhSO_2N_3$ + Styrene	-3625.74595		19.5030108	
^{4}B + Styrene	-3625.7471		18.7813743	
^{4}TS1 + Styrene	-3625.73247		27.9618456	
^{4}C + Styrene + N_2	-3625.79161		-9.1490958	
^{4}TS2 + N_2	-3625.77608		0.5961345	
^{4}D + N_2	-3625.81024		-20.8396071	
		ΔS gas phase cal K^{-1} mol^{-1}	*ΔS solution cal K^{-1} mol^{-1}*	
A + PhSO2N3 + Styrene	0.000485671	0	0	
B + Styrene	0.000425235	-37.92434597	-29.58857416	
TS1 + Styrene	0.00042094	-40.61969094	-32.28391913	
C + Styrene + N2	0.000481409	-2.674287584	5.661484228	
TS2 + N2	0.000408826	-48.22140604	-31.54986242	
D + N2	0.000411678	-46.43152852	-29.7599849	
TS3 + N2	0.000404698	-50.81146409	-34.13992047	
E + N2	0.000401879	-52.58028423	-35.9087406	
A + Aziridine_product_cis + N2	0.000473926	-7.370083893	0.965687919	
A + Aziridine_product_trans + N2	0.000473221	-7.812288926	0.523482886	
4A + PhSO2N3 + Styrene	0.00049245	4.253591275	4.253591275	
4B + Styrene	0.000433322	-32.84951678	-24.51374497	
4TS1 + Styrene	0.000420268	-41.04083859	-32.70506678	
4C + Styrene + N2	0.000486477	0.50537718	8.841148992	
4TS2 + N2	0.000411711	-46.41047114	-38.07469933	
4D + N2	0.000406611	-49.61119329	-32.93964967	

Table S4. Co(PorAmide) species: Relative free energies, enthalpies and entropies.

	a.u	*ΔG 298K kcal mol^{-1}*	*ΔG 298K solution kcal mol^{-1}*	Barriers
A + $PhSO_2N_3$ + Styrene	-4065.04124	0	0	
B + Styrene	-4065.02424	10.66767	8.18361	
TS1 + Styrene	-4065.00415	23.2743459	20.7902859	**20.79029**
C + Styrene + N_2	-4065.07592	-21.7620468	-24.2461068	
TS2 + N_2	-4065.03559	3.5454315	-1.4226885	**22.82342**
D + N_2	-4065.0575	-10.2033126	-15.1714326	
TS3 + N_2	-4065.05653	-9.5946279	-14.5627479	**0.608685**
E + N_2	-4065.07397	-20.5384023	-25.5065223	
A + Aziridine_product_cis + N_2	-4065.10	-35.3350881	-37.8191481	
A + Aziridine_product_trans + N_2	-4065.11	-40.223391	-42.707451	
^{4}C + Styrene + N_2	-4065.06	-10.7994471	-13.2835071	
^{4}TS2 + N_2	-4065.02254	11.734437	9.250377	**22.53388**
^{4}D + N_2	-4065.04561	-2.7422187	-5.2262787	

		ΔH kcal mol^{-1}
A + $PhSO_2N_3$ + Styrene	-4064.90076	0
B + Styrene	-4064.91774	-10.6551198
TS1 + Styrene	-4064.89825	1.5750501
C + Styrene + N_2	-4064.95019	-31.0178193
TS2 + N_2	-4064.93799	-23.3621973
D + N_2	-4064.95895	-36.5148069
TS3 + N_2	-4064.96053	-37.5062727
E + N_2	-4064.97867	-48.8893041
A + Aziridine_product_cis + N_2	-4064.96057	-37.5313731
A + Aziridine_product_trans + N_2	-4064.96857	-42.5514531
^{4}C + Styrene + N_2	-4064.89407	4.1980419
^{4}TS2 + N_2	-4064.87986	13.114959
^{4}D + N_2	-4064.94957	-30.6287631

		ΔS gas phase cal K^{-1} mol^{-1}	*ΔS solution cal K^{-1} mol^{-1}*
A + $PhSO_2N_3$ + Styrene	0.000471409	0	0
B + Styrene	0.000357383	-71.55298591	-63.21721409
TS1 + Styrene	0.000355369	-72.81642886	-64.48065705
C + Styrene + N_2	0.000421913	-31.05963926	-22.72386745
TS2 + N_2	0.000327517	-90.29405638	-73.62251275
D + N_2	0.000330705	-88.29360503	-71.62206141
TS3 + N_2	0.000322148	-93.66323758	-76.99169396
E + N_2	0.000319799	-95.13725436	-78.46571074
A + Aziridine_product_cis + N_2	0.000459664	-7.370083893	0.965687919
A + Aziridine_product_trans + N_2	0.00045896	-7.812288926	0.523482886
^{4}C + Styrene + N_2	0.000551611	50.3271443	44.57552718
^{4}TS2 + N_2	0.000478792	4.63262416	12.96839597
^{4}D + N_2	0.000322282	-93.57900805	17.53784799

Figure S1. Relative free energy profiles (ΔG in kcal mol^{-1}) for aziridination of styrene by $PhSO_2N_3$ mediated by the Co(por) and Co(PorAmide) species.

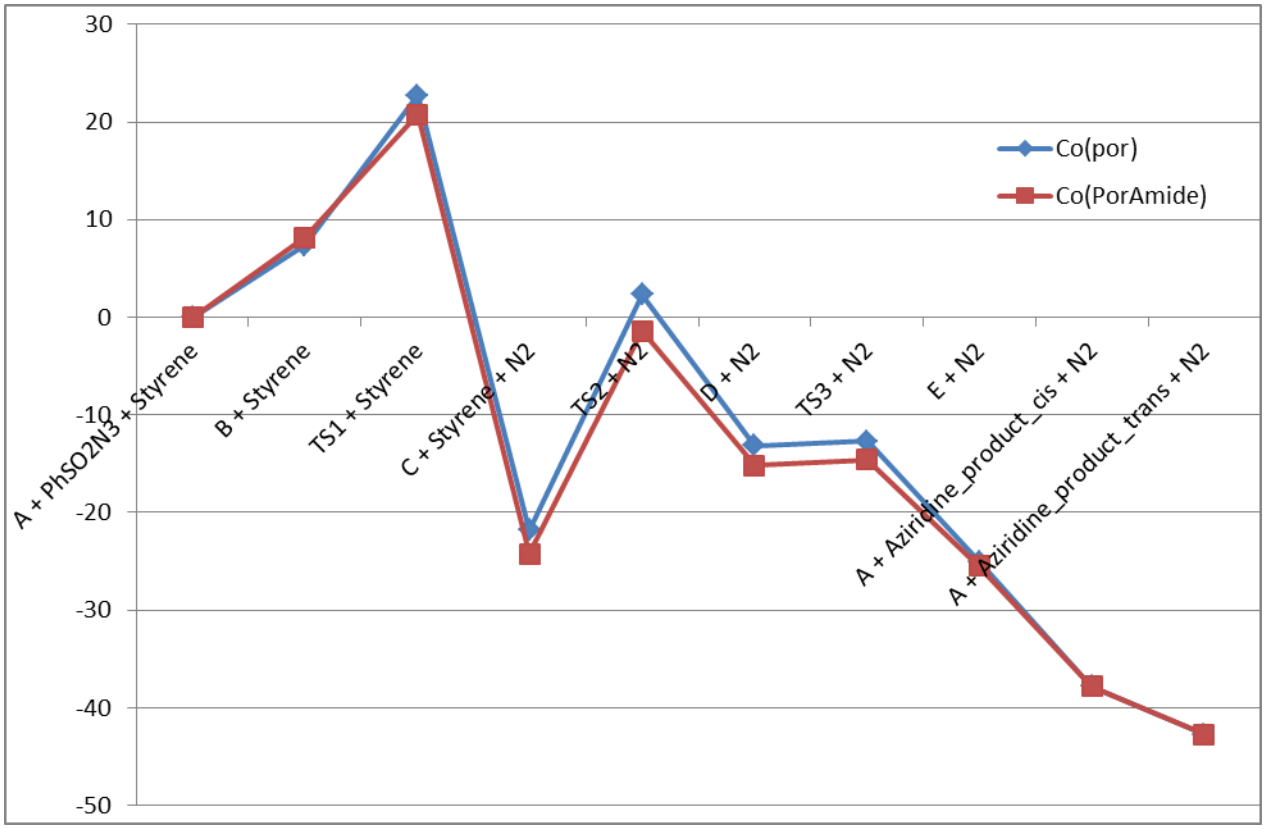


Figure S2. Relative enthalpy profiles (ΔG in kcal mol^{-1}) for aziridination of styrene by $PhSO_2N_3$ mediated by the Co(por) and Co(PorAmide) species.

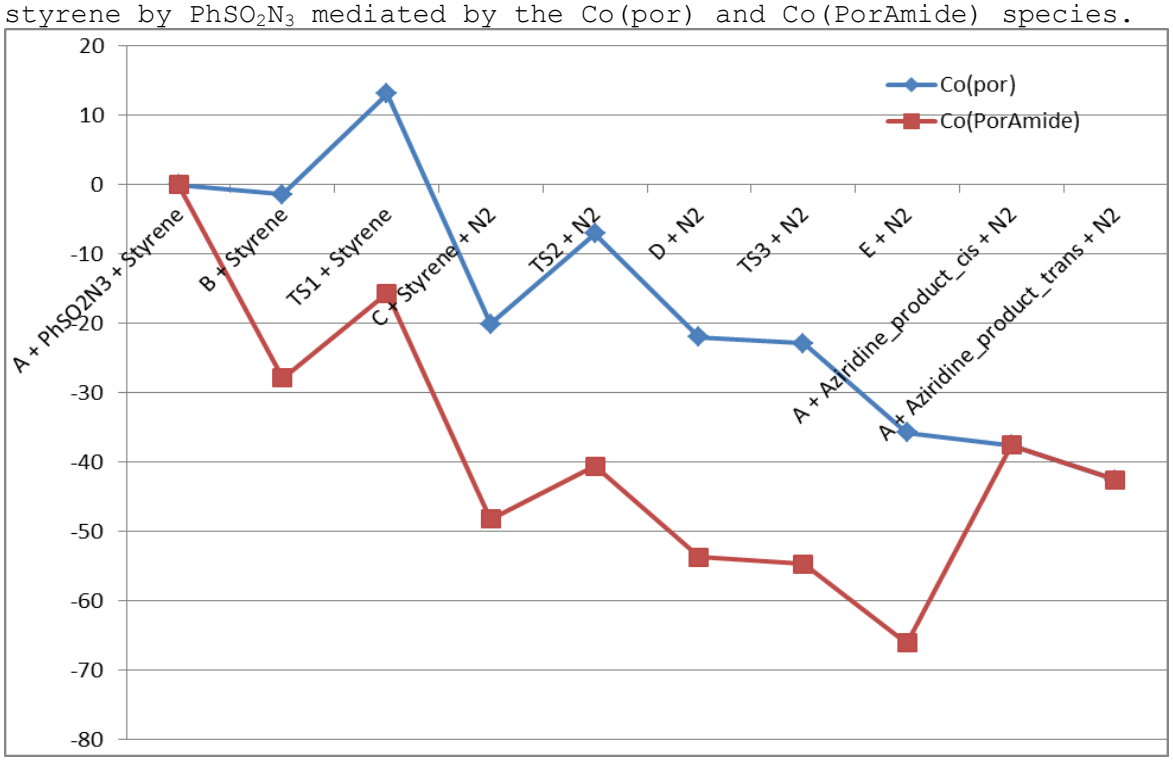
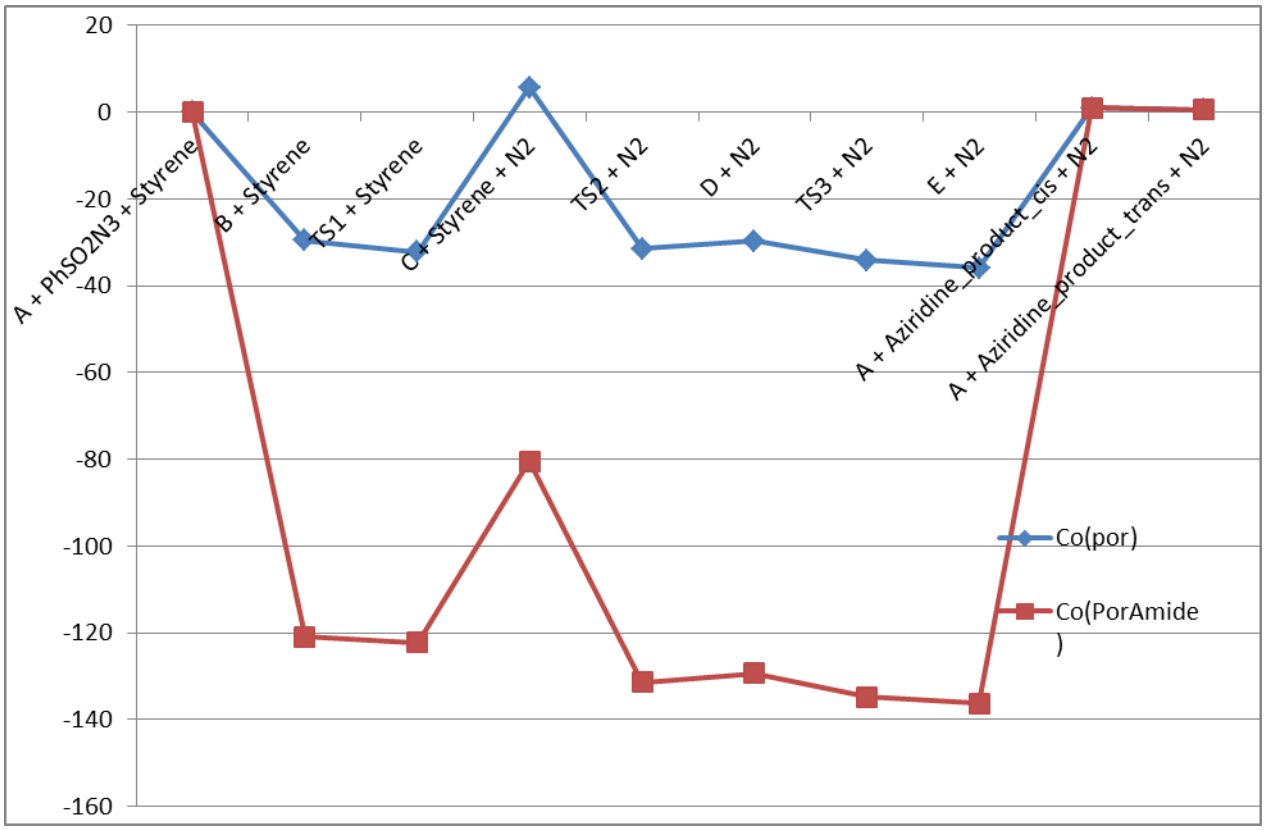


Figure S3. Relative enthalpy profiles (ΔG in kcal mol^{-1}) for aziridination of styrene by $PhSO_2N_3$ mediated by the Co(por) and Co(PorAmide) species.



Optimized Geometries

PhSO2N3

Xyz file

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O    -1.5924444   -2.0342745    2.5487076
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C    -1.0354048   -3.6447338    4.5997483
C    -1.5334949   -6.0263381    5.9433320
C    -0.7693912   -3.7131483    5.9773419
C    -1.5540106   -4.7334425    3.8784374
C    -1.8000127   -5.9325227    4.5649611
C    -1.0236718   -4.9206854    6.6474616
H    -0.3841732   -2.8298217    6.5095696
H    -1.7672947   -4.6320871    2.8032361
H    -2.2086099   -6.7985605    4.0193503
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pdb File

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ATOM      3  O   111     1      -1.592  -2.034   2.549  1.00  0.00
ATOM      4  O   111     1      -0.591  -1.007   4.710  1.00  0.00
ATOM      5  C   111     1      -1.035  -3.645   4.600  1.00  0.00
ATOM      6  C   111     1      -1.533  -6.026   5.943  1.00  0.00
ATOM      7  C   111     1      -0.769  -3.713   5.977  1.00  0.00
ATOM      8  C   111     1      -1.554  -4.733   3.878  1.00  0.00
ATOM      9  C   111     1      -1.800  -5.933   4.565  1.00  0.00
ATOM     10  C   111     1      -1.024  -4.921   6.647  1.00  0.00
ATOM     11  H   111     1      -0.384  -2.830   6.510  1.00  0.00
ATOM     12  H   111     1      -1.767  -4.632   2.803  1.00  0.00
ATOM     13  H   111     1      -2.209  -6.799   4.019  1.00  0.00
ATOM     14  H   111     1      -0.827  -4.995   7.729  1.00  0.00
ATOM     15  H   111     1      -1.731  -6.971   6.476  1.00  0.00
ATOM     16  N   111     1       2.773  -1.422   4.138  1.00  0.00
ATOM     17  N   111     1       1.844  -1.890   3.645  1.00  0.00
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CONECT    2    3    4    5
CONECT    5    7    8
CONECT    6    9   10   15
CONECT    7   10   11
CONECT    8    9   12
CONECT    9   13
CONECT   10   14
CONECT   16   17
END
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Styrene
Xyz file
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C     0.3533030   -0.0005233    3.9557215
C     1.1590344   -0.0005984    1.6325807
C    -1.2438235    0.0012447    2.1255730
C    -0.9783040    0.0015890    3.5084830
C     1.4060815   -0.0013803    3.0274300
H    -2.2861162    0.0020563    1.7652410
H    -1.8092469    0.0021131    4.2332214
H     2.4500471   -0.0039707    3.3856056
H     0.5750395   -0.0014232    5.0360195
C     2.3048469    0.0003334    0.7040109
H     3.2943425    0.0027941    1.1998021
C     2.2774250   -0.0000210   -0.6480522
H     3.2144833    0.0002092   -1.2305551
H     1.3365994   -0.0013509   -1.2265161

Pdb file
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COMPND B2Pdb
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ATOM      2  C   111     1      -0.192  -0.000   1.201  1.00  0.00
ATOM      3  C   111     1       0.353  -0.001   3.956  1.00  0.00
ATOM      4  C   111     1       1.159  -0.001   1.633  1.00  0.00
ATOM      5  C   111     1      -1.244   0.001   2.126  1.00  0.00
ATOM      6  C   111     1      -0.978   0.002   3.508  1.00  0.00
ATOM      7  C   111     1       1.406  -0.001   3.027  1.00  0.00
ATOM      8  H   111     1      -2.286   0.002   1.765  1.00  0.00
ATOM      9  H   111     1      -1.809   0.002   4.233  1.00  0.00
ATOM     10  H   111     1       2.450  -0.004   3.386  1.00  0.00
ATOM     11  H   111     1       0.575  -0.001   5.036  1.00  0.00
ATOM     12  C   111     1       2.305   0.000   0.704  1.00  0.00
ATOM     13  H   111     1       3.294   0.003   1.200  1.00  0.00
ATOM     14  C   111     1       2.277  -0.000  -0.648  1.00  0.00
ATOM     15  H   111     1       3.214   0.000  -1.231  1.00  0.00
ATOM     16  H   111     1       1.337  -0.001  -1.227  1.00  0.00
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CONECT    2    4    5
CONECT    3    6    7   11
CONECT    4    7   12
CONECT    5    6    8
CONECT    6    9
CONECT    7   10
CONECT   12   13   14
CONECT   14   15   16
END

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Pdb file
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CONECT    1    2
END

Aziridine product cis
Xyz file
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O    -1.7209956   -1.2090327    4.2502473
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C     3.3761497   -1.8581066    5.2854752
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C     1.3478867   -1.3484216    4.0354192
C     2.7179263   -1.1484738    4.2628670
C     2.6674427   -2.7696953    6.0871424
H     0.7126083   -3.6844835    6.4839087
H     0.8106680   -0.7947543    3.2501569
H     3.2762166   -0.4292322    3.6414854
H     3.1837907   -3.3164724    6.8931121
H     4.4521822   -1.6937766    5.4613283
H    -0.5214414   -5.4221544    2.4719683
C    -1.2187349   -4.8451810    3.1068239
H    -1.4403566   -5.2806051    4.0996631
C    -2.2814905   -3.9850764    2.5014970
H    -2.2762820   -3.8758100    1.3987622
C    -3.6468701   -3.8289219    3.1148945
C    -6.2681961   -3.5347973    4.1298154
C    -4.2805517   -4.8960241    3.7836122
C    -4.3460473   -2.6125541    2.9537149
C    -5.6452747   -2.4658837    3.4617975
C    -5.5831589   -4.7505982    4.2885695
H    -3.7516110   -5.8552312    3.9069482
H    -3.8571743   -1.7686893    2.4412604
H    -6.1754157   -1.5070598    3.3376837
H    -6.0644812   -5.5940904    4.8107207
H    -7.2898000   -3.4187445    4.5283927

Pdb file
HEADER B2Pdb
COMPND B2Pdb
ATOM      1  N   111     1       0.910  -2.430   3.035  1.00  0.00
ATOM      2  S   111     1      -0.725  -2.103   3.730  1.00  0.00
ATOM      3  O   111     1      -1.592  -2.034   2.549  1.00  0.00
ATOM      4  O   111     1      -0.591  -1.007   4.710  1.00  0.00
ATOM      5  C   111     1      -1.035  -3.645   4.600  1.00  0.00
ATOM      6  C   111     1      -1.533  -6.026   5.943  1.00  0.00
ATOM      7  C   111     1      -0.769  -3.713   5.977  1.00  0.00
ATOM      8  C   111     1      -1.554  -4.733   3.878  1.00  0.00
ATOM      9  C   111     1      -1.800  -5.933   4.565  1.00  0.00
ATOM     10  C   111     1      -1.024  -4.921   6.647  1.00  0.00
ATOM     11  H   111     1      -0.384  -2.830   6.510  1.00  0.00
ATOM     12  H   111     1      -1.767  -4.632   2.803  1.00  0.00
ATOM     13  H   111     1      -2.209  -6.799   4.019  1.00  0.00
ATOM     14  H   111     1      -0.827  -4.995   7.729  1.00  0.00
ATOM     15  H   111     1      -1.731  -6.971   6.476  1.00  0.00
```

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ATOM     16  N   111     1       2.773  -1.422   4.138  1.00  0.00
ATOM     17  N   111     1       1.844  -1.890   3.645  1.00  0.00
CONECT    1    2   17
CONECT    2    3    4    5
CONECT    5    7    8
CONECT    6    9   10   15
CONECT    7   10   11
CONECT    8    9   12
CONECT    9   13
CONECT   10   14
CONECT   16   17
END

Aziridine product trans
Xyz file
31
 Energy =   -1144.9466427160
N    -1.0585288   -3.5377197    2.6834811
S    -0.0178447   -2.1661284    2.3605186
O    -0.8229094   -0.9992022    1.9149186
O     1.0784496   -2.6953730    1.5253954
C     0.6010358   -1.8339888    4.0180337
C     1.5951715   -1.2964750    6.5617362
C     0.0870025   -0.7404230    4.7317034
C     1.6117663   -2.6581546    4.5414858
C     2.1041722   -2.3834009    5.8263726
C     0.5930257   -0.4759483    6.0156477
H    -0.6883954   -0.1067971    4.2744651
H     2.0063357   -3.4933366    3.9422917
H     2.8963104   -3.0187444    6.2552845
H     0.2030261    0.3802369    6.5901829
H     1.9890454   -1.0837432    7.5692910
H    -1.7274459   -3.4431703    0.5692422
C    -1.8298512   -4.0001533    1.5202189
H    -1.8926028   -5.0999723    1.4269945
C    -2.5166662   -3.2938544    2.6579125
H    -2.8146697   -2.2555213    2.4156830
C    -3.3644640   -3.9858344    3.6782843
C    -5.0298453   -5.2945850    5.5501739
C    -4.6973909   -3.5651468    3.8693974
C    -2.8714089   -5.0646229    4.4417038
C    -3.6996185   -5.7139481    5.3705995
C    -5.5263674   -4.2169397    4.7969309
H    -5.0898375   -2.7163537    3.2830903
H    -1.8223320   -5.3755542    4.3094762
H    -3.3006454   -6.5527648    5.9652381
H    -6.5665456   -3.8775975    4.9348263
H    -5.6781292   -5.8051647    6.2815832

Pdb file
HEADER B2Pdb
COMPND B2Pdb
ATOM      1  N   111     1      -1.059  -3.538   2.683  1.00  0.00
ATOM      2  S   111     1      -0.018  -2.166   2.361  1.00  0.00
ATOM      3  O   111     1      -0.823  -0.999   1.915  1.00  0.00
ATOM      4  O   111     1       1.078  -2.695   1.525  1.00  0.00
ATOM      5  C   111     1       0.601  -1.834   4.018  1.00  0.00
ATOM      6  C   111     1       1.595  -1.296   6.562  1.00  0.00
ATOM      7  C   111     1       0.087  -0.740   4.732  1.00  0.00
ATOM      8  C   111     1       1.612  -2.658   4.541  1.00  0.00
```

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ATOM      9  C   111     1       2.104  -2.383   5.826  1.00  0.00
ATOM     10  C   111     1       0.593  -0.476   6.016  1.00  0.00
ATOM     11  H   111     1      -0.688  -0.107   4.274  1.00  0.00
ATOM     12  H   111     1       2.006  -3.493   3.942  1.00  0.00
ATOM     13  H   111     1       2.896  -3.019   6.255  1.00  0.00
ATOM     14  H   111     1       0.203   0.380   6.590  1.00  0.00
ATOM     15  H   111     1       1.989  -1.084   7.569  1.00  0.00
ATOM     16  H   111     1      -1.727  -3.443   0.569  1.00  0.00
ATOM     17  C   111     1      -1.830  -4.000   1.520  1.00  0.00
ATOM     18  H   111     1      -1.893  -5.100   1.427  1.00  0.00
ATOM     19  C   111     1      -2.517  -3.294   2.658  1.00  0.00
ATOM     20  H   111     1      -2.815  -2.256   2.416  1.00  0.00
ATOM     21  C   111     1      -3.364  -3.986   3.678  1.00  0.00
ATOM     22  C   111     1      -5.030  -5.295   5.550  1.00  0.00
ATOM     23  C   111     1      -4.697  -3.565   3.869  1.00  0.00
ATOM     24  C   111     1      -2.871  -5.065   4.442  1.00  0.00
ATOM     25  C   111     1      -3.700  -5.714   5.371  1.00  0.00
ATOM     26  C   111     1      -5.526  -4.217   4.797  1.00  0.00
ATOM     27  H   111     1      -5.090  -2.716   3.283  1.00  0.00
ATOM     28  H   111     1      -1.822  -5.376   4.309  1.00  0.00
ATOM     29  H   111     1      -3.301  -6.553   5.965  1.00  0.00
ATOM     30  H   111     1      -6.567  -3.878   4.935  1.00  0.00
ATOM     31  H   111     1      -5.678  -5.805   6.282  1.00  0.00
CONECT    1    2   17   19
CONECT    2    3    4    5
CONECT    5    7    8
CONECT    6    9   10   15
CONECT    7   10   11
CONECT    8    9   12
CONECT    9   13
CONECT   10   14
CONECT   16   17
CONECT   17   18   19
CONECT   19   20   21
CONECT   21   23   24
CONECT   22   25   26   31
CONECT   23   26   27
CONECT   24   25   28
CONECT   25   29
CONECT   26   30
END


A_Co(por)
Xyz file
37
Energy =   -2370.655550939
C     0.7723160   0.5410334   0.5260294
N     0.4957726  -0.8108628   0.6753610
H    -0.4798713   2.4025864   0.2727174
C    -0.8895864  -0.8886978   0.6438885
C    -1.4825378   0.4197089   0.4742534
H    -2.5627125   0.6110993   0.4207267
C    -0.4447042   1.3123522   0.4006299
C    -1.6320397  -2.0601917   0.7574987
H    -2.7291801  -1.9831420   0.7149583
N     0.2889937  -3.5926107   0.9954630
C     0.3628998  -4.9691101   1.1563181
C    -0.9555925  -5.5634486   1.1826069
H    -1.1516255  -6.6378008   1.2992880
```

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C    -1.8505049  -4.5353998   1.0357528
H    -2.9476658  -4.5745043   1.0047988
C    -1.0703894  -3.3229199   0.9210873
C     2.0448676   1.1035983   0.4992284
H     2.126189    2.1943060   0.3757623
H     6.5317773  -0.0246800   0.7712629
C     5.4346097  -0.0637655   0.7404768
C     4.6544986  -1.2762628   0.8549496
H     4.7357002   2.0387258   0.4776956
N     3.295102   -1.0065385   0.7808514
C     3.2211889   0.3700040   0.6203797
C     4.5396795   0.9643397   0.5940958
C     1.5392122  -5.7026852   1.2776141
H     1.4578799  -6.7933652   1.4013282
H     6.1468304  -5.2103382   1.3548620
C     5.0666471  -5.0189190   1.3016074
C     4.0287973  -5.9115109   1.3756466
H     4.0639543  -7.0017290   1.5037019
C     2.8117778  -5.1401621   1.2504537
N     3.0883289  -3.7882983   1.1008703
C     4.4736983  -3.7105086   1.1319872
C     5.2161575  -2.5390302   1.0182352
H     6.3133082  -2.6161036   1.0605128
Co    1.7920498  -2.2995778   0.8881391
```

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Pdb file
HEADER B2Pdb
COMPND B2Pdb
ATOM      1  C   111     1       0.772   0.541   0.526  1.00  0.00
ATOM      2  N   111     1       0.496  -0.811   0.675  1.00  0.00
ATOM      3  H   111     1      -0.480   2.403   0.273  1.00  0.00
ATOM      4  C   111     1      -0.890  -0.889   0.644  1.00  0.00
ATOM      5  C   111     1      -1.483   0.420   0.474  1.00  0.00
ATOM      6  H   111     1      -2.563   0.611   0.421  1.00  0.00
ATOM      7  C   111     1      -0.445   1.312   0.401  1.00  0.00
ATOM      8  C   111     1      -1.632  -2.060   0.757  1.00  0.00
ATOM      9  H   111     1      -2.729  -1.983   0.715  1.00  0.00
ATOM     10  N   111     1       0.289  -3.593   0.995  1.00  0.00
ATOM     11  C   111     1       0.363  -4.969   1.156  1.00  0.00
ATOM     12  C   111     1      -0.956  -5.563   1.183  1.00  0.00
ATOM     13  H   111     1      -1.152  -6.638   1.299  1.00  0.00
ATOM     14  C   111     1      -1.851  -4.535   1.036  1.00  0.00
ATOM     15  H   111     1      -2.948  -4.575   1.005  1.00  0.00
ATOM     16  C   111     1      -1.070  -3.323   0.921  1.00  0.00
ATOM     17  C   111     1       2.045   1.104   0.499  1.00  0.00
ATOM     18  H   111     1       2.126   2.194   0.376  1.00  0.00
ATOM     19  H   111     1       6.532  -0.025   0.771  1.00  0.00
ATOM     20  C   111     1       5.435  -0.064   0.740  1.00  0.00
ATOM     21  C   111     1       4.654  -1.276   0.855  1.00  0.00
ATOM     22  H   111     1       4.736   2.039   0.478  1.00  0.00
ATOM     23  N   111     1       3.295  -1.007   0.781  1.00  0.00
ATOM     24  C   111     1       3.221   0.370   0.620  1.00  0.00
ATOM     25  C   111     1       4.540   0.964   0.594  1.00  0.00
ATOM     26  C   111     1       1.539  -5.703   1.278  1.00  0.00
ATOM     27  H   111     1       1.458  -6.793   1.401  1.00  0.00
ATOM     28  H   111     1       6.147  -5.210   1.355  1.00  0.00
ATOM     29  C   111     1       5.067  -5.019   1.302  1.00  0.00
ATOM     30  C   111     1       4.029  -5.912   1.376  1.00  0.00
ATOM     31  H   111     1       4.064  -7.002   1.504  1.00  0.00
```

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ATOM     32  C   111     1       2.812  -5.140   1.250  1.00  0.00
ATOM     33  N   111     1       3.088  -3.788   1.101  1.00  0.00
ATOM     34  C   111     1       4.474  -3.711   1.132  1.00  0.00
ATOM     35  C   111     1       5.216  -2.539   1.018  1.00  0.00
ATOM     36  H   111     1       6.313  -2.616   1.061  1.00  0.00
ATOM     37 Co   111     1       1.792  -2.300   0.888  1.00  0.00
CONECT    1    2    7   17
CONECT    2    4   37
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   37
CONECT   11   12   26
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   18   24
CONECT   19   20
CONECT   20   21   25
CONECT   21   23   35
CONECT   22   25
CONECT   23   24   37
CONECT   24   25
CONECT   26   27   32
CONECT   28   29
CONECT   29   30   34
CONECT   30   31   32
CONECT   32   33
CONECT   33   34   37
CONECT   34   35
CONECT   35   36
END

H   111     1      -0.480   2.403   0.273  1.00  0.00
ATOM      4  C   111     1      -0.890  -0.889   0.644  1.00  0.00
ATOM      5  C   111     1      -1.483   0.420   0.474  1.00  0.00
ATOM      6  H   111     1      -2.563   0.611   0.421  1.00  0.00
ATOM      7  C   111     1      -0.445   1.312   0.401  1.00  0.00
ATOM      8  C   111     1      -1.632  -2.060   0.757  1.00  0.00
ATOM      9  H   111     1      -2.729  -1.983   0.715  1.00  0.00
ATOM     10  N   111     1       0.289  -3.593   0.995  1.00  0.00
ATOM     11  C   111     1       0.363  -4.969   1.156  1.00  0.00
ATOM     12  C   111     1      -0.956  -5.563   1.183  1.00  0.00
ATOM     13  H   111     1      -1.152  -6.638   1.299  1.00  0.00
ATOM     14  C   111     1      -1.851  -4.535   1.036  1.00  0.00
ATOM     15  H   111     1      -2.948  -4.575   1.005  1.00  0.00
ATOM     16  C   111     1      -1.070  -3.323   0.921  1.00  0.00
ATOM     17  C   111     1       2.045   1.104   0.499  1.00  0.00
ATOM     18  H   111     1       2.126   2.194   0.376  1.00  0.00
ATOM     19  H   111     1       6.532  -0.025   0.771  1.00  0.00
ATOM     20  C   111     1       5.435  -0.064   0.740  1.00  0.00
ATOM     21  C   111     1       4.654  -1.276   0.855  1.00  0.00
ATOM     22  H   111     1       4.736   2.039   0.478  1.00  0.00
ATOM     23  N   111     1       3.295  -1.007   0.781  1.00  0.00
ATOM     24  C   111     1       3.221   0.370   0.620  1.00  0.00
ATOM     25  C   111     1       4.540   0.964   0.594  1.00  0.00
ATOM     26  C   111     1       1.539  -5.703   1.278  1.00  0.00
ATOM     27  H   111     1       1.458  -6.793   1.401  1.00  0.00
ATOM     28  H   111     1       6.147  -5.210   1.355  1.00  0.00
ATOM     29  C   111     1       5.067  -5.019   1.302  1.00  0.00
```

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ATOM     30  C   111     1        4.029  -5.912   1.376  1.00  0.00
ATOM     31  H   111     1        4.064  -7.002   1.504  1.00  0.00
ATOM     32  C   111     1        2.812  -5.140   1.250  1.00  0.00
ATOM     33  N   111     1        3.088  -3.788   1.101  1.00  0.00
ATOM     34  C   111     1        4.474  -3.711   1.132  1.00  0.00
ATOM     35  C   111     1        5.216  -2.539   1.018  1.00  0.00
ATOM     36  H   111     1        6.313  -2.616   1.061  1.00  0.00
ATOM     37 Co   111     1        1.792  -2.300   0.888  1.00  0.00
CONECT    1    2    7   17
CONECT    2    4   37
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   37
CONECT   11   12   26
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   18   24
CONECT   19   20
CONECT   20   21   25
CONECT   21   23   35
CONECT   22   25
CONECT   23   24   37
CONECT   24   25
CONECT   26   27   32
CONECT   28   29
CONECT   29   30   34
CONECT   30   31   32
CONECT   32   33
CONECT   33   34   37
CONECT   34   35
CONECT   35   36
END
```

```
B_ Co(por)
Xyz file
54
 Energy =   -3316.5739685690
C     0.8564576   -0.1246196   -0.7200833
N     0.3610350   -1.4045365   -0.5202346
H     0.1708468    1.6718221   -1.9068655
C    -0.8137247   -1.4514545   -1.2533721
C    -1.0640758   -0.1864279   -1.9107379
H    -1.9325003    0.0231025   -2.5497275
C    -0.0114224    0.6345700   -1.5948447
C    -1.6120618   -2.5829470   -1.4148680
H    -2.5268438   -2.4879539   -2.0200283
N    -0.1568291   -4.1396655   -0.1720091
C    -0.1723306   -5.5168648   -0.0283828
C    -1.2963284   -6.0986812   -0.7315255
H    -1.5169246   -7.1738340   -0.7721556
C    -1.9938363   -5.0561928   -1.2843585
H    -2.9094402   -5.0838752   -1.8905360
C    -1.2692092   -3.8489450   -0.9436570
C     2.0010656    0.3952699   -0.1177066
H     2.2863040    1.4301795   -0.3603880
H     5.1670587   -0.6037945    3.1243684
```

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C     4.3354700   -0.6630125    2.4090652
C     3.5078281   -1.8328972    2.2046470
H     4.2625340    1.3118366    1.3727191
N     2.5471517   -1.5965748    1.2340208
C     2.7720831   -0.2930127    0.8185715
C     3.8882724    0.2913866    1.5305926
C     0.7240612   -6.2541868    0.7403679
H     0.6001032   -7.3474027    0.7731427
H     4.1826581   -5.7121404    3.7886071
C     3.3904119   -5.5308156    3.0492657
C     2.5811112   -6.4415970    2.4148537
H     2.5528583   -7.5338935    2.5284553
C     1.7275038   -5.6859347    1.5234537
N     2.0157911   -4.3324112    1.5929742
C     3.0422599   -4.2295471    2.5186385
C     3.7157397   -3.0530021    2.8460829
H     4.5168014   -3.1099776    3.5994709
Co    1.1215559   -2.8485132    0.6223335
N    -0.1836790   -2.2692407    2.3131524
S    -1.3502993   -3.2527721    3.3349911
O    -1.2733071   -4.5946319    2.7497238
O    -2.5954012   -2.4673597    3.4199372
C    -0.5385485   -3.2445441    4.9381880
C     0.6835472   -3.2579434    7.4341481
C    -0.9869417   -2.3407490    5.9168505
C     0.5023042   -4.1589385    5.1760259
C     1.1127442   -4.1564119    6.4398143
C    -0.3628353   -2.3547099    7.1749163
H    -1.8187193   -1.6549499    5.6960036
H     0.8228042   -4.8604976    4.3903067
H     1.9291421   -4.8668333    6.6474275
H    -0.7023449   -1.6585231    7.9588524
H     1.1675596   -3.2647792    8.4244695
N    -0.3297314   -1.0439676    2.4979445
N    -0.3899082    0.0998410    2.5974136
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Pdb file
HEADER B2Pdb
COMPND B2Pdb
ATOM      1  C   111     1       0.856  -0.125  -0.720  1.00  0.00
ATOM      2  N   111     1       0.361  -1.405  -0.520  1.00  0.00
ATOM      3  H   111     1       0.171   1.672  -1.907  1.00  0.00
ATOM      4  C   111     1      -0.814  -1.451  -1.253  1.00  0.00
ATOM      5  C   111     1      -1.064  -0.186  -1.911  1.00  0.00
ATOM      6  H   111     1      -1.933   0.023  -2.550  1.00  0.00
ATOM      7  C   111     1      -0.011   0.635  -1.595  1.00  0.00
ATOM      8  C   111     1      -1.612  -2.583  -1.415  1.00  0.00
ATOM      9  H   111     1      -2.527  -2.488  -2.020  1.00  0.00
ATOM     10  N   111     1      -0.157  -4.140  -0.172  1.00  0.00
ATOM     11  C   111     1      -0.172  -5.517  -0.028  1.00  0.00
ATOM     12  C   111     1      -1.296  -6.099  -0.732  1.00  0.00
ATOM     13  H   111     1      -1.517  -7.174  -0.772  1.00  0.00
ATOM     14  C   111     1      -1.994  -5.056  -1.284  1.00  0.00
ATOM     15  H   111     1      -2.909  -5.084  -1.891  1.00  0.00
ATOM     16  C   111     1      -1.269  -3.849  -0.944  1.00  0.00
ATOM     17  C   111     1       2.001   0.395  -0.118  1.00  0.00
ATOM     18  H   111     1       2.286   1.430  -0.360  1.00  0.00
ATOM     19  H   111     1       5.167  -0.604   3.124  1.00  0.00
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ATOM     20  C   111     1        4.335  -0.663   2.409  1.00  0.00
ATOM     21  C   111     1        3.508  -1.833   2.205  1.00  0.00
ATOM     22  H   111     1        4.263   1.312   1.373  1.00  0.00
ATOM     23  N   111     1        2.547  -1.597   1.234  1.00  0.00
ATOM     24  C   111     1        2.772  -0.293   0.819  1.00  0.00
ATOM     25  C   111     1        3.888   0.291   1.531  1.00  0.00
ATOM     26  C   111     1        0.724  -6.254   0.740  1.00  0.00
ATOM     27  H   111     1        0.600  -7.347   0.773  1.00  0.00
ATOM     28  H   111     1        4.183  -5.712   3.789  1.00  0.00
ATOM     29  C   111     1        3.390  -5.531   3.049  1.00  0.00
ATOM     30  C   111     1        2.581  -6.442   2.415  1.00  0.00
ATOM     31  H   111     1        2.553  -7.534   2.528  1.00  0.00
ATOM     32  C   111     1        1.728  -5.686   1.523  1.00  0.00
ATOM     33  N   111     1        2.016  -4.332   1.593  1.00  0.00
ATOM     34  C   111     1        3.042  -4.230   2.519  1.00  0.00
ATOM     35  C   111     1        3.716  -3.053   2.846  1.00  0.00
ATOM     36  H   111     1        4.517  -3.110   3.599  1.00  0.00
ATOM     37 Co   111     1        1.122  -2.849   0.622  1.00  0.00
ATOM     38  N   111     1       -0.184  -2.269   2.313  1.00  0.00
ATOM     39  S   111     1       -1.350  -3.253   3.335  1.00  0.00
ATOM     40  O   111     1       -1.273  -4.595   2.750  1.00  0.00
ATOM     41  O   111     1       -2.595  -2.467   3.420  1.00  0.00
ATOM     42  C   111     1       -0.539  -3.245   4.938  1.00  0.00
ATOM     43  C   111     1        0.684  -3.258   7.434  1.00  0.00
ATOM     44  C   111     1       -0.987  -2.341   5.917  1.00  0.00
ATOM     45  C   111     1        0.502  -4.159   5.176  1.00  0.00
ATOM     46  C   111     1        1.113  -4.156   6.440  1.00  0.00
ATOM     47  C   111     1       -0.363  -2.355   7.175  1.00  0.00
ATOM     48  H   111     1       -1.819  -1.655   5.696  1.00  0.00
ATOM     49  H   111     1        0.823  -4.860   4.390  1.00  0.00
ATOM     50  H   111     1        1.929  -4.867   6.647  1.00  0.00
ATOM     51  H   111     1       -0.702  -1.659   7.959  1.00  0.00
ATOM     52  H   111     1        1.168  -3.265   8.424  1.00  0.00
ATOM     53  N   111     1       -0.330  -1.044   2.498  1.00  0.00
ATOM     54  N   111     1       -0.390   0.100   2.597  1.00  0.00
CONECT    1    2    7   17
CONECT    2    4   37
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   37
CONECT   11   12   26
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   18   24
CONECT   19   20
CONECT   20   21   25
CONECT   21   23   35
CONECT   22   25
CONECT   23   24   37
CONECT   24   25
CONECT   26   27   32
CONECT   28   29
CONECT   29   30   34
CONECT   30   31   32
CONECT   32   33
CONECT   33   34   37
CONECT   34   35
CONECT   35   36
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CONECT   38   39   53
CONECT   39   40   41   42
CONECT   42   44   45
CONECT   43   46   47   52
CONECT   44   47   48
CONECT   45   46   49
CONECT   46   50
CONECT   47   51
CONECT   53   54
END



TS1_ Co(por)
Xyz file
54
 Energy =   -3316.5471059920
C     0.2077268    0.1249423    0.7091604
N     0.1693963   -1.1966840    0.2959149
H    -1.1428114    1.9096935    0.4114539
C    -0.9825884   -1.3082738   -0.4651116
C    -1.6667153   -0.0362972   -0.5433160
H    -2.5974065    0.1360829   -1.1000228
C    -0.9443704    0.8474324    0.2169429
C    -1.4587090   -2.4909887   -1.0238023
H    -2.3868876   -2.4499806   -1.6132890
N     0.2659566   -3.9586211   -0.0511655
C     0.3618903   -5.3339079    0.0844914
C    -0.7483099   -5.9876690   -0.5724822
H    -0.8934613   -7.0754634   -0.6181716
C    -1.5124175   -4.9954284   -1.1350397
H    -2.4325651   -5.0888945   -1.7270756
C    -0.8960931   -3.7398125   -0.7709790
C     1.2778224    0.7208359    1.3712068
H     1.1888875    1.7812890    1.6515197
H     5.8012853   -0.0096944    2.0963787
C     4.7327591   -0.1467831    1.8829442
C     4.1314777   -1.3972194    1.4795584
H     3.7678141    1.8306984    2.2539400
N     2.7694013   -1.2381888    1.2683338
C     2.5063402    0.0894793    1.5648999
C     3.7145929    0.7711350    1.9701409
C     1.4394930   -6.0079576    0.6576807
H     1.3971877   -7.1068862    0.7049005
H     5.9194731   -5.2520956    1.5855285
C     4.8448696   -5.1204143    1.4006831
C     3.8677837   -6.0788004    1.2942939
H     3.9682714   -7.1710345    1.3523986
C     2.6306070   -5.3789514    1.0211610
N     2.8342396   -4.0111378    1.0080158
C     4.1881432   -3.8399833    1.2492441
C     4.8190254   -2.6085906    1.4105123
H     5.9038276   -2.5998662    1.5945016
Co    1.4220326   -2.6223791    0.8152354
N     0.7883927   -2.9552705    2.5530723
S    -0.8345369   -2.4790475    3.0608696
O    -1.7425590   -3.0439515    2.0347035
O    -0.9282318   -1.0529004    3.4541029
C    -1.0487611   -3.4775502    4.5607651
C    -1.4839682   -4.9994492    6.8549076
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C    -1.0508658   -2.8410060    5.8111369
C    -1.2713454   -4.8587584    4.4313869
C    -1.4846208   -5.6197092    5.5915747
C    -1.2717859   -3.6137480    6.9637200
H    -0.8883753   -1.7535481    5.8654644
H    -1.2818079   -5.3223170    3.4328144
H    -1.6586535   -6.7052992    5.5085469
H    -1.2802699   -3.1279496    7.9535210
H    -1.6549284   -5.6019372    7.7623264
N     2.7999684   -2.5968760    4.0442096
N     1.6656487   -2.6054744    3.8885465
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Pdb file
HEADER B2Pdb
COMPND B2Pdb
ATOM      1  C   111     1       0.208   0.125   0.709  1.00  0.00
ATOM      2  N   111     1       0.169  -1.197   0.296  1.00  0.00
ATOM      3  H   111     1      -1.143   1.910   0.411  1.00  0.00
ATOM      4  C   111     1      -0.983  -1.308  -0.465  1.00  0.00
ATOM      5  C   111     1      -1.667  -0.036  -0.543  1.00  0.00
ATOM      6  H   111     1      -2.597   0.136  -1.100  1.00  0.00
ATOM      7  C   111     1      -0.944   0.847   0.217  1.00  0.00
ATOM      8  C   111     1      -1.459  -2.491  -1.024  1.00  0.00
ATOM      9  H   111     1      -2.387  -2.450  -1.613  1.00  0.00
ATOM     10  N   111     1       0.266  -3.959  -0.051  1.00  0.00
ATOM     11  C   111     1       0.362  -5.334   0.084  1.00  0.00
ATOM     12  C   111     1      -0.748  -5.988  -0.572  1.00  0.00
ATOM     13  H   111     1      -0.893  -7.075  -0.618  1.00  0.00
ATOM     14  C   111     1      -1.512  -4.995  -1.135  1.00  0.00
ATOM     15  H   111     1      -2.433  -5.089  -1.727  1.00  0.00
ATOM     16  C   111     1      -0.896  -3.740  -0.771  1.00  0.00
ATOM     17  C   111     1       1.278   0.721   1.371  1.00  0.00
ATOM     18  H   111     1       1.189   1.781   1.652  1.00  0.00
ATOM     19  H   111     1       5.801  -0.010   2.096  1.00  0.00
ATOM     20  C   111     1       4.733  -0.147   1.883  1.00  0.00
ATOM     21  C   111     1       4.131  -1.397   1.480  1.00  0.00
ATOM     22  H   111     1       3.768   1.831   2.254  1.00  0.00
ATOM     23  N   111     1       2.769  -1.238   1.268  1.00  0.00
ATOM     24  C   111     1       2.506   0.089   1.565  1.00  0.00
ATOM     25  C   111     1       3.715   0.771   1.970  1.00  0.00
ATOM     26  C   111     1       1.439  -6.008   0.658  1.00  0.00
ATOM     27  H   111     1       1.397  -7.107   0.705  1.00  0.00
ATOM     28  H   111     1       5.919  -5.252   1.586  1.00  0.00
ATOM     29  C   111     1       4.845  -5.120   1.401  1.00  0.00
ATOM     30  C   111     1       3.868  -6.079   1.294  1.00  0.00
ATOM     31  H   111     1       3.968  -7.171   1.352  1.00  0.00
ATOM     32  C   111     1       2.631  -5.379   1.021  1.00  0.00
ATOM     33  N   111     1       2.834  -4.011   1.008  1.00  0.00
ATOM     34  C   111     1       4.188  -3.840   1.249  1.00  0.00
ATOM     35  C   111     1       4.819  -2.609   1.411  1.00  0.00
ATOM     36  H   111     1       5.904  -2.600   1.595  1.00  0.00
ATOM     37 Co   111     1       1.422  -2.622   0.815  1.00  0.00
ATOM     38  N   111     1       0.788  -2.955   2.553  1.00  0.00
ATOM     39  S   111     1      -0.835  -2.479   3.061  1.00  0.00
ATOM     40  O   111     1      -1.743  -3.044   2.035  1.00  0.00
ATOM     41  O   111     1      -0.928  -1.053   3.454  1.00  0.00
ATOM     42  C   111     1      -1.049  -3.478   4.561  1.00  0.00
ATOM     43  C   111     1      -1.484  -4.999   6.855  1.00  0.00
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ATOM     44  C   111     1       -1.051  -2.841   5.811  1.00  0.00
ATOM     45  C   111     1       -1.271  -4.859   4.431  1.00  0.00
ATOM     46  C   111     1       -1.485  -5.620   5.592  1.00  0.00
ATOM     47  C   111     1       -1.272  -3.614   6.964  1.00  0.00
ATOM     48  H   111     1       -0.888  -1.754   5.865  1.00  0.00
ATOM     49  H   111     1       -1.282  -5.322   3.433  1.00  0.00
ATOM     50  H   111     1       -1.659  -6.705   5.509  1.00  0.00
ATOM     51  H   111     1       -1.280  -3.128   7.954  1.00  0.00
ATOM     52  H   111     1       -1.655  -5.602   7.762  1.00  0.00
ATOM     53  N   111     1        2.800  -2.597   4.044  1.00  0.00
ATOM     54  N   111     1        1.666  -2.605   3.889  1.00  0.00
CONECT    1    2    7   17
CONECT    2    4   37
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   37
CONECT   11   12   26
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   18   24
CONECT   19   20
CONECT   20   21   25
CONECT   21   23   35
CONECT   22   25
CONECT   23   24   37
CONECT   24   25
CONECT   26   27   32
CONECT   28   29
CONECT   29   30   34
CONECT   30   31   32
CONECT   32   33
CONECT   33   34   37
CONECT   34   35
CONECT   35   36
CONECT   37   38
CONECT   38   39   54
CONECT   39   40   41   42
CONECT   42   44   45
CONECT   43   46   47   52
CONECT   44   47   48
CONECT   45   46   49
CONECT   46   50
CONECT   47   51
CONECT   53   54
END



2C_ Co(por)
Xyz file
52
 Energy =   -3207.0247187560
C     0.2853322   -0.1824436    0.0192826
N     0.1018876   -1.5560165   -0.0544117
H    -0.9097225    1.6124277   -0.6382560
C    -1.1189933   -1.7171639   -0.6945731
C    -1.6913311   -0.4372147   -1.0419302
H    -2.6472581   -0.3067299   -1.5660922
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C    -0.8273506    0.5193780   -0.5756545
C    -1.7408081   -2.9348534   -0.9426827
H    -2.7140252   -2.9250902   -1.4554573
N    -0.0397358   -4.3378538    0.1592054
C    -0.0210633   -5.6797021    0.5101761
C    -1.2195572   -6.3460942    0.0537489
H    -1.4316949   -7.4136342    0.2002143
C    -1.9726054   -5.4001755   -0.5938046
H    -2.9471586   -5.5134865   -1.0866897
C    -1.2480799   -4.1547825   -0.4932460
C     1.4248069    0.4489718    0.5027308
H     1.4392085    1.5488606    0.5224665
H     5.7911435   -0.4896215    1.7452861
C     4.7325993   -0.5759681    1.4657967
C     4.0314035   -1.8285757    1.2918260
H     3.9622496    1.5091657    1.2706326
N     2.7174721   -1.6084602    0.9110218
C     2.5763933   -0.2307574    0.8876406
C     3.8191838    0.4208963    1.2336061
C     1.0392292   -6.3352793    1.1290262
H     0.9242337   -7.4067816    1.3532777
H     5.5037040   -5.7006934    2.2131319
C     4.4581571   -5.5455919    1.9149511
C     3.4340168   -6.4564083    1.8604924
H     3.4531246   -7.5292320    2.0944422
C     2.2688554   -5.7376207    1.3924236
N     2.5658147   -4.4057708    1.1687549
C     3.8988890   -4.2727192    1.5124975
C     4.6048551   -3.0731693    1.5381711
H     5.6647432   -3.1030864    1.8325480
Co    1.2536098   -2.9541290    0.7356772
N     0.7356492   -2.8595061    2.4519142
S    -0.7326879   -2.1476703    2.8899897
O    -1.9235031   -2.7867524    2.2605809
O    -0.6276541   -0.6596529    2.8922948
C    -0.6982260   -2.6777176    4.6278310
C    -0.6866441   -3.4662233    7.3037224
C     0.0184139   -1.9130816    5.5640344
C    -1.4132386   -3.8254399    5.0060521
C    -1.4054570   -4.2163048    6.3551216
C     0.0221427   -2.3163609    6.9086271
H     0.5524968   -1.0091040    5.2329461
H    -1.9756475   -4.3872386    4.2441415
H    -1.9679354   -5.1114819    6.6691292
H     0.5785933   -1.7260417    7.6554780
H    -0.6820130   -3.7778407    8.3615270
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Pdb file
HEADER B2Pdb
COMPND B2Pdb
ATOM      1  C   111     1       0.285  -0.182   0.019  1.00  0.00
ATOM      2  N   111     1       0.102  -1.556  -0.054  1.00  0.00
ATOM      3  H   111     1      -0.910   1.612  -0.638  1.00  0.00
ATOM      4  C   111     1      -1.119  -1.717  -0.695  1.00  0.00
ATOM      5  C   111     1      -1.691  -0.437  -1.042  1.00  0.00
ATOM      6  H   111     1      -2.647  -0.307  -1.566  1.00  0.00
ATOM      7  C   111     1      -0.827   0.519  -0.576  1.00  0.00
ATOM      8  C   111     1      -1.741  -2.935  -0.943  1.00  0.00
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ATOM      9  H   111     1      -2.714  -2.925  -1.455  1.00  0.00
ATOM     10  N   111     1      -0.040  -4.338   0.159  1.00  0.00
ATOM     11  C   111     1      -0.021  -5.680   0.510  1.00  0.00
ATOM     12  C   111     1      -1.220  -6.346   0.054  1.00  0.00
ATOM     13  H   111     1      -1.432  -7.414   0.200  1.00  0.00
ATOM     14  C   111     1      -1.973  -5.400  -0.594  1.00  0.00
ATOM     15  H   111     1      -2.947  -5.513  -1.087  1.00  0.00
ATOM     16  C   111     1      -1.248  -4.155  -0.493  1.00  0.00
ATOM     17  C   111     1       1.425   0.449   0.503  1.00  0.00
ATOM     18  H   111     1       1.439   1.549   0.522  1.00  0.00
ATOM     19  H   111     1       5.791  -0.490   1.745  1.00  0.00
ATOM     20  C   111     1       4.733  -0.576   1.466  1.00  0.00
ATOM     21  C   111     1       4.031  -1.829   1.292  1.00  0.00
ATOM     22  H   111     1       3.962   1.509   1.271  1.00  0.00
ATOM     23  N   111     1       2.717  -1.608   0.911  1.00  0.00
ATOM     24  C   111     1       2.576  -0.231   0.888  1.00  0.00
ATOM     25  C   111     1       3.819   0.421   1.234  1.00  0.00
ATOM     26  C   111     1       1.039  -6.335   1.129  1.00  0.00
ATOM     27  H   111     1       0.924  -7.407   1.353  1.00  0.00
ATOM     28  H   111     1       5.504  -5.701   2.213  1.00  0.00
ATOM     29  C   111     1       4.458  -5.546   1.915  1.00  0.00
ATOM     30  C   111     1       3.434  -6.456   1.860  1.00  0.00
ATOM     31  H   111     1       3.453  -7.529   2.094  1.00  0.00
ATOM     32  C   111     1       2.269  -5.738   1.392  1.00  0.00
ATOM     33  N   111     1       2.566  -4.406   1.169  1.00  0.00
ATOM     34  C   111     1       3.899  -4.273   1.512  1.00  0.00
ATOM     35  C   111     1       4.605  -3.073   1.538  1.00  0.00
ATOM     36  H   111     1       5.665  -3.103   1.833  1.00  0.00
ATOM     37 Co   111     1       1.254  -2.954   0.736  1.00  0.00
ATOM     38  N   111     1       0.736  -2.860   2.452  1.00  0.00
ATOM     39  S   111     1      -0.733  -2.148   2.890  1.00  0.00
ATOM     40  O   111     1      -1.924  -2.787   2.261  1.00  0.00
ATOM     41  O   111     1      -0.628  -0.660   2.892  1.00  0.00
ATOM     42  C   111     1      -0.698  -2.678   4.628  1.00  0.00
ATOM     43  C   111     1      -0.687  -3.466   7.304  1.00  0.00
ATOM     44  C   111     1       0.018  -1.913   5.564  1.00  0.00
ATOM     45  C   111     1      -1.413  -3.825   5.006  1.00  0.00
ATOM     46  C   111     1      -1.405  -4.216   6.355  1.00  0.00
ATOM     47  C   111     1       0.022  -2.316   6.909  1.00  0.00
ATOM     48  H   111     1       0.552  -1.009   5.233  1.00  0.00
ATOM     49  H   111     1      -1.976  -4.387   4.244  1.00  0.00
ATOM     50  H   111     1      -1.968  -5.111   6.669  1.00  0.00
ATOM     51  H   111     1       0.579  -1.726   7.655  1.00  0.00
ATOM     52  H   111     1      -0.682  -3.778   8.362  1.00  0.00
CONECT    1    2    7   17
CONECT    2    4   37
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   37
CONECT   11   12   26
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   18   24
CONECT   19   20
CONECT   20   21   25
CONECT   21   23   35
CONECT   22   25
CONECT   23   24   37
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CONECT   24   25
CONECT   26   27   32
CONECT   28   29
CONECT   29   30   34
CONECT   30   31   32
CONECT   32   33
CONECT   33   34   37
CONECT   34   35
CONECT   35   36
CONECT   37   38
CONECT   38   39
CONECT   39   40   41   42
CONECT   42   44   45
CONECT   43   46   47   52
CONECT   44   47   48
CONECT   45   46   49
CONECT   46   50
CONECT   47   51
END



TS2_ Co(por)
Xyz file
68
 Energy =   -3516.7575731470
C    -0.4378971   -0.3007667    0.7692505
N    -0.3413324   -1.6781181    0.8918205
H    -2.0082007    1.1071960   -0.0342571
C    -1.5394662   -2.1683007    0.3974381
C    -2.4031124   -1.0874715   -0.0233290
H    -3.4067687   -1.2220564   -0.4479148
C    -1.7025796    0.0737539    0.1764050
C    -1.8197380   -3.5134781    0.1811282
H    -2.8094582   -3.7804517   -0.2187312
N     0.4148220   -4.3419125    0.8077523
C     1.0468187   -5.5650315    0.6337897
C     0.1587213   -6.5132512   -0.0002411
H     0.4319506   -7.5444090   -0.2613682
C    -1.0432181   -5.8713729   -0.1761052
H    -1.9674239   -6.2562733   -0.6277444
C    -0.8667323   -4.5219813    0.3111208
C     0.5141816    0.6119063    1.2109203
H     4.2017769    0.8085142    4.0140039
C     3.3899172    0.4570633    3.3631485
C     3.0947609   -0.9342093    3.0955609
H     2.4117453    2.2869694    2.5441895
N     2.0244380   -1.0480635    2.2245089
C     1.6360498    0.2510011    1.9519878
C     2.5023622    1.1954090    2.6221157
C     2.3322693   -5.8782561    1.0763400
H     2.7164887   -6.8891175    0.8717591
H     5.6275666   -4.2407903    3.9053780
C     4.7389463   -4.3394495    3.2672420
C     4.3559407   -5.4036057    2.4885710
H     4.8513412   -6.3756512    2.3611488
C     3.1154217   -5.0215930    1.8483365
N     2.7669868   -3.7240803    2.1893255
C     3.7568312   -3.2978782    3.0558478
C     3.8735570   -1.9977934    3.5486050
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H	4.7039202	-1.7755157	4.2360865
Co	1.1069807	-2.7194274	1.7243398
N	0.3966769	-3.0160232	3.4226581
S	-0.9386979	-2.0857003	3.9301501
O	-2.2651018	-2.5690957	3.4555262
O	-0.6067461	-0.6409232	3.7565594
C	-0.8802206	-2.3429125	5.7313164
C	-0.9002546	-2.4240550	8.5250509
C	0.3186228	-2.1249050	6.4350459
C	-2.0859144	-2.5964808	6.4020604
C	-2.0914084	-2.6279398	7.8085399
C	0.3046317	-2.1782145	7.8373473
H	1.2476770	-1.9177427	5.8814263
H	-3.0032268	-2.7591823	5.8157327
H	-3.0356991	-2.8189064	8.3450861
H	1.2389423	-2.0161772	8.4006167
H	-0.9077826	-2.4537524	9.6274279
C	-0.9979856	-5.5946485	3.7755178
C	0.2236657	-5.0291700	4.1139555
H	1.0832761	-5.1834311	3.4499329
H	0.4699490	-4.7982520	5.1641077
H	-1.1528429	-5.8519751	2.7124242
C	-2.1253694	-5.8821668	4.6465394
C	-4.3611304	-6.5851040	6.2650625
C	-3.3715162	-6.2550492	4.0674007
C	-2.0359236	-5.8787936	6.0671174
C	-3.1354111	-6.2279771	6.8598265
C	-4.4725565	-6.5949415	4.8616224
H	-3.4624138	-6.2633720	2.9683466
H	-1.0819349	-5.6196805	6.5528367
H	-3.0354967	-6.2274555	7.9581268
H	-5.4279337	-6.8722581	4.3854735
H	-5.2240071	-6.8612175	6.8935475
H	0.3177188	1.6832001	1.0544442

Pdb file
HEADER B2Pdb
COMPND B2Pdb

ATOM	1	C	111	1	-0.438	-0.301	0.769	1.00	0.00
ATOM	2	N	111	1	-0.341	-1.678	0.892	1.00	0.00
ATOM	3	H	111	1	-2.008	1.107	-0.034	1.00	0.00
ATOM	4	C	111	1	-1.539	-2.168	0.397	1.00	0.00
ATOM	5	C	111	1	-2.403	-1.087	-0.023	1.00	0.00
ATOM	6	H	111	1	-3.407	-1.222	-0.448	1.00	0.00
ATOM	7	C	111	1	-1.703	0.074	0.176	1.00	0.00
ATOM	8	C	111	1	-1.820	-3.513	0.181	1.00	0.00
ATOM	9	H	111	1	-2.809	-3.780	-0.219	1.00	0.00
ATOM	10	N	111	1	0.415	-4.342	0.808	1.00	0.00
ATOM	11	C	111	1	1.047	-5.565	0.634	1.00	0.00
ATOM	12	C	111	1	0.159	-6.513	-0.000	1.00	0.00
ATOM	13	H	111	1	0.432	-7.544	-0.261	1.00	0.00
ATOM	14	C	111	1	-1.043	-5.871	-0.176	1.00	0.00
ATOM	15	H	111	1	-1.967	-6.256	-0.628	1.00	0.00
ATOM	16	C	111	1	-0.867	-4.522	0.311	1.00	0.00
ATOM	17	C	111	1	0.514	0.612	1.211	1.00	0.00
ATOM	18	H	111	1	4.202	0.809	4.014	1.00	0.00
ATOM	19	C	111	1	3.390	0.457	3.363	1.00	0.00
ATOM	20	C	111	1	3.095	-0.934	3.096	1.00	0.00

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ATOM     21  H   111     1       2.412   2.287   2.544  1.00  0.00
ATOM     22  N   111     1       2.024  -1.048   2.225  1.00  0.00
ATOM     23  C   111     1       1.636   0.251   1.952  1.00  0.00
ATOM     24  C   111     1       2.502   1.195   2.622  1.00  0.00
ATOM     25  C   111     1       2.332  -5.878   1.076  1.00  0.00
ATOM     26  H   111     1       2.716  -6.889   0.872  1.00  0.00
ATOM     27  H   111     1       5.628  -4.241   3.905  1.00  0.00
ATOM     28  C   111     1       4.739  -4.339   3.267  1.00  0.00
ATOM     29  C   111     1       4.356  -5.404   2.489  1.00  0.00
ATOM     30  H   111     1       4.851  -6.376   2.361  1.00  0.00
ATOM     31  C   111     1       3.115  -5.022   1.848  1.00  0.00
ATOM     32  N   111     1       2.767  -3.724   2.189  1.00  0.00
ATOM     33  C   111     1       3.757  -3.298   3.056  1.00  0.00
ATOM     34  C   111     1       3.874  -1.998   3.549  1.00  0.00
ATOM     35  H   111     1       4.704  -1.776   4.236  1.00  0.00
ATOM     36 Co   111     1       1.107  -2.719   1.724  1.00  0.00
ATOM     37  N   111     1       0.397  -3.016   3.423  1.00  0.00
ATOM     38  S   111     1      -0.939  -2.086   3.930  1.00  0.00
ATOM     39  O   111     1      -2.265  -2.569   3.456  1.00  0.00
ATOM     40  O   111     1      -0.607  -0.641   3.757  1.00  0.00
ATOM     41  C   111     1      -0.880  -2.343   5.731  1.00  0.00
ATOM     42  C   111     1      -0.900  -2.424   8.525  1.00  0.00
ATOM     43  C   111     1       0.319  -2.125   6.435  1.00  0.00
ATOM     44  C   111     1      -2.086  -2.596   6.402  1.00  0.00
ATOM     45  C   111     1      -2.091  -2.628   7.809  1.00  0.00
ATOM     46  C   111     1       0.305  -2.178   7.837  1.00  0.00
ATOM     47  H   111     1       1.248  -1.918   5.881  1.00  0.00
ATOM     48  H   111     1      -3.003  -2.759   5.816  1.00  0.00
ATOM     49  H   111     1      -3.036  -2.819   8.345  1.00  0.00
ATOM     50  H   111     1       1.239  -2.016   8.401  1.00  0.00
ATOM     51  H   111     1      -0.908  -2.454   9.627  1.00  0.00
ATOM     52  C   111     1      -0.998  -5.595   3.776  1.00  0.00
ATOM     53  C   111     1       0.224  -5.029   4.114  1.00  0.00
ATOM     54  H   111     1       1.083  -5.183   3.450  1.00  0.00
ATOM     55  H   111     1       0.470  -4.798   5.164  1.00  0.00
ATOM     56  H   111     1      -1.153  -5.852   2.712  1.00  0.00
ATOM     57  C   111     1      -2.125  -5.882   4.647  1.00  0.00
ATOM     58  C   111     1      -4.361  -6.585   6.265  1.00  0.00
ATOM     59  C   111     1      -3.372  -6.255   4.067  1.00  0.00
ATOM     60  C   111     1      -2.036  -5.879   6.067  1.00  0.00
ATOM     61  C   111     1      -3.135  -6.228   6.860  1.00  0.00
ATOM     62  C   111     1      -4.473  -6.595   4.862  1.00  0.00
ATOM     63  H   111     1      -3.462  -6.263   2.968  1.00  0.00
ATOM     64  H   111     1      -1.082  -5.620   6.553  1.00  0.00
ATOM     65  H   111     1      -3.035  -6.227   7.958  1.00  0.00
ATOM     66  H   111     1      -5.428  -6.872   4.385  1.00  0.00
ATOM     67  H   111     1      -5.224  -6.861   6.894  1.00  0.00
ATOM     68  H   111     1       0.318   1.683   1.054  1.00  0.00
CONECT    1    2    7   17
CONECT    2    4   36
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   36
CONECT   11   12   25
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   23   68
CONECT   18   19
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CONECT   19   20   24
CONECT   20   22   34
CONECT   21   24
CONECT   22   23   36
CONECT   23   24
CONECT   25   26   31
CONECT   27   28
CONECT   28   29   33
CONECT   29   30   31
CONECT   31   32
CONECT   32   33   36
CONECT   33   34
CONECT   34   35
CONECT   36   37
CONECT   37   38
CONECT   38   39   40   41
CONECT   41   43   44
CONECT   42   45   46   51
CONECT   43   46   47
CONECT   44   45   48
CONECT   45   49
CONECT   46   50
CONECT   52   53   56   57
CONECT   53   54   55
CONECT   57   59   60
CONECT   58   61   62   67
CONECT   59   62   63
CONECT   60   61   64
CONECT   61   65
CONECT   62   66
END



2D_Co(por)
Xyz file
68
 Energy =   -3516.7832811130
C    -0.1946079   -1.0268681   -0.6110940
N    -0.5015862   -2.3534625   -0.3744620
H    -1.2221658    0.6656316   -1.6991490
C    -1.7160822   -2.5618296   -1.0021948
C    -2.1977622   -1.3381053   -1.6103379
H    -3.1414705   -1.2473207   -2.1648545
C    -1.2384570   -0.3857059   -1.3823357
C    -2.3390897   -3.7979162   -1.1642477
N    -0.6191154   -5.1466583   -0.0195598
C    -0.4433983   -6.5122859    0.1326082
C    -1.4978611   -7.2436217   -0.5343398
H    -1.5714867   -8.3388863   -0.5698956
C    -2.3409997   -6.3060457   -1.0793269
H    -3.2550342   -6.4634708   -1.6677779
C    -1.7826422   -5.0111960   -0.7573723
C     0.9614237   -0.3797436   -0.1844330
H     4.6795512   -0.9930665    2.5140334
C     3.7544922   -1.1486121    1.9426684
C     3.0102352   -2.3903884    1.9034068
H     3.3393369    0.7728677    0.8880724
N     1.8990777   -2.2733163    1.0882624
C     1.9305413   -0.9718884    0.6202028
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C     3.0887045   -0.2690948    1.1277999
C     0.5707265   -7.1167070    0.8763794
H     0.5834989   -8.2158238    0.9326155
H     4.2248145   -6.1056002    3.5533250
C     3.3427674   -6.0346986    2.9024821
C     2.5742646   -7.0463553    2.3839581
H     2.6794924   -8.1309274    2.5212375
C     1.5541724   -6.4157494    1.5733640
N     1.6930565   -5.0370985    1.5916948
C     2.8008218   -4.7961594    2.3847324
C     3.4070672   -3.5530761    2.5637341
H     4.3059218   -3.5048199    3.1973348
Co    0.4771341   -3.6521036    0.7827779
N    -0.6533166   -3.4521221    2.4570153
S    -1.1506736   -1.9862182    3.1604299
O    -2.6261950   -1.9221844    3.3359619
O    -0.4491744   -0.8977959    2.4467138
C    -0.4524417   -2.0512886    4.8466143
C     0.6069420   -2.0419159    7.4345556
C     0.9404062   -2.1215683    5.0205462
C    -1.3213127   -1.9644984    5.9461455
C    -0.7835579   -1.9593111    7.2458373
C     1.4659853   -2.1220432    6.3223867
H     1.6024354   -2.1761701    4.1426852
H    -2.4054948   -1.8898739    5.7667626
H    -1.4566466   -1.8861552    8.1163628
H     2.5572251   -2.1813706    6.4703917
H     1.0260013   -2.0401143    8.4546283
H    -0.6157108   -5.5144880    2.8190699
C    -1.2301808   -4.6377177    3.1210015
H    -1.1543888   -4.5713798    4.2315125
C    -2.6373887   -4.7854398    2.6408492
H    -2.7436216   -4.8278030    1.5443469
C    -3.8383683   -4.7926738    3.4017921
C    -6.3045482   -4.9162236    4.8212431
C    -3.8732992   -4.7372677    4.8322410
C    -5.0919191   -4.9020535    2.7146127
C    -6.2987045   -4.9649890    3.4115209
C    -5.0850899   -4.8028641    5.5221487
H    -2.9334573   -4.6312125    5.3958918
H    -5.0859046   -4.9349729    1.6124429
H    -7.2493666   -5.0460005    2.8585520
H    -5.0891437   -4.7566867    6.6238245
H    -7.2580903   -4.9589486    5.3730520
H    -3.2881258   -3.8267951   -1.7211955
H     1.0972175    0.6755424   -0.4656154
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Pdb file
HEADER B2Pdb
COMPND B2Pdb
ATOM      1  C   111     1      -0.195  -1.027  -0.611  1.00  0.00
ATOM      2  N   111     1      -0.502  -2.353  -0.374  1.00  0.00
ATOM      3  H   111     1      -1.222   0.666  -1.699  1.00  0.00
ATOM      4  C   111     1      -1.716  -2.562  -1.002  1.00  0.00
ATOM      5  C   111     1      -2.198  -1.338  -1.610  1.00  0.00
ATOM      6  H   111     1      -3.141  -1.247  -2.165  1.00  0.00
ATOM      7  C   111     1      -1.238  -0.386  -1.382  1.00  0.00
ATOM      8  C   111     1      -2.339  -3.798  -1.164  1.00  0.00
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ATOM	9	N	111	1	-0.619	-5.147	-0.020	1.00	0.00
ATOM	10	C	111	1	-0.443	-6.512	0.133	1.00	0.00
ATOM	11	C	111	1	-1.498	-7.244	-0.534	1.00	0.00
ATOM	12	H	111	1	-1.571	-8.339	-0.570	1.00	0.00
ATOM	13	C	111	1	-2.341	-6.306	-1.079	1.00	0.00
ATOM	14	H	111	1	-3.255	-6.463	-1.668	1.00	0.00
ATOM	15	C	111	1	-1.783	-5.011	-0.757	1.00	0.00
ATOM	16	C	111	1	0.961	-0.380	-0.184	1.00	0.00
ATOM	17	H	111	1	4.680	-0.993	2.514	1.00	0.00
ATOM	18	C	111	1	3.754	-1.149	1.943	1.00	0.00
ATOM	19	C	111	1	3.010	-2.390	1.903	1.00	0.00
ATOM	20	H	111	1	3.339	0.773	0.888	1.00	0.00
ATOM	21	N	111	1	1.899	-2.273	1.088	1.00	0.00
ATOM	22	C	111	1	1.931	-0.972	0.620	1.00	0.00
ATOM	23	C	111	1	3.089	-0.269	1.128	1.00	0.00
ATOM	24	C	111	1	0.571	-7.117	0.876	1.00	0.00
ATOM	25	H	111	1	0.583	-8.216	0.933	1.00	0.00
ATOM	26	H	111	1	4.225	-6.106	3.553	1.00	0.00
ATOM	27	C	111	1	3.343	-6.035	2.902	1.00	0.00
ATOM	28	C	111	1	2.574	-7.046	2.384	1.00	0.00
ATOM	29	H	111	1	2.679	-8.131	2.521	1.00	0.00
ATOM	30	C	111	1	1.554	-6.416	1.573	1.00	0.00
ATOM	31	N	111	1	1.693	-5.037	1.592	1.00	0.00
ATOM	32	C	111	1	2.801	-4.796	2.385	1.00	0.00
ATOM	33	C	111	1	3.407	-3.553	2.564	1.00	0.00
ATOM	34	H	111	1	4.306	-3.505	3.197	1.00	0.00
ATOM	35	Co	111	1	0.477	-3.652	0.783	1.00	0.00
ATOM	36	N	111	1	-0.653	-3.452	2.457	1.00	0.00
ATOM	37	S	111	1	-1.151	-1.986	3.160	1.00	0.00
ATOM	38	O	111	1	-2.626	-1.922	3.336	1.00	0.00
ATOM	39	O	111	1	-0.449	-0.898	2.447	1.00	0.00
ATOM	40	C	111	1	-0.452	-2.051	4.847	1.00	0.00
ATOM	41	C	111	1	0.607	-2.042	7.435	1.00	0.00
ATOM	42	C	111	1	0.940	-2.122	5.021	1.00	0.00
ATOM	43	C	111	1	-1.321	-1.964	5.946	1.00	0.00
ATOM	44	C	111	1	-0.784	-1.959	7.246	1.00	0.00
ATOM	45	C	111	1	1.466	-2.122	6.322	1.00	0.00
ATOM	46	H	111	1	1.602	-2.176	4.143	1.00	0.00
ATOM	47	H	111	1	-2.405	-1.890	5.767	1.00	0.00
ATOM	48	H	111	1	-1.457	-1.886	8.116	1.00	0.00
ATOM	49	H	111	1	2.557	-2.181	6.470	1.00	0.00
ATOM	50	H	111	1	1.026	-2.040	8.455	1.00	0.00
ATOM	51	H	111	1	-0.616	-5.514	2.819	1.00	0.00
ATOM	52	C	111	1	-1.230	-4.638	3.121	1.00	0.00
ATOM	53	H	111	1	-1.154	-4.571	4.232	1.00	0.00
ATOM	54	C	111	1	-2.637	-4.785	2.641	1.00	0.00
ATOM	55	H	111	1	-2.744	-4.828	1.544	1.00	0.00
ATOM	56	C	111	1	-3.838	-4.793	3.402	1.00	0.00
ATOM	57	C	111	1	-6.305	-4.916	4.821	1.00	0.00
ATOM	58	C	111	1	-3.873	-4.737	4.832	1.00	0.00
ATOM	59	C	111	1	-5.092	-4.902	2.715	1.00	0.00
ATOM	60	C	111	1	-6.299	-4.965	3.412	1.00	0.00
ATOM	61	C	111	1	-5.085	-4.803	5.522	1.00	0.00
ATOM	62	H	111	1	-2.933	-4.631	5.396	1.00	0.00
ATOM	63	H	111	1	-5.086	-4.935	1.612	1.00	0.00
ATOM	64	H	111	1	-7.249	-5.046	2.859	1.00	0.00
ATOM	65	H	111	1	-5.089	-4.757	6.624	1.00	0.00
ATOM	66	H	111	1	-7.258	-4.959	5.373	1.00	0.00
ATOM	67	H	111	1	-3.288	-3.827	-1.721	1.00	0.00
ATOM	68	H	111	1	1.097	0.676	-0.466	1.00	0.00

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CONECT    2    4   35
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8   15   67
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CONECT   10   11   24
CONECT   11   12   13
CONECT   13   14   15
CONECT   16   22   68
CONECT   17   18
CONECT   18   19   23
CONECT   19   21   33
CONECT   20   23
CONECT   21   22   35
CONECT   22   23
CONECT   24   25   30
CONECT   26   27
CONECT   27   28   32
CONECT   28   29   30
CONECT   30   31
CONECT   31   32   35
CONECT   32   33
CONECT   33   34
CONECT   35   36
CONECT   36   37   52
CONECT   37   38   39   40
CONECT   40   42   43
CONECT   41   44   45   50
CONECT   42   45   46
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CONECT   45   49
CONECT   51   52
CONECT   52   53   54
CONECT   54   55   56
CONECT   56   58   59
CONECT   57   60   61   66
CONECT   58   61   62
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CONECT   60   64
CONECT   61   65
END
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TS3_ Co(por)
Xyz file
68
 Energy =   -3516.7839029750
C    -0.7569850   -0.8702460   -0.4334694
N    -0.9581023   -2.2200962   -0.2166526
H    -1.9553481    0.7719615   -1.4229370
C    -2.1960756   -2.4921527   -0.7676036
C    -2.7950947   -1.2903753   -1.3154801
H    -3.7769648   -1.2505528   -1.8059694
C    -1.8842382   -0.2841861   -1.1303655
C    -2.7458436   -3.7636003   -0.9163534
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H	-3.7372248	-3.8461917	-1.3874437
N	-0.8155214	-5.0093718	-0.0161349
C	-0.4949239	-6.3578236	0.0066546
C	-1.5389531	-7.1445252	-0.6117409
H	-1.5113298	-8.2361450	-0.7303143
C	-2.5242339	-6.2626767	-0.9878799
H	-3.4745733	-6.4713016	-1.4979597
C	-2.0581576	-4.9425439	-0.6245484
C	0.3527657	-0.1443881	-0.0115951
H	0.3952609	0.9266470	-0.2611342
H	4.1496670	-0.5302948	2.6253971
C	3.2317322	-0.7439842	2.0610824
C	2.6101241	-2.0482023	1.9630368
H	2.6256651	1.1778896	1.1032528
N	1.4739688	-1.9944101	1.1734765
C	1.3798087	-0.6758202	0.7655849
C	2.4745994	0.1072407	1.2960875
C	0.6329783	-6.9045866	0.6201538
H	0.7656530	-7.9964848	0.5747469
H	4.2792756	-5.7334683	3.2426522
C	3.3686477	-5.7028112	2.6289880
C	2.6995107	-6.7424067	2.0330931
H	2.9321857	-7.8155700	2.0594052
C	1.5799156	-6.1609395	1.3228101
N	1.5646484	-4.7817546	1.4701500
C	2.6719932	-4.4911996	2.2499212
C	3.1426676	-3.2079132	2.5271905
H	4.0496165	-3.1132847	3.1439625
Co	0.1952572	-3.4822912	0.7988912
N	-0.8887097	-3.4825066	2.6014758
S	-1.6317041	-2.1032014	3.3077153
O	-3.0692748	-2.3220380	3.6102348
O	-1.2331276	-0.9497293	2.4755348
C	-0.8044609	-1.8997539	4.9240956
C	0.4135134	-1.4433311	7.3984784
C	0.5825057	-1.6801829	4.9770242
C	-1.5924525	-1.8798454	6.0862030
C	-0.9753085	-1.6493310	7.3286467
C	1.1888588	-1.4584060	6.2239570
H	1.1780049	-1.6815508	4.0512322
H	-2.6802259	-2.0280235	5.9987403
H	-1.5857375	-1.6257070	8.2467340
H	2.2769216	-1.2887205	6.2774971
H	0.8954190	-1.2641721	8.3740074
H	-0.0111125	-5.3058860	3.2345573
C	-0.8975498	-4.6831251	3.4681471
H	-0.8844818	-4.4529038	4.5563531
C	-2.1758864	-5.2293495	2.9605173
H	-2.1470538	-5.5609344	1.9119614
C	-3.4369091	-5.3115298	3.6252046
C	-5.9563907	-5.6864059	4.8802042
C	-3.6126948	-5.0404279	5.0166406
C	-4.5720688	-5.7680547	2.8853624
C	-5.8097276	-5.9536672	3.5041207
C	-4.8516655	-5.2325832	5.6302857
H	-2.7622583	-4.6773889	5.6136495
H	-4.4503567	-5.9753125	1.8091747
H	-6.6726157	-6.3061621	2.9153974
H	-4.9684086	-5.0215878	6.7061846
H	-6.9338866	-5.8294840	5.3699113

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Pdb file
HEADER B2Pdb
COMPND B2Pdb
ATOM      1  C   111     1      -0.757  -0.870  -0.433  1.00  0.00
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ATOM      3  H   111     1      -1.955   0.772  -1.423  1.00  0.00
ATOM      4  C   111     1      -2.196  -2.492  -0.768  1.00  0.00
ATOM      5  C   111     1      -2.795  -1.290  -1.315  1.00  0.00
ATOM      6  H   111     1      -3.777  -1.251  -1.806  1.00  0.00
ATOM      7  C   111     1      -1.884  -0.284  -1.130  1.00  0.00
ATOM      8  C   111     1      -2.746  -3.764  -0.916  1.00  0.00
ATOM      9  H   111     1      -3.737  -3.846  -1.387  1.00  0.00
ATOM     10  N   111     1      -0.816  -5.009  -0.016  1.00  0.00
ATOM     11  C   111     1      -0.495  -6.358   0.007  1.00  0.00
ATOM     12  C   111     1      -1.539  -7.145  -0.612  1.00  0.00
ATOM     13  H   111     1      -1.511  -8.236  -0.730  1.00  0.00
ATOM     14  C   111     1      -2.524  -6.263  -0.988  1.00  0.00
ATOM     15  H   111     1      -3.475  -6.471  -1.498  1.00  0.00
ATOM     16  C   111     1      -2.058  -4.943  -0.625  1.00  0.00
ATOM     17  C   111     1       0.353  -0.144  -0.012  1.00  0.00
ATOM     18  H   111     1       0.395   0.927  -0.261  1.00  0.00
ATOM     19  H   111     1       4.150  -0.530   2.625  1.00  0.00
ATOM     20  C   111     1       3.232  -0.744   2.061  1.00  0.00
ATOM     21  C   111     1       2.610  -2.048   1.963  1.00  0.00
ATOM     22  H   111     1       2.626   1.178   1.103  1.00  0.00
ATOM     23  N   111     1       1.474  -1.994   1.173  1.00  0.00
ATOM     24  C   111     1       1.380  -0.676   0.766  1.00  0.00
ATOM     25  C   111     1       2.475   0.107   1.296  1.00  0.00
ATOM     26  C   111     1       0.633  -6.905   0.620  1.00  0.00
ATOM     27  H   111     1       0.766  -7.996   0.575  1.00  0.00
ATOM     28  H   111     1       4.279  -5.733   3.243  1.00  0.00
ATOM     29  C   111     1       3.369  -5.703   2.629  1.00  0.00
ATOM     30  C   111     1       2.700  -6.742   2.033  1.00  0.00
ATOM     31  H   111     1       2.932  -7.816   2.059  1.00  0.00
ATOM     32  C   111     1       1.580  -6.161   1.323  1.00  0.00
ATOM     33  N   111     1       1.565  -4.782   1.470  1.00  0.00
ATOM     34  C   111     1       2.672  -4.491   2.250  1.00  0.00
ATOM     35  C   111     1       3.143  -3.208   2.527  1.00  0.00
ATOM     36  H   111     1       4.050  -3.113   3.144  1.00  0.00
ATOM     37 Co   111     1       0.195  -3.482   0.799  1.00  0.00
ATOM     38  N   111     1      -0.889  -3.483   2.601  1.00  0.00
ATOM     39  S   111     1      -1.632  -2.103   3.308  1.00  0.00
ATOM     40  O   111     1      -3.069  -2.322   3.610  1.00  0.00
ATOM     41  O   111     1      -1.233  -0.950   2.476  1.00  0.00
ATOM     42  C   111     1      -0.804  -1.900   4.924  1.00  0.00
ATOM     43  C   111     1       0.414  -1.443   7.398  1.00  0.00
ATOM     44  C   111     1       0.583  -1.680   4.977  1.00  0.00
ATOM     45  C   111     1      -1.592  -1.880   6.086  1.00  0.00
ATOM     46  C   111     1      -0.975  -1.649   7.329  1.00  0.00
ATOM     47  C   111     1       1.189  -1.458   6.224  1.00  0.00
ATOM     48  H   111     1       1.178  -1.682   4.051  1.00  0.00
ATOM     49  H   111     1      -2.680  -2.028   5.999  1.00  0.00
ATOM     50  H   111     1      -1.586  -1.626   8.247  1.00  0.00
ATOM     51  H   111     1       2.277  -1.289   6.277  1.00  0.00
ATOM     52  H   111     1       0.895  -1.264   8.374  1.00  0.00
ATOM     53  H   111     1      -0.011  -5.306   3.235  1.00  0.00
ATOM     54  C   111     1      -0.898  -4.683   3.468  1.00  0.00
ATOM     55  H   111     1      -0.884  -4.453   4.556  1.00  0.00
ATOM     56  C   111     1      -2.176  -5.229   2.961  1.00  0.00
ATOM     57  H   111     1      -2.147  -5.561   1.912  1.00  0.00
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ATOM     58  C   111     1       -3.437  -5.312   3.625  1.00  0.00
ATOM     59  C   111     1       -5.956  -5.686   4.880  1.00  0.00
ATOM     60  C   111     1       -3.613  -5.040   5.017  1.00  0.00
ATOM     61  C   111     1       -4.572  -5.768   2.885  1.00  0.00
ATOM     62  C   111     1       -5.810  -5.954   3.504  1.00  0.00
ATOM     63  C   111     1       -4.852  -5.233   5.630  1.00  0.00
ATOM     64  H   111     1       -2.762  -4.677   5.614  1.00  0.00
ATOM     65  H   111     1       -4.450  -5.975   1.809  1.00  0.00
ATOM     66  H   111     1       -6.673  -6.306   2.915  1.00  0.00
ATOM     67  H   111     1       -4.968  -5.022   6.706  1.00  0.00
ATOM     68  H   111     1       -6.934  -5.829   5.370  1.00  0.00
CONECT    1    2    7   17
CONECT    2    4   37
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   37
CONECT   11   12   26
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   18   24
CONECT   19   20
CONECT   20   21   25
CONECT   21   23   35
CONECT   22   25
CONECT   23   24   37
CONECT   24   25
CONECT   26   27   32
CONECT   28   29
CONECT   29   30   34
CONECT   30   31   32
CONECT   32   33
CONECT   33   34   37
CONECT   34   35
CONECT   35   36
CONECT   37   38
CONECT   38   39   54
CONECT   39   40   41   42
CONECT   42   44   45
CONECT   43   46   47   52
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CONECT   46   50
CONECT   47   51
CONECT   53   54
CONECT   54   55   56
CONECT   56   57   58
CONECT   58   60   61
CONECT   59   62   63   68
CONECT   60   63   64
CONECT   61   62   65
CONECT   62   66
CONECT   63   67
END

E_ Co(por)
Xyz file
68
 Energy =   -3516.8076917220
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C	-0.3861610	-0.8069094	-0.4951784
N	-0.7856026	-2.1217313	-0.3213095
H	-1.3495194	1.0450882	-1.3587124
C	-2.0847005	-2.1621162	-0.8004224
C	-2.4993886	-0.8651182	-1.2914232
H	-3.4864703	-0.6490407	-1.7217336
C	-1.4337249	-0.0221903	-1.1132840
C	-2.8909703	-3.2957521	-0.8399243
H	-3.9189315	-3.1853311	-1.2170835
N	-1.1878235	-4.8841827	-0.0269796
C	-1.1700261	-6.2697092	0.0525151
C	-2.4449665	-6.8288233	-0.3430550
H	-2.6740876	-7.9028549	-0.3678511
C	-3.2511746	-5.7681412	-0.6720197
H	-4.2876544	-5.7774626	-1.0355953
C	-2.4557868	-4.5723948	-0.4919993
C	0.8318915	-0.2762973	-0.0816393
H	1.0137892	0.7951336	-0.2564791
H	4.7907330	-1.4426468	2.0338561
C	3.7877847	-1.4650869	1.5864539
C	2.9807901	-2.6584204	1.4380440
H	3.3454780	0.6200603	0.9279267
N	1.7669329	-2.3665647	0.8344059
C	1.8215961	-1.0083630	0.5684634
C	3.0687002	-0.4377960	1.0313706
C	-0.0771327	-7.0380295	0.4529824
H	-0.1866783	-8.1333147	0.4437843
H	4.2356028	-6.6573130	2.1204357
C	3.2356089	-6.4366156	1.7227197
C	2.2568586	-7.3115102	1.3225823
H	2.2719200	-8.4097635	1.3242669
C	1.1401236	-6.5074050	0.8771493
N	1.4277340	-5.1521080	0.9830425
C	2.7147110	-5.1053435	1.5030566
C	3.4276905	-3.9367814	1.7695346
H	4.4315191	-4.0338294	2.2111145
Co	0.2537899	-3.6076521	0.4875413
N	-0.6247849	-3.4105857	2.7093781
S	-1.6487008	-1.9866652	3.0045390
O	-2.9438644	-2.2908141	2.3651183
O	-0.7982265	-0.8526715	2.5989656
C	-1.9311120	-1.7671487	4.7846148
C	-2.4361827	-1.2307741	7.4746184
C	-0.9585771	-1.0887456	5.5431178
C	-3.1587068	-2.1608295	5.3408144
C	-3.4068958	-1.8845816	6.6952554
C	-1.2147083	-0.8336562	6.8998219
H	-0.0291057	-0.7441119	5.0638200
H	-3.9074526	-2.6655598	4.7121756
H	-4.3692289	-2.1819471	7.1423626
H	-0.4615411	-0.3056823	7.5073901
H	-2.6370244	-1.0182582	8.5376949
H	1.2990069	-4.1144685	3.4588107
C	0.2662640	-3.8990661	3.7806140
H	0.1678029	-3.4129269	4.7696985
C	-0.8726942	-4.7522335	3.3264116
H	-0.6325856	-5.5308032	2.5805224
C	-2.0511739	-5.1088023	4.1852269
C	-4.2539665	-5.9643467	5.7360436
C	-1.9061755	-5.3438922	5.5677766

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C    -3.3111183   -5.3229626    3.5819917
C    -4.4058217   -5.7386240    4.3555261
C    -3.0002958   -5.7702252    6.3395211
H    -0.9233751   -5.2006917    6.0466679
H    -3.4302957   -5.1521311    2.4999168
H    -5.3853038   -5.8955622    3.8741042
H    -2.8697684   -5.9541848    7.4189295
H    -5.1133152   -6.2998935    6.3401990
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Pdb file
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COMPND B2Pdb
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ATOM      2  N   111     1      -0.786  -2.122  -0.321  1.00  0.00
ATOM      3  H   111     1      -1.350   1.045  -1.359  1.00  0.00
ATOM      4  C   111     1      -2.085  -2.162  -0.800  1.00  0.00
ATOM      5  C   111     1      -2.499  -0.865  -1.291  1.00  0.00
ATOM      6  H   111     1      -3.486  -0.649  -1.722  1.00  0.00
ATOM      7  C   111     1      -1.434  -0.022  -1.113  1.00  0.00
ATOM      8  C   111     1      -2.891  -3.296  -0.840  1.00  0.00
ATOM      9  H   111     1      -3.919  -3.185  -1.217  1.00  0.00
ATOM     10  N   111     1      -1.188  -4.884  -0.027  1.00  0.00
ATOM     11  C   111     1      -1.170  -6.270   0.053  1.00  0.00
ATOM     12  C   111     1      -2.445  -6.829  -0.343  1.00  0.00
ATOM     13  H   111     1      -2.674  -7.903  -0.368  1.00  0.00
ATOM     14  C   111     1      -3.251  -5.768  -0.672  1.00  0.00
ATOM     15  H   111     1      -4.288  -5.777  -1.036  1.00  0.00
ATOM     16  C   111     1      -2.456  -4.572  -0.492  1.00  0.00
ATOM     17  C   111     1       0.832  -0.276  -0.082  1.00  0.00
ATOM     18  H   111     1       1.014   0.795  -0.256  1.00  0.00
ATOM     19  H   111     1       4.791  -1.443   2.034  1.00  0.00
ATOM     20  C   111     1       3.788  -1.465   1.586  1.00  0.00
ATOM     21  C   111     1       2.981  -2.658   1.438  1.00  0.00
ATOM     22  H   111     1       3.345   0.620   0.928  1.00  0.00
ATOM     23  N   111     1       1.767  -2.367   0.834  1.00  0.00
ATOM     24  C   111     1       1.822  -1.008   0.568  1.00  0.00
ATOM     25  C   111     1       3.069  -0.438   1.031  1.00  0.00
ATOM     26  C   111     1      -0.077  -7.038   0.453  1.00  0.00
ATOM     27  H   111     1      -0.187  -8.133   0.444  1.00  0.00
ATOM     28  H   111     1       4.236  -6.657   2.120  1.00  0.00
ATOM     29  C   111     1       3.236  -6.437   1.723  1.00  0.00
ATOM     30  C   111     1       2.257  -7.312   1.323  1.00  0.00
ATOM     31  H   111     1       2.272  -8.410   1.324  1.00  0.00
ATOM     32  C   111     1       1.140  -6.507   0.877  1.00  0.00
ATOM     33  N   111     1       1.428  -5.152   0.983  1.00  0.00
ATOM     34  C   111     1       2.715  -5.105   1.503  1.00  0.00
ATOM     35  C   111     1       3.428  -3.937   1.770  1.00  0.00
ATOM     36  H   111     1       4.432  -4.034   2.211  1.00  0.00
ATOM     37 Co   111     1       0.254  -3.608   0.488  1.00  0.00
ATOM     38  N   111     1      -0.625  -3.411   2.709  1.00  0.00
ATOM     39  S   111     1      -1.649  -1.987   3.005  1.00  0.00
ATOM     40  O   111     1      -2.944  -2.291   2.365  1.00  0.00
ATOM     41  O   111     1      -0.798  -0.853   2.599  1.00  0.00
ATOM     42  C   111     1      -1.931  -1.767   4.785  1.00  0.00
ATOM     43  C   111     1      -2.436  -1.231   7.475  1.00  0.00
ATOM     44  C   111     1      -0.959  -1.089   5.543  1.00  0.00
ATOM     45  C   111     1      -3.159  -2.161   5.341  1.00  0.00
ATOM     46  C   111     1      -3.407  -1.885   6.695  1.00  0.00
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ATOM     47  C   111     1       -1.215  -0.834   6.900  1.00  0.00
ATOM     48  H   111     1       -0.029  -0.744   5.064  1.00  0.00
ATOM     49  H   111     1       -3.907  -2.666   4.712  1.00  0.00
ATOM     50  H   111     1       -4.369  -2.182   7.142  1.00  0.00
ATOM     51  H   111     1       -0.462  -0.306   7.507  1.00  0.00
ATOM     52  H   111     1       -2.637  -1.018   8.538  1.00  0.00
ATOM     53  H   111     1        1.299  -4.114   3.459  1.00  0.00
ATOM     54  C   111     1        0.266  -3.899   3.781  1.00  0.00
ATOM     55  H   111     1        0.168  -3.413   4.770  1.00  0.00
ATOM     56  C   111     1       -0.873  -4.752   3.326  1.00  0.00
ATOM     57  H   111     1       -0.633  -5.531   2.581  1.00  0.00
ATOM     58  C   111     1       -2.051  -5.109   4.185  1.00  0.00
ATOM     59  C   111     1       -4.254  -5.964   5.736  1.00  0.00
ATOM     60  C   111     1       -1.906  -5.344   5.568  1.00  0.00
ATOM     61  C   111     1       -3.311  -5.323   3.582  1.00  0.00
ATOM     62  C   111     1       -4.406  -5.739   4.356  1.00  0.00
ATOM     63  C   111     1       -3.000  -5.770   6.340  1.00  0.00
ATOM     64  H   111     1       -0.923  -5.201   6.047  1.00  0.00
ATOM     65  H   111     1       -3.430  -5.152   2.500  1.00  0.00
ATOM     66  H   111     1       -5.385  -5.896   3.874  1.00  0.00
ATOM     67  H   111     1       -2.870  -5.954   7.419  1.00  0.00
ATOM     68  H   111     1       -5.113  -6.300   6.340  1.00  0.00
CONECT    1    2    7   17
CONECT    2    4   37
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   37
CONECT   11   12   26
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   18   24
CONECT   19   20
CONECT   20   21   25
CONECT   21   23   35
CONECT   22   25
CONECT   23   24   37
CONECT   24   25
CONECT   26   27   32
CONECT   28   29
CONECT   29   30   34
CONECT   30   31   32
CONECT   32   33
CONECT   33   34   37
CONECT   34   35
CONECT   35   36
CONECT   38   39   54   56
CONECT   39   40   41   42
CONECT   42   44   45
CONECT   43   46   47   52
CONECT   44   47   48
CONECT   45   46   49
CONECT   46   50
CONECT   47   51
CONECT   53   54
CONECT   54   55   56
CONECT   56   57   58
CONECT   58   60   61
CONECT   59   62   63   68
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CONECT   60   63   64
CONECT   61   62   65
CONECT   62   66
CONECT   63   67
END


A_Co(PorAmide)
Xyz file
54
 Energy =   -2811.1075001490
C     0.3363138   -0.3121408    0.7816775
N     0.1964114   -1.6695270    0.5280665
H    -0.9660693    1.5062858    0.4727998
C    -1.0641691   -1.7897464   -0.0379822
C    -1.7121259   -0.5016511   -0.1518494
H    -2.7144790   -0.3437875   -0.5722288
C    -0.8421072    0.4196791    0.3715414
C    -1.6641030   -2.9902562   -0.4045894
N     0.1832686   -4.4773158    0.3003062
C     0.2966973   -5.8634520    0.3312757
C    -0.9184484   -6.4922278   -0.1466751
H    -1.0758876   -7.5755288   -0.2083072
C    -1.7700045   -5.4797451   -0.5024220
H    -2.7853665   -5.5479202   -0.9154385
C    -1.0845327   -4.2412602   -0.2143009
C     1.4642613    0.2900410    1.3309289
H     5.8186787   -0.6624574    2.6000851
C     4.7764425   -0.7444343    2.2637841
C     4.1362149   -1.9807037    1.8720435
H     3.9261243    1.3168896    2.3360323
N     2.8185709   -1.7663972    1.4956441
C     2.6307859   -0.3996616    1.6474074
C     3.8323570    0.2412799    2.1348712
C     1.4361418   -6.5854395    0.7213562
H     5.8407334   -5.8478421    1.9996238
C     4.7883483   -5.7071408    1.7187606
C     3.8463606   -6.6555568    1.4180823
H     3.9545958   -7.7465273    1.3879105
C     2.6239991   -5.9419931    1.1078607
N     2.8077709   -4.5684648    1.2230337
C     4.1348857   -4.4238949    1.6060226
C     4.7680417   -3.2197125    1.8994479
Co    1.5021587   -3.1202261    0.8848174
C     1.3978901   -8.0868491    0.6925234
C     1.3333776  -10.9064247    0.6134159
C     1.5628136   -8.7795014   -0.5230488
C     1.1940312   -8.8339088    1.8917455
C     1.1644739  -10.2475154    1.8397322
C     1.5327103  -10.1823530   -0.5739735
H     1.7222797   -8.1940409   -1.4435915
H     1.0071191  -10.8019758    2.7733861
H     1.6666170  -10.7043636   -1.5353473
H     1.3072200  -12.0087201    0.5913650
N     1.0228821   -8.1137579    3.0899531
C     0.8489078   -8.5840889    4.3870398
O     0.7976751   -9.7727704    4.6869416
C     0.7393683   -7.4641491    5.4228761
H     1.6995899   -6.9066054    5.5061359
H     0.5039835   -7.9182894    6.4048568
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H    -0.0558041   -6.7319035    5.1582568
H     1.0547060   -7.0947262    2.9725449
H     5.8249358   -3.2552500    2.2043525
H     1.4455216    1.3788554    1.4907989
H    -2.6761676   -2.9528261   -0.8355491
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Pdb file
HEADER B2Pdb
COMPND B2Pdb
ATOM      1  C   111     1       0.336  -0.312   0.782  1.00  0.00
ATOM      2  N   111     1       0.196  -1.670   0.528  1.00  0.00
ATOM      3  H   111     1      -0.966   1.506   0.473  1.00  0.00
ATOM      4  C   111     1      -1.064  -1.790  -0.038  1.00  0.00
ATOM      5  C   111     1      -1.712  -0.502  -0.152  1.00  0.00
ATOM      6  H   111     1      -2.714  -0.344  -0.572  1.00  0.00
ATOM      7  C   111     1      -0.842   0.420   0.372  1.00  0.00
ATOM      8  C   111     1      -1.664  -2.990  -0.405  1.00  0.00
ATOM      9  N   111     1       0.183  -4.477   0.300  1.00  0.00
ATOM     10  C   111     1       0.297  -5.863   0.331  1.00  0.00
ATOM     11  C   111     1      -0.918  -6.492  -0.147  1.00  0.00
ATOM     12  H   111     1      -1.076  -7.576  -0.208  1.00  0.00
ATOM     13  C   111     1      -1.770  -5.480  -0.502  1.00  0.00
ATOM     14  H   111     1      -2.785  -5.548  -0.915  1.00  0.00
ATOM     15  C   111     1      -1.085  -4.241  -0.214  1.00  0.00
ATOM     16  C   111     1       1.464   0.290   1.331  1.00  0.00
ATOM     17  H   111     1       5.819  -0.662   2.600  1.00  0.00
ATOM     18  C   111     1       4.776  -0.744   2.264  1.00  0.00
ATOM     19  C   111     1       4.136  -1.981   1.872  1.00  0.00
ATOM     20  H   111     1       3.926   1.317   2.336  1.00  0.00
ATOM     21  N   111     1       2.819  -1.766   1.496  1.00  0.00
ATOM     22  C   111     1       2.631  -0.400   1.647  1.00  0.00
ATOM     23  C   111     1       3.832   0.241   2.135  1.00  0.00
ATOM     24  C   111     1       1.436  -6.585   0.721  1.00  0.00
ATOM     25  H   111     1       5.841  -5.848   2.000  1.00  0.00
ATOM     26  C   111     1       4.788  -5.707   1.719  1.00  0.00
ATOM     27  C   111     1       3.846  -6.656   1.418  1.00  0.00
ATOM     28  H   111     1       3.955  -7.747   1.388  1.00  0.00
ATOM     29  C   111     1       2.624  -5.942   1.108  1.00  0.00
ATOM     30  N   111     1       2.808  -4.568   1.223  1.00  0.00
ATOM     31  C   111     1       4.135  -4.424   1.606  1.00  0.00
ATOM     32  C   111     1       4.768  -3.220   1.899  1.00  0.00
ATOM     33 Co   111     1       1.502  -3.120   0.885  1.00  0.00
ATOM     34  C   111     1       1.398  -8.087   0.693  1.00  0.00
ATOM     35  C   111     1       1.333 -10.906   0.613  1.00  0.00
ATOM     36  C   111     1       1.563  -8.780  -0.523  1.00  0.00
ATOM     37  C   111     1       1.194  -8.834   1.892  1.00  0.00
ATOM     38  C   111     1       1.164 -10.248   1.840  1.00  0.00
ATOM     39  C   111     1       1.533 -10.182  -0.574  1.00  0.00
ATOM     40  H   111     1       1.722  -8.194  -1.444  1.00  0.00
ATOM     41  H   111     1       1.007 -10.802   2.773  1.00  0.00
ATOM     42  H   111     1       1.667 -10.704  -1.535  1.00  0.00
ATOM     43  H   111     1       1.307 -12.009   0.591  1.00  0.00
ATOM     44  N   111     1       1.023  -8.114   3.090  1.00  0.00
ATOM     45  C   111     1       0.849  -8.584   4.387  1.00  0.00
ATOM     46  O   111     1       0.798  -9.773   4.687  1.00  0.00
ATOM     47  C   111     1       0.739  -7.464   5.423  1.00  0.00
ATOM     48  H   111     1       1.700  -6.907   5.506  1.00  0.00
ATOM     49  H   111     1       0.504  -7.918   6.405  1.00  0.00
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ATOM     50  H   111     1       -0.056  -6.732   5.158  1.00  0.00
ATOM     51  H   111     1        1.055  -7.095   2.973  1.00  0.00
ATOM     52  H   111     1        5.825  -3.255   2.204  1.00  0.00
ATOM     53  H   111     1        1.446   1.379   1.491  1.00  0.00
ATOM     54  H   111     1       -2.676  -2.953  -0.836  1.00  0.00
CONECT    1    2    7   16
CONECT    2    4   33
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8   15   54
CONECT    9   10   15   33
CONECT   10   11   24
CONECT   11   12   13
CONECT   13   14   15
CONECT   16   22   53
CONECT   17   18
CONECT   18   19   23
CONECT   19   21   32
CONECT   20   23
CONECT   21   22   33
CONECT   22   23
CONECT   24   29   34
CONECT   25   26
CONECT   26   27   31
CONECT   27   28   29
CONECT   29   30
CONECT   30   31   33
CONECT   31   32
CONECT   32   52
CONECT   34   36   37
CONECT   35   38   39   43
CONECT   36   39   40
CONECT   37   38   44
CONECT   38   41
CONECT   39   42
CONECT   44   45   51
CONECT   45   46   47
CONECT   47   48   49   50
END


B_ Co(PorAmide)
Xyz file
71
 Energy =   -3755.8140616240
C     0.7292434    0.0243372   -0.0655284
N     0.3779670   -1.3123060   -0.1775781
H    -0.0370833    1.9438359   -0.9806001
C    -0.6775140   -1.3347827   -1.0773047
C    -0.9882823    0.0051847   -1.5346377
C    -0.1235394    0.8523698   -0.8894066
C    -1.4086874   -2.4726983   -1.4601221
N    -0.1956967   -4.0261315    0.0554091
C    -0.3948952   -5.3599424    0.3754856
C    -1.5114801   -5.9086522   -0.3623472
H    -1.8595395   -6.9475024   -0.2863177
C    -1.9782193   -4.9055025   -1.1703024
H    -2.7967496   -4.9383677   -1.8993289
C    -1.1730627   -3.7331063   -0.8853283
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C	1.8029513	0.5227212	0.6715330
H	1.9685454	1.6110795	0.6649434
H	5.6504102	-0.8997395	2.8367771
C	4.6678489	-0.8640314	2.3471513
C	3.8550371	-2.0243183	2.0503874
H	4.2432569	1.2908308	1.9558058
N	2.6768003	-1.6552992	1.4189172
C	2.7403955	-0.2754971	1.3242675
C	3.9624466	0.2297899	1.9128651
C	0.4168945	-6.1256236	1.2103091
H	4.5916202	-6.0382338	3.2305517
C	3.6590253	-5.7552910	2.7241224
C	2.5633556	-6.5316296	2.4433930
H	2.4008159	-7.5965838	2.6574048
C	1.6193588	-5.6783454	1.7541532
N	2.1110734	-4.3887574	1.6336217
C	3.3609256	-4.4265682	2.2345826
C	4.1989056	-3.3265606	2.4090031
H	5.1679922	-3.4875011	2.9056223
Co	1.1766318	-2.8240021	0.8221551
N	0.0560791	-2.4601238	2.6852093
S	-1.6936360	-2.0404979	2.9666036
O	-2.2346595	-3.0248274	3.9208866
O	-2.2236265	-1.8774268	1.6040772
C	-1.5843839	-0.4365556	3.7633575
C	-1.4303274	2.0407912	5.0092217
C	-1.6974689	-0.3753219	5.1632969
C	-1.4018550	0.7083339	2.9678363
C	-1.3258122	1.9544110	3.6085912
C	-1.6171937	0.8817930	5.7835197
H	-1.8607250	-1.2940261	5.7468954
H	-1.3259360	0.6226992	1.8724139
H	-1.1868178	2.8661813	3.0058824
H	-1.7078340	0.9545672	6.8794166
H	-1.3696389	3.0244461	5.5031338
N	0.6349380	-2.7752402	3.7476558
N	1.2695744	-3.0830819	4.6553757
H	0.1342947	-7.1761378	1.3779258
H	-1.7770844	0.2491346	-2.2562334
C	-2.4866721	-2.3281179	-2.4941657
C	-4.4472064	-2.0755449	-4.5071935
C	-2.1227875	-2.2070682	-3.8509395
C	-3.8713714	-2.3089805	-2.1423537
C	-4.8425246	-2.1871732	-3.1666276
C	-3.0880731	-2.0809066	-4.8615810
H	-1.0506060	-2.2232036	-4.1065860
H	-5.9016189	-2.1852310	-2.8814406
H	-2.7792285	-1.9933177	-5.9158422
H	-5.2225937	-1.9811264	-5.2860425
N	-4.2195367	-2.4063680	-0.7805124
H	-3.4285759	-2.3989496	-0.1220274
C	-5.4864917	-2.5170361	-0.2174935
O	-6.5303391	-2.5384169	-0.8653056
C	-5.4832450	-2.5793216	1.3089685
H	-5.4484011	-1.5469895	1.7250840
H	-4.6192821	-3.1378896	1.7251518
H	-6.4318685	-3.0487046	1.6367886

Pdb file
HEADER B2Pdb
COMPND B2Pdb

ATOM	1	C	111	1	0.729	0.024	-0.066	1.00	0.00
ATOM	2	N	111	1	0.378	-1.312	-0.178	1.00	0.00
ATOM	3	H	111	1	-0.037	1.944	-0.981	1.00	0.00
ATOM	4	C	111	1	-0.678	-1.335	-1.077	1.00	0.00
ATOM	5	C	111	1	-0.988	0.005	-1.535	1.00	0.00
ATOM	6	C	111	1	-0.124	0.852	-0.889	1.00	0.00
ATOM	7	C	111	1	-1.409	-2.473	-1.460	1.00	0.00
ATOM	8	N	111	1	-0.196	-4.026	0.055	1.00	0.00
ATOM	9	C	111	1	-0.395	-5.360	0.375	1.00	0.00
ATOM	10	C	111	1	-1.511	-5.909	-0.362	1.00	0.00
ATOM	11	H	111	1	-1.860	-6.948	-0.286	1.00	0.00
ATOM	12	C	111	1	-1.978	-4.906	-1.170	1.00	0.00
ATOM	13	H	111	1	-2.797	-4.938	-1.899	1.00	0.00
ATOM	14	C	111	1	-1.173	-3.733	-0.885	1.00	0.00
ATOM	15	C	111	1	1.803	0.523	0.672	1.00	0.00
ATOM	16	H	111	1	1.969	1.611	0.665	1.00	0.00
ATOM	17	H	111	1	5.650	-0.900	2.837	1.00	0.00
ATOM	18	C	111	1	4.668	-0.864	2.347	1.00	0.00
ATOM	19	C	111	1	3.855	-2.024	2.050	1.00	0.00
ATOM	20	H	111	1	4.243	1.291	1.956	1.00	0.00
ATOM	21	N	111	1	2.677	-1.655	1.419	1.00	0.00
ATOM	22	C	111	1	2.740	-0.275	1.324	1.00	0.00
ATOM	23	C	111	1	3.962	0.230	1.913	1.00	0.00
ATOM	24	C	111	1	0.417	-6.126	1.210	1.00	0.00
ATOM	25	H	111	1	4.592	-6.038	3.231	1.00	0.00
ATOM	26	C	111	1	3.659	-5.755	2.724	1.00	0.00
ATOM	27	C	111	1	2.563	-6.532	2.443	1.00	0.00
ATOM	28	H	111	1	2.401	-7.597	2.657	1.00	0.00
ATOM	29	C	111	1	1.619	-5.678	1.754	1.00	0.00
ATOM	30	N	111	1	2.111	-4.389	1.634	1.00	0.00
ATOM	31	C	111	1	3.361	-4.427	2.235	1.00	0.00
ATOM	32	C	111	1	4.199	-3.327	2.409	1.00	0.00
ATOM	33	H	111	1	5.168	-3.488	2.906	1.00	0.00
ATOM	34	Co	111	1	1.177	-2.824	0.822	1.00	0.00
ATOM	35	N	111	1	0.056	-2.460	2.685	1.00	0.00
ATOM	36	S	111	1	-1.694	-2.040	2.967	1.00	0.00
ATOM	37	O	111	1	-2.235	-3.025	3.921	1.00	0.00
ATOM	38	O	111	1	-2.224	-1.877	1.604	1.00	0.00
ATOM	39	C	111	1	-1.584	-0.437	3.763	1.00	0.00
ATOM	40	C	111	1	-1.430	2.041	5.009	1.00	0.00
ATOM	41	C	111	1	-1.697	-0.375	5.163	1.00	0.00
ATOM	42	C	111	1	-1.402	0.708	2.968	1.00	0.00
ATOM	43	C	111	1	-1.326	1.954	3.609	1.00	0.00
ATOM	44	C	111	1	-1.617	0.882	5.784	1.00	0.00
ATOM	45	H	111	1	-1.861	-1.294	5.747	1.00	0.00
ATOM	46	H	111	1	-1.326	0.623	1.872	1.00	0.00
ATOM	47	H	111	1	-1.187	2.866	3.006	1.00	0.00
ATOM	48	H	111	1	-1.708	0.955	6.879	1.00	0.00
ATOM	49	H	111	1	-1.370	3.024	5.503	1.00	0.00
ATOM	50	N	111	1	0.635	-2.775	3.748	1.00	0.00
ATOM	51	N	111	1	1.270	-3.083	4.655	1.00	0.00
ATOM	52	H	111	1	0.134	-7.176	1.378	1.00	0.00
ATOM	53	H	111	1	-1.777	0.249	-2.256	1.00	0.00
ATOM	54	C	111	1	-2.487	-2.328	-2.494	1.00	0.00
ATOM	55	C	111	1	-4.447	-2.076	-4.507	1.00	0.00
ATOM	56	C	111	1	-2.123	-2.207	-3.851	1.00	0.00
ATOM	57	C	111	1	-3.871	-2.309	-2.142	1.00	0.00

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ATOM     58  C   111     1       -4.843  -2.187  -3.167  1.00  0.00
ATOM     59  C   111     1       -3.088  -2.081  -4.862  1.00  0.00
ATOM     60  H   111     1       -1.051  -2.223  -4.107  1.00  0.00
ATOM     61  H   111     1       -5.902  -2.185  -2.881  1.00  0.00
ATOM     62  H   111     1       -2.779  -1.993  -5.916  1.00  0.00
ATOM     63  H   111     1       -5.223  -1.981  -5.286  1.00  0.00
ATOM     64  N   111     1       -4.220  -2.406  -0.781  1.00  0.00
ATOM     65  H   111     1       -3.429  -2.399  -0.122  1.00  0.00
ATOM     66  C   111     1       -5.486  -2.517  -0.217  1.00  0.00
ATOM     67  O   111     1       -6.530  -2.538  -0.865  1.00  0.00
ATOM     68  C   111     1       -5.483  -2.579   1.309  1.00  0.00
ATOM     69  H   111     1       -5.448  -1.547   1.725  1.00  0.00
ATOM     70  H   111     1       -4.619  -3.138   1.725  1.00  0.00
ATOM     71  H   111     1       -6.432  -3.049   1.637  1.00  0.00
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CONECT    2    4   34
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CONECT    4    5    7
CONECT    5    6   53
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CONECT   10   11   12
CONECT   12   13   14
CONECT   15   16   22
CONECT   17   18
CONECT   18   19   23
CONECT   19   21   32
CONECT   20   23
CONECT   21   22   34
CONECT   22   23
CONECT   24   29   52
CONECT   25   26
CONECT   26   27   31
CONECT   27   28   29
CONECT   29   30
CONECT   30   31   34
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CONECT   32   33
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CONECT   39   41   42
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CONECT   50   51
CONECT   54   56   57
CONECT   55   58   59   63
CONECT   56   59   60
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CONECT   58   61
CONECT   59   62
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CONECT   66   67   68
CONECT   68   69   70   71
END
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TS1_ Co(PorAmide)
Xyz file
71
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C	0.8911866	0.0039595	-0.4676614
N	0.5240908	-1.3331334	-0.4521470
H	0.2055401	1.8129603	-1.6300550
C	-0.5165906	-1.4372526	-1.3643417
C	-0.7594722	-0.1614222	-2.0021521
C	0.0948758	0.7404885	-1.4206375
C	-1.3265001	-2.5662462	-1.5618625
N	-0.2371279	-3.9068261	0.2205000
C	-0.5453287	-5.1303096	0.7957844
C	-1.7249840	-5.6990328	0.1866571
H	-2.1654061	-6.6654897	0.4650401
C	-2.1136681	-4.8340575	-0.8023292
H	-2.9472443	-4.9297119	-1.5083321
C	-1.2023073	-3.7088659	-0.7556870
C	1.9478992	0.5615079	0.2501201
H	2.1254484	1.6429921	0.1481404
H	5.8857480	-0.8041051	2.2764620
C	4.8668963	-0.7716768	1.8679017
C	4.0048440	-1.9243009	1.7186196
H	4.4625530	1.3657233	1.3741715
N	2.7923303	-1.5594745	1.1563236
C	2.8802971	-0.1945479	0.9584279
C	4.1521652	0.3135230	1.4259897
C	0.2488629	-5.8080530	1.7162554
H	4.6187201	-5.8197315	3.2735587
C	3.6594974	-5.5244957	2.8278844
C	2.4768525	-6.2221774	2.7942933
H	2.2577351	-7.2224932	3.1911518
C	1.5307264	-5.3973341	2.0800390
N	2.1090505	-4.1952922	1.7050472
C	3.4123188	-4.2564769	2.1834634
C	4.3304830	-3.2088960	2.1456933
H	5.3340562	-3.3817908	2.5627779
Co	1.1798752	-2.6838603	0.8145998
N	0.2945611	-1.9993896	2.3282896
S	-1.4563199	-1.9247870	2.4435612
O	-2.0993658	-3.2078378	2.8228989
O	-1.8982056	-1.2261060	1.2015162
C	-1.6965629	-0.7580285	3.8075348
C	-2.1522039	1.0461965	5.8796545
C	-2.1761738	-1.2390018	5.0357463
C	-1.4481521	0.6074562	3.5880959
C	-1.6770241	1.5098531	4.6386978
C	-2.4039011	-0.3231906	6.0764104
H	-2.3714956	-2.3151978	5.1597854
H	-1.0866064	0.9521245	2.6071197
H	-1.4873342	2.5850781	4.4857717
H	-2.7831319	-0.6835034	7.0467188
H	-2.3313342	1.7605843	6.6999920
N	0.6896454	-2.4222011	3.8434773
N	1.6876215	-2.8009233	4.2621130
H	-0.1092730	-6.7793181	2.0889482
H	-1.5134455	0.0094176	-2.7797614
C	-2.4274750	-2.5068903	-2.5763369
C	-4.4609721	-2.4561164	-4.5232129
C	-2.1300160	-2.7228708	-3.9366488

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C    -3.7759941   -2.2421582   -2.1842047
C    -4.7861593   -2.2286976   -3.1786612
C    -3.1346374   -2.6999819   -4.9163426
H    -1.0833664   -2.9238834   -4.2191590
H    -5.8201378   -2.0409841   -2.8647010
H    -2.8822656   -2.8772473   -5.9743996
H    -5.2665703   -2.4382319   -5.2764709
N    -4.0476152   -1.9992428   -0.8253659
H    -3.2270388   -1.8901809   -0.2051719
C    -5.2902837   -1.8864816   -0.2050338
O    -6.3647671   -1.9710117   -0.7952552
C    -5.2007928   -1.6382928    1.2983823
H    -4.7593953   -0.6381860    1.5042769
H    -4.5570908   -2.3897962    1.8050333
H    -6.2259271   -1.6771249    1.7156120
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Pdb file
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COMPND B2Pdb
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ATOM      2  N   111     1       0.524  -1.333  -0.452  1.00  0.00
ATOM      3  H   111     1       0.206   1.813  -1.630  1.00  0.00
ATOM      4  C   111     1      -0.517  -1.437  -1.364  1.00  0.00
ATOM      5  C   111     1      -0.759  -0.161  -2.002  1.00  0.00
ATOM      6  C   111     1       0.095   0.740  -1.421  1.00  0.00
ATOM      7  C   111     1      -1.327  -2.566  -1.562  1.00  0.00
ATOM      8  N   111     1      -0.237  -3.907   0.220  1.00  0.00
ATOM      9  C   111     1      -0.545  -5.130   0.796  1.00  0.00
ATOM     10  C   111     1      -1.725  -5.699   0.187  1.00  0.00
ATOM     11  H   111     1      -2.165  -6.665   0.465  1.00  0.00
ATOM     12  C   111     1      -2.114  -4.834  -0.802  1.00  0.00
ATOM     13  H   111     1      -2.947  -4.930  -1.508  1.00  0.00
ATOM     14  C   111     1      -1.202  -3.709  -0.756  1.00  0.00
ATOM     15  C   111     1       1.948   0.562   0.250  1.00  0.00
ATOM     16  H   111     1       2.125   1.643   0.148  1.00  0.00
ATOM     17  H   111     1       5.886  -0.804   2.276  1.00  0.00
ATOM     18  C   111     1       4.867  -0.772   1.868  1.00  0.00
ATOM     19  C   111     1       4.005  -1.924   1.719  1.00  0.00
ATOM     20  H   111     1       4.463   1.366   1.374  1.00  0.00
ATOM     21  N   111     1       2.792  -1.559   1.156  1.00  0.00
ATOM     22  C   111     1       2.880  -0.195   0.958  1.00  0.00
ATOM     23  C   111     1       4.152   0.314   1.426  1.00  0.00
ATOM     24  C   111     1       0.249  -5.808   1.716  1.00  0.00
ATOM     25  H   111     1       4.619  -5.820   3.274  1.00  0.00
ATOM     26  C   111     1       3.659  -5.524   2.828  1.00  0.00
ATOM     27  C   111     1       2.477  -6.222   2.794  1.00  0.00
ATOM     28  H   111     1       2.258  -7.222   3.191  1.00  0.00
ATOM     29  C   111     1       1.531  -5.397   2.080  1.00  0.00
ATOM     30  N   111     1       2.109  -4.195   1.705  1.00  0.00
ATOM     31  C   111     1       3.412  -4.256   2.183  1.00  0.00
ATOM     32  C   111     1       4.330  -3.209   2.146  1.00  0.00
ATOM     33  H   111     1       5.334  -3.382   2.563  1.00  0.00
ATOM     34 Co   111     1       1.180  -2.684   0.815  1.00  0.00
ATOM     35  N   111     1       0.295  -1.999   2.328  1.00  0.00
ATOM     36  S   111     1      -1.456  -1.925   2.444  1.00  0.00
ATOM     37  O   111     1      -2.099  -3.208   2.823  1.00  0.00
ATOM     38  O   111     1      -1.898  -1.226   1.202  1.00  0.00
ATOM     39  C   111     1      -1.697  -0.758   3.808  1.00  0.00
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ATOM     40  C   111     1       -2.152   1.046   5.880  1.00  0.00
ATOM     41  C   111     1       -2.176  -1.239   5.036  1.00  0.00
ATOM     42  C   111     1       -1.448   0.607   3.588  1.00  0.00
ATOM     43  C   111     1       -1.677   1.510   4.639  1.00  0.00
ATOM     44  C   111     1       -2.404  -0.323   6.076  1.00  0.00
ATOM     45  H   111     1       -2.371  -2.315   5.160  1.00  0.00
ATOM     46  H   111     1       -1.087   0.952   2.607  1.00  0.00
ATOM     47  H   111     1       -1.487   2.585   4.486  1.00  0.00
ATOM     48  H   111     1       -2.783  -0.684   7.047  1.00  0.00
ATOM     49  H   111     1       -2.331   1.761   6.700  1.00  0.00
ATOM     50  N   111     1        0.690  -2.422   3.843  1.00  0.00
ATOM     51  N   111     1        1.688  -2.801   4.262  1.00  0.00
ATOM     52  H   111     1       -0.109  -6.779   2.089  1.00  0.00
ATOM     53  H   111     1       -1.513   0.009  -2.780  1.00  0.00
ATOM     54  C   111     1       -2.427  -2.507  -2.576  1.00  0.00
ATOM     55  C   111     1       -4.461  -2.456  -4.523  1.00  0.00
ATOM     56  C   111     1       -2.130  -2.723  -3.937  1.00  0.00
ATOM     57  C   111     1       -3.776  -2.242  -2.184  1.00  0.00
ATOM     58  C   111     1       -4.786  -2.229  -3.179  1.00  0.00
ATOM     59  C   111     1       -3.135  -2.700  -4.916  1.00  0.00
ATOM     60  H   111     1       -1.083  -2.924  -4.219  1.00  0.00
ATOM     61  H   111     1       -5.820  -2.041  -2.865  1.00  0.00
ATOM     62  H   111     1       -2.882  -2.877  -5.974  1.00  0.00
ATOM     63  H   111     1       -5.267  -2.438  -5.276  1.00  0.00
ATOM     64  N   111     1       -4.048  -1.999  -0.825  1.00  0.00
ATOM     65  H   111     1       -3.227  -1.890  -0.205  1.00  0.00
ATOM     66  C   111     1       -5.290  -1.886  -0.205  1.00  0.00
ATOM     67  O   111     1       -6.365  -1.971  -0.795  1.00  0.00
ATOM     68  C   111     1       -5.201  -1.638   1.298  1.00  0.00
ATOM     69  H   111     1       -4.759  -0.638   1.504  1.00  0.00
ATOM     70  H   111     1       -4.557  -2.390   1.805  1.00  0.00
ATOM     71  H   111     1       -6.226  -1.677   1.716  1.00  0.00
CONECT    1    2    6   15
CONECT    2    4   34
CONECT    3    6
CONECT    4    5    7
CONECT    5    6   53
CONECT    7   14   54
CONECT    8    9   14   34
CONECT    9   10   24
CONECT   10   11   12
CONECT   12   13   14
CONECT   15   16   22
CONECT   17   18
CONECT   18   19   23
CONECT   19   21   32
CONECT   20   23
CONECT   21   22   34
CONECT   22   23
CONECT   24   29   52
CONECT   25   26
CONECT   26   27   31
CONECT   27   28   29
CONECT   29   30
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CONECT   31   32
CONECT   32   33
CONECT   34   35
CONECT   35   36   50
CONECT   36   37   38   39
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CONECT   41   44   45
CONECT   42   43   46
CONECT   43   47
CONECT   44   48
CONECT   50   51
CONECT   54   56   57
CONECT   55   58   59   63
CONECT   56   59   60
CONECT   57   58   64
CONECT   58   61
CONECT   59   62
CONECT   64   65   66
CONECT   66   67   68
CONECT   68   69   70   71
END



2C_ Co(PorAmide)
Xyz file
69
 Energy =   -3646.2699024550
C     0.1636357   -0.4307013   -0.0713677
N    -0.0215220   -1.8087844   -0.0318554
H    -1.0907526    1.3068802   -0.7726185
C    -1.3134325   -2.0070801   -0.5033622
C    -1.9322356   -0.7533404   -0.8542951
H    -2.9462416   -0.6544222   -1.2631307
C    -1.0066746    0.2259631   -0.6105110
C    -1.9238784   -3.2379304   -0.7078148
N     0.0317293   -4.6144059   -0.1335118
C     0.2655727   -5.9792041   -0.1911202
C    -0.8933050   -6.6798245   -0.6968936
H    -0.9440533   -7.7656982   -0.8529560
C    -1.8628885   -5.7327266   -0.9084424
H    -2.8857853   -5.8647122   -1.2853383
C    -1.2766555   -4.4596266   -0.5579065
C     1.2979601    0.2612651    0.3758041
H     5.2496733   -0.5785151    2.6584267
C     4.3058647   -0.6962046    2.1095606
C     3.6849718   -1.9645091    1.8147808
H     3.6359762    1.3598266    1.5712020
N     2.5131015   -1.7863494    1.0907787
C     2.3829792   -0.4100047    0.9557803
C     3.5042879    0.2716950    1.5631680
C     1.4297050   -6.6179082    0.2245781
H     1.4870747   -7.7115229    0.1159088
H     5.3827981   -5.7917852    2.4982303
C     4.4251219   -5.6792156    1.9728265
C     3.6517043   -6.6417119    1.3760477
H     3.8272445   -7.7237211    1.3085504
C     2.4953444   -5.9625946    0.8329440
N     2.5738506   -4.5980322    1.0516406
C     3.7471604   -4.4194861    1.7610175
C     4.2526520   -3.1866622    2.1600970
H     5.1938783   -3.1722084    2.7303032
Co    1.1815845   -3.1932009    0.6895968
N     0.4821960   -3.3497017    2.3304858
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S    -0.3719740   -2.0976333    3.0553111
O    -1.7736501   -1.9985936    2.5495827
O     0.4081874   -0.8187079    3.1842020
C    -0.4463532   -2.8181336    4.7172070
C    -0.5887279   -3.9020539    7.2824040
C     0.5668003   -2.5179402    5.6436219
C    -1.5301273   -3.6482276    5.0493229
C    -1.5953800   -4.1911582    6.3426410
C     0.4877801   -3.0654703    6.9342374
H     1.3937115   -1.8528305    5.3510437
H    -2.3126227   -3.8475070    4.3011257
H    -2.4414270   -4.8409517    6.6207792
H     1.2705798   -2.8336966    7.6754571
H    -0.6459690   -4.3293917    8.2972334
H    -2.9637503   -3.2421527   -1.0665929
C     1.3149590    1.7573412    0.3050100
C     1.3458030    4.5638416    0.0694281
C     0.5250583    2.5504514    1.1954762
C     2.1173796    2.3931250   -0.6647437
C     2.1412951    3.7899514   -0.7922756
C     0.5475166    3.9609622    1.0511156
H     2.7210207    1.7642527   -1.3400252
H     2.7691062    4.2667192   -1.5623497
H    -0.0794611    4.5601805    1.7226709
H     1.3459093    5.6635200   -0.0163184
N    -0.2379780    1.9064422    2.1854362
H    -0.0294954    0.9058311    2.3581126
C    -1.2476235    2.4543584    2.9758696
O    -1.6032229    3.6294699    2.9191886
C    -1.8787363    1.4550667    3.9403934
H    -2.1637372    0.5059169    3.4367620
H    -2.7716095    1.9297605    4.3920203
H    -1.1598993    1.1902133    4.7473682
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COMPND B2Pdb
ATOM      1  C   111     1       0.164  -0.431  -0.071  1.00  0.00
ATOM      2  N   111     1      -0.022  -1.809  -0.032  1.00  0.00
ATOM      3  H   111     1      -1.091   1.307  -0.773  1.00  0.00
ATOM      4  C   111     1      -1.313  -2.007  -0.503  1.00  0.00
ATOM      5  C   111     1      -1.932  -0.753  -0.854  1.00  0.00
ATOM      6  H   111     1      -2.946  -0.654  -1.263  1.00  0.00
ATOM      7  C   111     1      -1.007   0.226  -0.611  1.00  0.00
ATOM      8  C   111     1      -1.924  -3.238  -0.708  1.00  0.00
ATOM      9  N   111     1       0.032  -4.614  -0.134  1.00  0.00
ATOM     10  C   111     1       0.266  -5.979  -0.191  1.00  0.00
ATOM     11  C   111     1      -0.893  -6.680  -0.697  1.00  0.00
ATOM     12  H   111     1      -0.944  -7.766  -0.853  1.00  0.00
ATOM     13  C   111     1      -1.863  -5.733  -0.908  1.00  0.00
ATOM     14  H   111     1      -2.886  -5.865  -1.285  1.00  0.00
ATOM     15  C   111     1      -1.277  -4.460  -0.558  1.00  0.00
ATOM     16  C   111     1       1.298   0.261   0.376  1.00  0.00
ATOM     17  H   111     1       5.250  -0.579   2.658  1.00  0.00
ATOM     18  C   111     1       4.306  -0.696   2.110  1.00  0.00
ATOM     19  C   111     1       3.685  -1.965   1.815  1.00  0.00
ATOM     20  H   111     1       3.636   1.360   1.571  1.00  0.00
ATOM     21  N   111     1       2.513  -1.786   1.091  1.00  0.00
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ATOM     22  C   111     1       2.383  -0.410   0.956  1.00  0.00
ATOM     23  C   111     1       3.504   0.272   1.563  1.00  0.00
ATOM     24  C   111     1       1.430  -6.618   0.225  1.00  0.00
ATOM     25  H   111     1       1.487  -7.712   0.116  1.00  0.00
ATOM     26  H   111     1       5.383  -5.792   2.498  1.00  0.00
ATOM     27  C   111     1       4.425  -5.679   1.973  1.00  0.00
ATOM     28  C   111     1       3.652  -6.642   1.376  1.00  0.00
ATOM     29  H   111     1       3.827  -7.724   1.309  1.00  0.00
ATOM     30  C   111     1       2.495  -5.963   0.833  1.00  0.00
ATOM     31  N   111     1       2.574  -4.598   1.052  1.00  0.00
ATOM     32  C   111     1       3.747  -4.419   1.761  1.00  0.00
ATOM     33  C   111     1       4.253  -3.187   2.160  1.00  0.00
ATOM     34  H   111     1       5.194  -3.172   2.730  1.00  0.00
ATOM     35 Co   111     1       1.182  -3.193   0.690  1.00  0.00
ATOM     36  N   111     1       0.482  -3.350   2.330  1.00  0.00
ATOM     37  S   111     1      -0.372  -2.098   3.055  1.00  0.00
ATOM     38  O   111     1      -1.774  -1.999   2.550  1.00  0.00
ATOM     39  O   111     1       0.408  -0.819   3.184  1.00  0.00
ATOM     40  C   111     1      -0.446  -2.818   4.717  1.00  0.00
ATOM     41  C   111     1      -0.589  -3.902   7.282  1.00  0.00
ATOM     42  C   111     1       0.567  -2.518   5.644  1.00  0.00
ATOM     43  C   111     1      -1.530  -3.648   5.049  1.00  0.00
ATOM     44  C   111     1      -1.595  -4.191   6.343  1.00  0.00
ATOM     45  C   111     1       0.488  -3.065   6.934  1.00  0.00
ATOM     46  H   111     1       1.394  -1.853   5.351  1.00  0.00
ATOM     47  H   111     1      -2.313  -3.848   4.301  1.00  0.00
ATOM     48  H   111     1      -2.441  -4.841   6.621  1.00  0.00
ATOM     49  H   111     1       1.271  -2.834   7.675  1.00  0.00
ATOM     50  H   111     1      -0.646  -4.329   8.297  1.00  0.00
ATOM     51  H   111     1      -2.964  -3.242  -1.067  1.00  0.00
ATOM     52  C   111     1       1.315   1.757   0.305  1.00  0.00
ATOM     53  C   111     1       1.346   4.564   0.069  1.00  0.00
ATOM     54  C   111     1       0.525   2.550   1.195  1.00  0.00
ATOM     55  C   111     1       2.117   2.393  -0.665  1.00  0.00
ATOM     56  C   111     1       2.141   3.790  -0.792  1.00  0.00
ATOM     57  C   111     1       0.548   3.961   1.051  1.00  0.00
ATOM     58  H   111     1       2.721   1.764  -1.340  1.00  0.00
ATOM     59  H   111     1       2.769   4.267  -1.562  1.00  0.00
ATOM     60  H   111     1      -0.079   4.560   1.723  1.00  0.00
ATOM     61  H   111     1       1.346   5.664  -0.016  1.00  0.00
ATOM     62  N   111     1      -0.238   1.906   2.185  1.00  0.00
ATOM     63  H   111     1      -0.029   0.906   2.358  1.00  0.00
ATOM     64  C   111     1      -1.248   2.454   2.976  1.00  0.00
ATOM     65  O   111     1      -1.603   3.629   2.919  1.00  0.00
ATOM     66  C   111     1      -1.879   1.455   3.940  1.00  0.00
ATOM     67  H   111     1      -2.164   0.506   3.437  1.00  0.00
ATOM     68  H   111     1      -2.772   1.930   4.392  1.00  0.00
ATOM     69  H   111     1      -1.160   1.190   4.747  1.00  0.00
CONECT    1    2    7   16
CONECT    2    4   35
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8   15   51
CONECT    9   10   15   35
CONECT   10   11   24
CONECT   11   12   13
CONECT   13   14   15
CONECT   16   22   52
CONECT   17   18
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CONECT   18   19   23
CONECT   19   21   33
CONECT   20   23
CONECT   21   22   35
CONECT   22   23
CONECT   24   25   30
CONECT   26   27
CONECT   27   28   32
CONECT   28   29   30
CONECT   30   31
CONECT   31   32   35
CONECT   32   33
CONECT   33   34
CONECT   35   36
CONECT   36   37
CONECT   37   38   39   40
CONECT   40   42   43
CONECT   41   44   45   50
CONECT   42   45   46
CONECT   43   44   47
CONECT   44   48
CONECT   45   49
CONECT   52   54   55
CONECT   53   56   57   61
CONECT   54   57   62
CONECT   55   56   58
CONECT   56   59
CONECT   57   60
CONECT   62   63   64
CONECT   64   65   66
CONECT   66   67   68   69
END



TS2_ Co(PorAmide)
Xyz file
85
 Energy =   -3956.0037718840
C    -0.4495550   -0.3320653    0.7308372
N    -0.3186874   -1.7089010    0.8552897
H    -2.0219789    1.0235035   -0.1558906
C    -1.4877141   -2.2318808    0.3214704
C    -2.3636295   -1.1766547   -0.1304033
H    -3.3439959   -1.3381650   -0.5976335
C    -1.7022439    0.0031204    0.0862907
C    -1.7323670   -3.5804030    0.0862879
H    -2.7053384   -3.8612902   -0.3440727
N     0.5006667   -4.3664177    0.7567375
C     1.1619579   -5.5757009    0.5880378
C     0.3100675   -6.5366581   -0.0747645
H     0.6114053   -7.5594978   -0.3374592
C    -0.9011054   -5.9194999   -0.2733047
H    -1.8061328   -6.3202622   -0.7492951
C    -0.7640746   -4.5715699    0.2287668
C     0.4582137    0.6246244    1.2090607
H     4.0825833    0.8250828    4.1044443
C     3.2964291    0.4688672    3.4253723
C     3.0399168   -0.9205426    3.1236850
H     2.2973466    2.2923935    2.6236958
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N	1.9977192	-1.0413578	2.2176020
C	1.5825549	0.2557805	1.9637138
C	2.4107171	1.2034317	2.6802294
C	2.4391325	-5.8676863	1.0660385
H	2.8507069	-6.8685669	0.8653174
H	5.6146401	-4.1786114	3.9992469
C	4.7463361	-4.2932333	3.3364395
C	4.4070004	-5.3611507	2.5431763
H	4.9258051	-6.3219939	2.4246288
C	3.1780289	-5.0009722	1.8690875
N	2.7927951	-3.7127080	2.2057014
C	3.7496162	-3.2714410	3.1001249
C	3.8251981	-1.9704088	3.5956696
H	4.6291224	-1.7317302	4.3085275
Co	1.1289148	-2.7275185	1.7023526
N	0.3873274	-3.0251601	3.3840068
S	-0.9286646	-2.0927872	3.9032920
O	-2.2732029	-2.5024300	3.4107782
O	-0.5672315	-0.6366982	3.7788295
C	-0.8836362	-2.3835190	5.6969523
C	-0.9104361	-2.5159383	8.4863150
C	0.3212730	-2.2152385	6.4041965
C	-2.0974868	-2.6171412	6.3599150
C	-2.1054752	-2.6746596	7.7653879
C	0.3023734	-2.2926279	7.8051734
H	1.2567736	-2.0257434	5.8553859
H	-3.0187901	-2.7452363	5.7714609
H	-3.0551565	-2.8505870	8.2968976
H	1.2396763	-2.1670799	8.3723849
H	-0.9208397	-2.5643424	9.5878769
C	-1.1400352	-5.5223402	3.7278883
C	0.1360834	-5.0513343	4.0093440
H	0.9387754	-5.2231540	3.2813463
H	0.4636714	-4.8886676	5.0501315
H	-1.3833991	-5.6969700	2.6642462
C	-2.2180649	-5.7987527	4.6619384
C	-4.3725687	-6.4630351	6.3999490
C	-3.5285908	-6.0365665	4.1583963
C	-2.0220458	-5.9097782	6.0674056
C	-3.0821821	-6.2408910	6.9190545
C	-4.5898051	-6.3563976	5.0128161
H	-3.7017756	-5.9522889	3.0726987
H	-1.0172007	-5.7554773	6.4921732
H	-2.9011756	-6.3323350	8.0030956
H	-5.5966805	-6.5272999	4.5969122
H	-5.2045954	-6.7252578	7.0743007
C	0.1675513	2.0795743	1.0027568
C	-0.3386116	4.8093041	0.5324248
C	0.9003974	2.7943951	0.0334452
C	-0.8332992	2.7548013	1.7689701
C	-1.0763383	4.1278744	1.5106405
C	0.6570687	4.1543371	-0.2113924
H	1.6693006	2.2549287	-0.5439986
H	-1.8547231	4.6332837	2.0949067
H	1.2364600	4.6931442	-0.9785639
H	-0.5488065	5.8775140	0.3548812
N	-1.5348037	2.0353341	2.7545511
H	-1.2017537	1.0747927	2.9514210
C	-2.6295250	2.4626258	3.5028308
O	-3.1315835	3.5817599	3.4159945

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C    -3.1908237    1.4053491    4.4472116
H    -3.3108129    1.8601371    5.4535091
H    -2.5662546    0.4925960    4.5153265
H    -4.2071067    1.1226248    4.0939566
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Pdb file

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HEADER B2Pdb
COMPND B2Pdb
ATOM      1  C   111     1      -0.450  -0.332   0.731  1.00  0.00
ATOM      2  N   111     1      -0.319  -1.709   0.855  1.00  0.00
ATOM      3  H   111     1      -2.022   1.024  -0.156  1.00  0.00
ATOM      4  C   111     1      -1.488  -2.232   0.321  1.00  0.00
ATOM      5  C   111     1      -2.364  -1.177  -0.130  1.00  0.00
ATOM      6  H   111     1      -3.344  -1.338  -0.598  1.00  0.00
ATOM      7  C   111     1      -1.702   0.003   0.086  1.00  0.00
ATOM      8  C   111     1      -1.732  -3.580   0.086  1.00  0.00
ATOM      9  H   111     1      -2.705  -3.861  -0.344  1.00  0.00
ATOM     10  N   111     1       0.501  -4.366   0.757  1.00  0.00
ATOM     11  C   111     1       1.162  -5.576   0.588  1.00  0.00
ATOM     12  C   111     1       0.310  -6.537  -0.075  1.00  0.00
ATOM     13  H   111     1       0.611  -7.559  -0.337  1.00  0.00
ATOM     14  C   111     1      -0.901  -5.919  -0.273  1.00  0.00
ATOM     15  H   111     1      -1.806  -6.320  -0.749  1.00  0.00
ATOM     16  C   111     1      -0.764  -4.572   0.229  1.00  0.00
ATOM     17  C   111     1       0.458   0.625   1.209  1.00  0.00
ATOM     18  H   111     1       4.083   0.825   4.104  1.00  0.00
ATOM     19  C   111     1       3.296   0.469   3.425  1.00  0.00
ATOM     20  C   111     1       3.040  -0.921   3.124  1.00  0.00
ATOM     21  H   111     1       2.297   2.292   2.624  1.00  0.00
ATOM     22  N   111     1       1.998  -1.041   2.218  1.00  0.00
ATOM     23  C   111     1       1.583   0.256   1.964  1.00  0.00
ATOM     24  C   111     1       2.411   1.203   2.680  1.00  0.00
ATOM     25  C   111     1       2.439  -5.868   1.066  1.00  0.00
ATOM     26  H   111     1       2.851  -6.869   0.865  1.00  0.00
ATOM     27  H   111     1       5.615  -4.179   3.999  1.00  0.00
ATOM     28  C   111     1       4.746  -4.293   3.336  1.00  0.00
ATOM     29  C   111     1       4.407  -5.361   2.543  1.00  0.00
ATOM     30  H   111     1       4.926  -6.322   2.425  1.00  0.00
ATOM     31  C   111     1       3.178  -5.001   1.869  1.00  0.00
ATOM     32  N   111     1       2.793  -3.713   2.206  1.00  0.00
ATOM     33  C   111     1       3.750  -3.271   3.100  1.00  0.00
ATOM     34  C   111     1       3.825  -1.970   3.596  1.00  0.00
ATOM     35  H   111     1       4.629  -1.732   4.309  1.00  0.00
ATOM     36 Co   111     1       1.129  -2.728   1.702  1.00  0.00
ATOM     37  N   111     1       0.387  -3.025   3.384  1.00  0.00
ATOM     38  S   111     1      -0.929  -2.093   3.903  1.00  0.00
ATOM     39  O   111     1      -2.273  -2.502   3.411  1.00  0.00
ATOM     40  O   111     1      -0.567  -0.637   3.779  1.00  0.00
ATOM     41  C   111     1      -0.884  -2.384   5.697  1.00  0.00
ATOM     42  C   111     1      -0.910  -2.516   8.486  1.00  0.00
ATOM     43  C   111     1       0.321  -2.215   6.404  1.00  0.00
ATOM     44  C   111     1      -2.097  -2.617   6.360  1.00  0.00
ATOM     45  C   111     1      -2.105  -2.675   7.765  1.00  0.00
ATOM     46  C   111     1       0.302  -2.293   7.805  1.00  0.00
ATOM     47  H   111     1       1.257  -2.026   5.855  1.00  0.00
ATOM     48  H   111     1      -3.019  -2.745   5.771  1.00  0.00
ATOM     49  H   111     1      -3.055  -2.851   8.297  1.00  0.00
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ATOM     50  H   111     1       1.240  -2.167   8.372  1.00  0.00
ATOM     51  H   111     1      -0.921  -2.564   9.588  1.00  0.00
ATOM     52  C   111     1      -1.140  -5.522   3.728  1.00  0.00
ATOM     53  C   111     1       0.136  -5.051   4.009  1.00  0.00
ATOM     54  H   111     1       0.939  -5.223   3.281  1.00  0.00
ATOM     55  H   111     1       0.464  -4.889   5.050  1.00  0.00
ATOM     56  H   111     1      -1.383  -5.697   2.664  1.00  0.00
ATOM     57  C   111     1      -2.218  -5.799   4.662  1.00  0.00
ATOM     58  C   111     1      -4.373  -6.463   6.400  1.00  0.00
ATOM     59  C   111     1      -3.529  -6.037   4.158  1.00  0.00
ATOM     60  C   111     1      -2.022  -5.910   6.067  1.00  0.00
ATOM     61  C   111     1      -3.082  -6.241   6.919  1.00  0.00
ATOM     62  C   111     1      -4.590  -6.356   5.013  1.00  0.00
ATOM     63  H   111     1      -3.702  -5.952   3.073  1.00  0.00
ATOM     64  H   111     1      -1.017  -5.755   6.492  1.00  0.00
ATOM     65  H   111     1      -2.901  -6.332   8.003  1.00  0.00
ATOM     66  H   111     1      -5.597  -6.527   4.597  1.00  0.00
ATOM     67  H   111     1      -5.205  -6.725   7.074  1.00  0.00
ATOM     68  C   111     1       0.168   2.080   1.003  1.00  0.00
ATOM     69  C   111     1      -0.339   4.809   0.532  1.00  0.00
ATOM     70  C   111     1       0.900   2.794   0.033  1.00  0.00
ATOM     71  C   111     1      -0.833   2.755   1.769  1.00  0.00
ATOM     72  C   111     1      -1.076   4.128   1.511  1.00  0.00
ATOM     73  C   111     1       0.657   4.154  -0.211  1.00  0.00
ATOM     74  H   111     1       1.669   2.255  -0.544  1.00  0.00
ATOM     75  H   111     1      -1.855   4.633   2.095  1.00  0.00
ATOM     76  H   111     1       1.236   4.693  -0.979  1.00  0.00
ATOM     77  H   111     1      -0.549   5.878   0.355  1.00  0.00
ATOM     78  N   111     1      -1.535   2.035   2.755  1.00  0.00
ATOM     79  H   111     1      -1.202   1.075   2.951  1.00  0.00
ATOM     80  C   111     1      -2.630   2.463   3.503  1.00  0.00
ATOM     81  O   111     1      -3.132   3.582   3.416  1.00  0.00
ATOM     82  C   111     1      -3.191   1.405   4.447  1.00  0.00
ATOM     83  H   111     1      -3.311   1.860   5.454  1.00  0.00
ATOM     84  H   111     1      -2.566   0.493   4.515  1.00  0.00
ATOM     85  H   111     1      -4.207   1.123   4.094  1.00  0.00
CONECT    1    2    7   17
CONECT    2    4   36
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   36
CONECT   11   12   25
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   23   68
CONECT   18   19
CONECT   19   20   24
CONECT   20   22   34
CONECT   21   24
CONECT   22   23   36
CONECT   23   24
CONECT   25   26   31
CONECT   27   28
CONECT   28   29   33
CONECT   29   30   31
CONECT   31   32
CONECT   32   33   36
CONECT   33   34
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CONECT   36   37
CONECT   37   38
CONECT   38   39   40   41
CONECT   41   43   44
CONECT   42   45   46   51
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CONECT   44   45   48
CONECT   45   49
CONECT   46   50
CONECT   52   53   56   57
CONECT   53   54   55
CONECT   57   59   60
CONECT   58   61   62   67
CONECT   59   62   63
CONECT   60   61   64
CONECT   61   65
CONECT   62   66
CONECT   68   70   71
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CONECT   70   73   74
CONECT   71   72   78
CONECT   72   75
CONECT   73   76
CONECT   78   79   80
CONECT   80   81   82
CONECT   82   83   84   85
END

2D_ Co(PorAmide)
Xyz file
85
 Energy =   -3956.0260680000
C    -0.6266049   -1.1578226   -0.5136435
N    -0.6750074   -2.5327461   -0.3415419
H    -1.9586179    0.3502405   -1.5386120
C    -1.8128518   -2.9413164   -1.0175690
C    -2.5056115   -1.8095573   -1.5910379
H    -3.4309818   -1.8773905   -2.1787184
C    -1.7717895   -0.6966112   -1.2720975
C    -2.2295015   -4.2601004   -1.1950164
N    -0.4697429   -5.3189205    0.1660136
C    -0.1989406   -6.6417451    0.4819294
C    -1.1405321   -7.5310220   -0.1621960
H    -1.1252572   -8.6256285   -0.0736270
C    -1.9980102   -6.7374615   -0.8824149
H    -2.8448656   -7.0359922   -1.5148949
C    -1.5758328   -5.3709167   -0.6646796
C     0.4249574   -0.3156542   -0.1188805
H     4.5339796   -0.5187324    2.0280258
C     3.5603912   -0.7777106    1.5906770
C     2.9619103   -2.0945699    1.6380468
H     2.7760364    1.0871671    0.6557727
N     1.7463261   -2.1124286    0.9779892
C     1.5569150   -0.8095659    0.5455741
C     2.6858768    0.0236107    0.9068830
C     0.8320959   -7.0756133    1.3141962
H     0.9145510   -8.1543212    1.5161511
H     4.6436802   -5.5422359    3.4624793
C     3.6935911   -5.5986173    2.9142336
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C	2.9183535	-6.6990549	2.6472124
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C	3.5568259	-3.1775143	2.2816437
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Co	0.4823065	-3.6570665	0.8324774
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S	-0.8965047	-2.0677564	3.4642357
O	-2.3375247	-1.7924180	3.7279761
O	-0.0660789	-0.9826704	2.8737280
C	-0.1584794	-2.4581948	5.0841790
C	0.9705963	-2.9908321	7.5845125
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C	-0.9700630	-2.4114106	6.2293820
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C	1.7714264	-3.0305919	6.4274285
H	1.8284052	-2.7888841	4.2572964
H	-2.0349995	-2.1523126	6.1240870
H	-1.0228526	-2.6410380	8.3918498
H	2.8442144	-3.2721759	6.5056144
H	1.4172738	-3.2014389	8.5703700
H	-0.9906855	-5.5256031	2.6751423
C	-1.4639389	-4.5887731	3.0411085
H	-1.4688872	-4.6528956	4.1538115
C	-2.8258220	-4.4098281	2.4574280
H	-2.8342295	-4.2924751	1.3609351
C	-4.0748171	-4.2903942	3.1241407
C	-6.6445263	-4.1344197	4.3332024
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H	-3.3470143	-4.5677225	5.1772585
H	-5.1484694	-3.9503794	1.2500136
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H	-3.1252808	-4.4348267	-1.8103726
C	0.3519283	1.1414988	-0.4728913
C	0.2030603	3.8430769	-1.2586765
C	0.8018299	1.5533203	-1.7443232
C	-0.1829792	2.1107894	0.4312143
C	-0.2525687	3.4649182	0.0112891
C	0.7368736	2.8955372	-2.1477923
H	1.2087528	0.7886891	-2.4267926
H	-0.6772625	4.1980614	0.7074270
H	1.0950056	3.1943247	-3.1464178
H	0.1357701	4.9037329	-1.5542027
N	-0.6241503	1.6935772	1.6999025
H	-0.4649641	0.7001715	1.9458119
C	-1.2264355	2.4670371	2.6919838
O	-1.4818828	3.6641014	2.5737007
C	-1.5394875	1.6958703	3.9698922
H	-2.1447734	0.7843097	3.7743356
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Pdb file
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COMPND B2Pdb
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ATOM      4  C   111     1      -1.813  -2.941  -1.018  1.00  0.00
ATOM      5  C   111     1      -2.506  -1.810  -1.591  1.00  0.00
ATOM      6  H   111     1      -3.431  -1.877  -2.179  1.00  0.00
ATOM      7  C   111     1      -1.772  -0.697  -1.272  1.00  0.00
ATOM      8  C   111     1      -2.230  -4.260  -1.195  1.00  0.00
ATOM      9  N   111     1      -0.470  -5.319   0.166  1.00  0.00
ATOM     10  C   111     1      -0.199  -6.642   0.482  1.00  0.00
ATOM     11  C   111     1      -1.141  -7.531  -0.162  1.00  0.00
ATOM     12  H   111     1      -1.125  -8.626  -0.074  1.00  0.00
ATOM     13  C   111     1      -1.998  -6.737  -0.882  1.00  0.00
ATOM     14  H   111     1      -2.845  -7.036  -1.515  1.00  0.00
ATOM     15  C   111     1      -1.576  -5.371  -0.665  1.00  0.00
ATOM     16  C   111     1       0.425  -0.316  -0.119  1.00  0.00
ATOM     17  H   111     1       4.534  -0.519   2.028  1.00  0.00
ATOM     18  C   111     1       3.560  -0.778   1.591  1.00  0.00
ATOM     19  C   111     1       2.962  -2.095   1.638  1.00  0.00
ATOM     20  H   111     1       2.776   1.087   0.656  1.00  0.00
ATOM     21  N   111     1       1.746  -2.112   0.978  1.00  0.00
ATOM     22  C   111     1       1.557  -0.810   0.546  1.00  0.00
ATOM     23  C   111     1       2.686   0.024   0.907  1.00  0.00
ATOM     24  C   111     1       0.832  -7.076   1.314  1.00  0.00
ATOM     25  H   111     1       0.915  -8.154   1.516  1.00  0.00
ATOM     26  H   111     1       4.644  -5.542   3.462  1.00  0.00
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ATOM     28  C   111     1       2.918  -6.699   2.647  1.00  0.00
ATOM     29  H   111     1       3.090  -7.747   2.927  1.00  0.00
ATOM     30  C   111     1       1.796  -6.232   1.862  1.00  0.00
ATOM     31  N   111     1       1.866  -4.862   1.668  1.00  0.00
ATOM     32  C   111     1       3.034  -4.470   2.294  1.00  0.00
ATOM     33  C   111     1       3.557  -3.178   2.282  1.00  0.00
ATOM     34  H   111     1       4.518  -3.006   2.790  1.00  0.00
ATOM     35 Co   111     1       0.482  -3.657   0.832  1.00  0.00
ATOM     36  N   111     1      -0.651  -3.455   2.548  1.00  0.00
ATOM     37  S   111     1      -0.897  -2.068   3.464  1.00  0.00
ATOM     38  O   111     1      -2.338  -1.792   3.728  1.00  0.00
ATOM     39  O   111     1      -0.066  -0.983   2.874  1.00  0.00
ATOM     40  C   111     1      -0.158  -2.458   5.084  1.00  0.00
ATOM     41  C   111     1       0.971  -2.991   7.585  1.00  0.00
ATOM     42  C   111     1       1.211  -2.762   5.169  1.00  0.00
ATOM     43  C   111     1      -0.970  -2.411   6.229  1.00  0.00
ATOM     44  C   111     1      -0.396  -2.680   7.485  1.00  0.00
ATOM     45  C   111     1       1.771  -3.031   6.427  1.00  0.00
ATOM     46  H   111     1       1.828  -2.789   4.257  1.00  0.00
ATOM     47  H   111     1      -2.035  -2.152   6.124  1.00  0.00
ATOM     48  H   111     1      -1.023  -2.641   8.392  1.00  0.00
ATOM     49  H   111     1       2.844  -3.272   6.506  1.00  0.00
ATOM     50  H   111     1       1.417  -3.201   8.570  1.00  0.00
ATOM     51  H   111     1      -0.991  -5.526   2.675  1.00  0.00
ATOM     52  C   111     1      -1.464  -4.589   3.041  1.00  0.00
ATOM     53  H   111     1      -1.469  -4.653   4.154  1.00  0.00
ATOM     54  C   111     1      -2.826  -4.410   2.457  1.00  0.00
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ATOM     61  C   111     1       -5.498  -4.348   5.128  1.00  0.00
ATOM     62  H   111     1       -3.347  -4.568   5.177  1.00  0.00
ATOM     63  H   111     1       -5.148  -3.950   1.250  1.00  0.00
ATOM     64  H   111     1       -7.408  -3.819   2.314  1.00  0.00
ATOM     65  H   111     1       -5.600  -4.448   6.221  1.00  0.00
ATOM     66  H   111     1       -7.639  -4.070   4.805  1.00  0.00
ATOM     67  H   111     1       -3.125  -4.435  -1.810  1.00  0.00
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ATOM     69  C   111     1        0.203   3.843  -1.259  1.00  0.00
ATOM     70  C   111     1        0.802   1.553  -1.744  1.00  0.00
ATOM     71  C   111     1       -0.183   2.111   0.431  1.00  0.00
ATOM     72  C   111     1       -0.253   3.465   0.011  1.00  0.00
ATOM     73  C   111     1        0.737   2.896  -2.148  1.00  0.00
ATOM     74  H   111     1        1.209   0.789  -2.427  1.00  0.00
ATOM     75  H   111     1       -0.677   4.198   0.707  1.00  0.00
ATOM     76  H   111     1        1.095   3.194  -3.146  1.00  0.00
ATOM     77  H   111     1        0.136   4.904  -1.554  1.00  0.00
ATOM     78  N   111     1       -0.624   1.694   1.700  1.00  0.00
ATOM     79  H   111     1       -0.465   0.700   1.946  1.00  0.00
ATOM     80  C   111     1       -1.226   2.467   2.692  1.00  0.00
ATOM     81  O   111     1       -1.482   3.664   2.574  1.00  0.00
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ATOM     85  H   111     1       -0.601   1.357   4.462  1.00  0.00
CONECT    1    2    7   16
CONECT    2    4   35
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8   15   67
CONECT    9   10   15   35
CONECT   10   11   24
CONECT   11   12   13
CONECT   13   14   15
CONECT   16   22   68
CONECT   17   18
CONECT   18   19   23
CONECT   19   21   33
CONECT   20   23
CONECT   21   22   35
CONECT   22   23
CONECT   24   25   30
CONECT   26   27
CONECT   27   28   32
CONECT   28   29   30
CONECT   30   31
CONECT   31   32   35
CONECT   32   33
CONECT   33   34
CONECT   35   36
CONECT   36   37   52
CONECT   37   38   39   40
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CONECT   42   45   46
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CONECT   59   60   63
CONECT   60   64
CONECT   61   65
CONECT   68   70   71
CONECT   69   72   73   77
CONECT   70   73   74
CONECT   71   72   78
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CONECT   80   81   82
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END
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TS3_ Co(PorAmide)
Xyz file
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C    -2.0038293   -2.5884131   -0.8226394
C    -2.5743959   -1.3717604   -1.3617047
H    -3.5467793   -1.3090389   -1.8683917
C    -1.6499716   -0.3832417   -1.1560404
C    -2.5848654   -3.8416599   -0.9999604
N    -0.7451951   -5.1584757   -0.0217855
C    -0.5061761   -6.5223414    0.0583862
C    -1.5695299   -7.2709554   -0.5735628
H    -1.6000498   -8.3660093   -0.6529043
C    -2.4839861   -6.3494988   -1.0240417
H    -3.4249125   -6.5221641   -1.5638462
C    -1.9587414   -5.0466940   -0.6813318
C     0.6096461   -0.2868578   -0.0597693
H     4.4678328   -0.8853087    2.4545395
C     3.5275515   -1.0545007    1.9126201
C     2.8395605   -2.3245225    1.8348762
H     2.9862221    0.8961033    0.9833214
N     1.6891957   -2.2207841    1.0701645
C     1.6438583   -0.8940064    0.6700200
C     2.7912991   -0.1657358    1.1744896
C     0.5732018   -7.1108909    0.7174164
H     0.6395042   -8.2096461    0.7200874
H     4.3157354   -6.0462164    3.2453546
C     3.3969553   -5.9888016    2.6460724
C     2.6506064   -7.0115182    2.1172115
H     2.8144106   -8.0948700    2.1943462
C     1.5606183   -6.3948895    1.3911573
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C	3.3230554	-3.4934349	2.4219239
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Co	0.3426234	-3.6530919	0.7495008
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S	-1.2313720	-2.1080499	3.3707757
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O	-0.5537693	-1.0163596	2.6277235
C	-0.4347139	-2.1867819	5.0067686
C	0.7764052	-2.1450390	7.5213399
C	0.9634147	-2.2998373	5.0946311
C	-1.2355881	-2.0434176	6.1513893
C	-0.6197219	-2.0217960	7.4151776
C	1.5643045	-2.2842374	6.3633542
H	1.5718437	-2.3967553	4.1814582
H	-2.3255041	-1.9340737	6.0375506
H	-1.2359483	-1.9015370	8.3214293
H	2.6597655	-2.3741033	6.4478453
H	1.2565527	-2.1272317	8.5137741
H	-0.2229012	-5.5451989	3.0450906
C	-0.9725844	-4.7910684	3.3553310
H	-0.9072634	-4.6507792	4.4562680
C	-2.3313192	-4.9943355	2.8142105
H	-2.3651270	-5.2645947	1.7487319
C	-3.5878174	-4.8360733	3.4815179
C	-6.1380041	-4.7208238	4.7171576
C	-3.7105797	-4.6742238	4.8938190
C	-4.7859038	-4.9309605	2.7102322
C	-6.0410730	-4.8743571	3.3199133
C	-4.9682448	-4.6249871	5.4986363
H	-2.8059109	-4.5932485	5.5157383
H	-4.7015870	-5.0512371	1.6178526
H	-6.9548461	-4.9476547	2.7079765
H	-5.0469558	-4.5061257	6.5918109
H	-7.1281520	-4.6747687	5.2001207
H	-3.5621063	-3.8860227	-1.5048240
C	0.7134837	1.1699034	-0.4020158
C	0.9161231	3.8826111	-1.1403770
C	1.5184753	1.5669067	-1.4886603
C	0.0030200	2.1621395	0.3413938
C	0.1126951	3.5204043	-0.0502732
C	1.6288226	2.9140582	-1.8662262
H	2.0595122	0.7873199	-2.0503455
H	-0.4488346	4.2705016	0.5199965
H	2.2606210	3.2005452	-2.7227402
H	0.9838992	4.9468778	-1.4224821
N	-0.7751778	1.7534713	1.4409654
H	-0.7019927	0.7574441	1.7069006
C	-1.6202713	2.5287354	2.2303861
O	-1.8226163	3.7286856	2.0539876
C	-2.2688400	1.7602644	3.3789619
H	-2.6147860	0.7468145	3.0878930
H	-3.1197733	2.3609516	3.7564006
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Pdb file
HEADER B2Pdb
COMPND B2Pdb
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ATOM      3  H   111     1      -1.696   0.672  -1.451  1.00  0.00
ATOM      4  C   111     1      -2.004  -2.588  -0.823  1.00  0.00
ATOM      5  C   111     1      -2.574  -1.372  -1.362  1.00  0.00
ATOM      6  H   111     1      -3.547  -1.309  -1.868  1.00  0.00
ATOM      7  C   111     1      -1.650  -0.383  -1.156  1.00  0.00
ATOM      8  C   111     1      -2.585  -3.842  -1.000  1.00  0.00
ATOM      9  N   111     1      -0.745  -5.158  -0.022  1.00  0.00
ATOM     10  C   111     1      -0.506  -6.522   0.058  1.00  0.00
ATOM     11  C   111     1      -1.570  -7.271  -0.574  1.00  0.00
ATOM     12  H   111     1      -1.600  -8.366  -0.653  1.00  0.00
ATOM     13  C   111     1      -2.484  -6.349  -1.024  1.00  0.00
ATOM     14  H   111     1      -3.425  -6.522  -1.564  1.00  0.00
ATOM     15  C   111     1      -1.959  -5.047  -0.681  1.00  0.00
ATOM     16  C   111     1       0.610  -0.287  -0.060  1.00  0.00
ATOM     17  H   111     1       4.468  -0.885   2.455  1.00  0.00
ATOM     18  C   111     1       3.528  -1.055   1.913  1.00  0.00
ATOM     19  C   111     1       2.840  -2.325   1.835  1.00  0.00
ATOM     20  H   111     1       2.986   0.896   0.983  1.00  0.00
ATOM     21  N   111     1       1.689  -2.221   1.070  1.00  0.00
ATOM     22  C   111     1       1.644  -0.894   0.670  1.00  0.00
ATOM     23  C   111     1       2.791  -0.166   1.174  1.00  0.00
ATOM     24  C   111     1       0.573  -7.111   0.717  1.00  0.00
ATOM     25  H   111     1       0.640  -8.210   0.720  1.00  0.00
ATOM     26  H   111     1       4.316  -6.046   3.245  1.00  0.00
ATOM     27  C   111     1       3.397  -5.989   2.646  1.00  0.00
ATOM     28  C   111     1       2.651  -7.012   2.117  1.00  0.00
ATOM     29  H   111     1       2.814  -8.095   2.194  1.00  0.00
ATOM     30  C   111     1       1.561  -6.395   1.391  1.00  0.00
ATOM     31  N   111     1       1.632  -5.011   1.470  1.00  0.00
ATOM     32  C   111     1       2.771  -4.757   2.216  1.00  0.00
ATOM     33  C   111     1       3.323  -3.493   2.422  1.00  0.00
ATOM     34  H   111     1       4.249  -3.426   3.013  1.00  0.00
ATOM     35 Co   111     1       0.343  -3.653   0.750  1.00  0.00
ATOM     36  N   111     1      -0.783  -3.554   2.563  1.00  0.00
ATOM     37  S   111     1      -1.231  -2.108   3.371  1.00  0.00
ATOM     38  O   111     1      -2.692  -1.991   3.612  1.00  0.00
ATOM     39  O   111     1      -0.554  -1.016   2.628  1.00  0.00
ATOM     40  C   111     1      -0.435  -2.187   5.007  1.00  0.00
ATOM     41  C   111     1       0.776  -2.145   7.521  1.00  0.00
ATOM     42  C   111     1       0.963  -2.300   5.095  1.00  0.00
ATOM     43  C   111     1      -1.236  -2.043   6.151  1.00  0.00
ATOM     44  C   111     1      -0.620  -2.022   7.415  1.00  0.00
ATOM     45  C   111     1       1.564  -2.284   6.363  1.00  0.00
ATOM     46  H   111     1       1.572  -2.397   4.181  1.00  0.00
ATOM     47  H   111     1      -2.326  -1.934   6.038  1.00  0.00
ATOM     48  H   111     1      -1.236  -1.902   8.321  1.00  0.00
ATOM     49  H   111     1       2.660  -2.374   6.448  1.00  0.00
ATOM     50  H   111     1       1.257  -2.127   8.514  1.00  0.00
ATOM     51  H   111     1      -0.223  -5.545   3.045  1.00  0.00
ATOM     52  C   111     1      -0.973  -4.791   3.355  1.00  0.00
ATOM     53  H   111     1      -0.907  -4.651   4.456  1.00  0.00
ATOM     54  C   111     1      -2.331  -4.994   2.814  1.00  0.00
ATOM     55  H   111     1      -2.365  -5.265   1.749  1.00  0.00
ATOM     56  C   111     1      -3.588  -4.836   3.482  1.00  0.00
ATOM     57  C   111     1      -6.138  -4.721   4.717  1.00  0.00
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ATOM     58  C   111     1       -3.711  -4.674   4.894  1.00  0.00
ATOM     59  C   111     1       -4.786  -4.931   2.710  1.00  0.00
ATOM     60  C   111     1       -6.041  -4.874   3.320  1.00  0.00
ATOM     61  C   111     1       -4.968  -4.625   5.499  1.00  0.00
ATOM     62  H   111     1       -2.806  -4.593   5.516  1.00  0.00
ATOM     63  H   111     1       -4.702  -5.051   1.618  1.00  0.00
ATOM     64  H   111     1       -6.955  -4.948   2.708  1.00  0.00
ATOM     65  H   111     1       -5.047  -4.506   6.592  1.00  0.00
ATOM     66  H   111     1       -7.128  -4.675   5.200  1.00  0.00
ATOM     67  H   111     1       -3.562  -3.886  -1.505  1.00  0.00
ATOM     68  C   111     1        0.713   1.170  -0.402  1.00  0.00
ATOM     69  C   111     1        0.916   3.883  -1.140  1.00  0.00
ATOM     70  C   111     1        1.518   1.567  -1.489  1.00  0.00
ATOM     71  C   111     1        0.003   2.162   0.341  1.00  0.00
ATOM     72  C   111     1        0.113   3.520  -0.050  1.00  0.00
ATOM     73  C   111     1        1.629   2.914  -1.866  1.00  0.00
ATOM     74  H   111     1        2.060   0.787  -2.050  1.00  0.00
ATOM     75  H   111     1       -0.449   4.271   0.520  1.00  0.00
ATOM     76  H   111     1        2.261   3.201  -2.723  1.00  0.00
ATOM     77  H   111     1        0.984   4.947  -1.422  1.00  0.00
ATOM     78  N   111     1       -0.775   1.753   1.441  1.00  0.00
ATOM     79  H   111     1       -0.702   0.757   1.707  1.00  0.00
ATOM     80  C   111     1       -1.620   2.529   2.230  1.00  0.00
ATOM     81  O   111     1       -1.823   3.729   2.054  1.00  0.00
ATOM     82  C   111     1       -2.269   1.760   3.379  1.00  0.00
ATOM     83  H   111     1       -2.615   0.747   3.088  1.00  0.00
ATOM     84  H   111     1       -3.120   2.361   3.756  1.00  0.00
ATOM     85  H   111     1       -1.535   1.631   4.206  1.00  0.00
CONECT    1    2    7   16
CONECT    2    4   35
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8   15   67
CONECT    9   10   15   35
CONECT   10   11   24
CONECT   11   12   13
CONECT   13   14   15
CONECT   16   22   68
CONECT   17   18
CONECT   18   19   23
CONECT   19   21   33
CONECT   20   23
CONECT   21   22   35
CONECT   22   23
CONECT   24   25   30
CONECT   26   27
CONECT   27   28   32
CONECT   28   29   30
CONECT   30   31
CONECT   31   32   35
CONECT   32   33
CONECT   33   34
CONECT   35   36
CONECT   36   37   52
CONECT   37   38   39   40
CONECT   40   42   43
CONECT   41   44   45   50
CONECT   42   45   46
CONECT   43   44   47
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CONECT   44   48
CONECT   45   49
CONECT   51   52
CONECT   52   53   54
CONECT   54   55   56
CONECT   56   58   59
CONECT   57   60   61   66
CONECT   58   61   62
CONECT   59   60   63
CONECT   60   64
CONECT   61   65
CONECT   68   70   71
CONECT   69   72   73   77
CONECT   70   73   74
CONECT   71   72   78
CONECT   72   75
CONECT   73   76
CONECT   78   79   80
CONECT   80   81   82
CONECT   82   83   84   85
END



E_ Co(PorAmide)
Xyz file
85
 Energy =   -3956.0493578510
C    -0.3858859   -0.8694190   -0.5199246
N    -0.8016670   -2.1784216   -0.3170056
H    -1.3345600    0.9618466   -1.4491382
C    -2.1083035   -2.2105438   -0.7789724
C    -2.5108793   -0.9211443   -1.2932148
H    -3.4966406   -0.7019823   -1.7246961
C    -1.4311209   -0.0903010   -1.1557525
C    -2.9351834   -3.3295718   -0.8010289
N    -1.2373802   -4.9510347   -0.0580529
C    -1.2324220   -6.3387359   -0.0112263
C    -2.5230896   -6.8758865   -0.3846616
H    -2.7636885   -7.9466872   -0.4288830
C    -3.3275706   -5.8000430   -0.6653580
H    -4.3730171   -5.7910386   -1.0021575
C    -2.5139868   -4.6175770   -0.4808783
C     0.8438056   -0.3252691   -0.1133960
H     4.7595179   -1.6002378    2.0446206
C     3.7651350   -1.6032680    1.5781163
C     2.9517775   -2.7832529    1.3844521
H     3.3534845    0.5016330    0.9799662
N     1.7493674   -2.4645133    0.7703272
C     1.8202630   -1.0991886    0.5359157
C     3.0656986   -0.5543967    1.0415764
C    -0.1383985   -7.1252475    0.3479713
H    -0.2565291   -8.2192110    0.3167836
H     4.1955533   -6.8036308    1.9712859
C     3.1931820   -6.5692110    1.5879042
C     2.2055674   -7.4300877    1.1790124
H     2.2141379   -8.5281973    1.1578281
C     1.0886652   -6.6108138    0.7628369
N     1.3859168   -5.2594745    0.8918904
C     2.6771185   -5.2312955    1.4007041
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C	3.3917806	-4.0700288	1.6899200
H	4.3945496	-4.1774796	2.1315746
Co	0.2294307	-3.6909302	0.4373773
N	-0.5837382	-3.5072113	2.7008581
S	-1.4382888	-2.0097959	3.0789758
O	-2.7629598	-2.1142742	2.4379750
O	-0.4623505	-0.9567760	2.7093127
C	-1.6761222	-1.8334630	4.8671046
C	-2.1027788	-1.3693271	7.5823149
C	-0.6255815	-1.3114313	5.6461278
C	-2.9387629	-2.1102579	5.4161500
C	-3.1463731	-1.8700450	6.7839089
C	-0.8452065	-1.0916904	7.0152980
H	0.3382503	-1.0585857	5.1772523
H	-3.7442588	-2.4961840	4.7736218
H	-4.1346633	-2.0738985	7.2266125
H	-0.0331989	-0.6837789	7.6391611
H	-2.2732226	-1.1831547	8.6554881
H	1.2563100	-4.4523721	3.3901855
C	0.2554637	-4.1457566	3.7376660
H	0.2166543	-3.7019927	4.7499897
C	-0.9716043	-4.8458771	3.2558072
H	-0.8224161	-5.6021637	2.4644737
C	-2.1785920	-5.1128664	4.1070633
C	-4.4584741	-5.7906724	5.6328426
C	-2.0592918	-5.4066695	5.4809086
C	-3.4527972	-5.1782769	3.4992546
C	-4.5851888	-5.5054641	4.2608425
C	-3.1924220	-5.7451469	6.2399496
H	-1.0678364	-5.3813655	5.9624248
H	-3.5516710	-4.9643611	2.4226586
H	-5.5746791	-5.5480063	3.7761596
H	-3.0828746	-5.9780161	7.3121193
H	-5.3482414	-6.0577944	6.2270159
H	-3.9675278	-3.1975547	-1.1592546
C	1.1217220	1.1250659	-0.3766240
C	1.6673657	3.8299646	-0.9715847
C	2.0482508	1.4766255	-1.3800723
C	0.4652695	2.1627936	0.3543502
C	0.7472501	3.5148177	0.0379618
C	2.3283090	2.8171734	-1.6858604
H	2.5457175	0.6655129	-1.9367831
H	0.2237625	4.2991433	0.5981414
H	3.0512309	3.0653502	-2.4799243
H	1.8691702	4.8904274	-1.1982428
N	-0.4383837	1.8013609	1.3726762
H	-0.4668166	0.7975656	1.6115030
C	-1.3236135	2.6179125	2.0677023
O	-1.4135027	3.8337203	1.9114009
C	-2.1912721	1.8626825	3.0739836
H	-2.7017729	0.9900297	2.6114056
H	-2.9450676	2.5679112	3.4757611
H	-1.5716395	1.4770489	3.9135139

Pdb file
HEADER B2Pdb
COMPND B2Pdb

ATOM	1	C	111	1	-0.386	-0.869	-0.520	1.00	0.00
ATOM	2	N	111	1	-0.802	-2.178	-0.317	1.00	0.00
ATOM	3	H	111	1	-1.335	0.962	-1.449	1.00	0.00
ATOM	4	C	111	1	-2.108	-2.211	-0.779	1.00	0.00
ATOM	5	C	111	1	-2.511	-0.921	-1.293	1.00	0.00
ATOM	6	H	111	1	-3.497	-0.702	-1.725	1.00	0.00
ATOM	7	C	111	1	-1.431	-0.090	-1.156	1.00	0.00
ATOM	8	C	111	1	-2.935	-3.330	-0.801	1.00	0.00
ATOM	9	N	111	1	-1.237	-4.951	-0.058	1.00	0.00
ATOM	10	C	111	1	-1.232	-6.339	-0.011	1.00	0.00
ATOM	11	C	111	1	-2.523	-6.876	-0.385	1.00	0.00
ATOM	12	H	111	1	-2.764	-7.947	-0.429	1.00	0.00
ATOM	13	C	111	1	-3.328	-5.800	-0.665	1.00	0.00
ATOM	14	H	111	1	-4.373	-5.791	-1.002	1.00	0.00
ATOM	15	C	111	1	-2.514	-4.618	-0.481	1.00	0.00
ATOM	16	C	111	1	0.844	-0.325	-0.113	1.00	0.00
ATOM	17	H	111	1	4.760	-1.600	2.045	1.00	0.00
ATOM	18	C	111	1	3.765	-1.603	1.578	1.00	0.00
ATOM	19	C	111	1	2.952	-2.783	1.384	1.00	0.00
ATOM	20	H	111	1	3.353	0.502	0.980	1.00	0.00
ATOM	21	N	111	1	1.749	-2.465	0.770	1.00	0.00
ATOM	22	C	111	1	1.820	-1.099	0.536	1.00	0.00
ATOM	23	C	111	1	3.066	-0.554	1.042	1.00	0.00
ATOM	24	C	111	1	-0.138	-7.125	0.348	1.00	0.00
ATOM	25	H	111	1	-0.257	-8.219	0.317	1.00	0.00
ATOM	26	H	111	1	4.196	-6.804	1.971	1.00	0.00
ATOM	27	C	111	1	3.193	-6.569	1.588	1.00	0.00
ATOM	28	C	111	1	2.206	-7.430	1.179	1.00	0.00
ATOM	29	H	111	1	2.214	-8.528	1.158	1.00	0.00
ATOM	30	C	111	1	1.089	-6.611	0.763	1.00	0.00
ATOM	31	N	111	1	1.386	-5.259	0.892	1.00	0.00
ATOM	32	C	111	1	2.677	-5.231	1.401	1.00	0.00
ATOM	33	C	111	1	3.392	-4.070	1.690	1.00	0.00
ATOM	34	H	111	1	4.395	-4.177	2.132	1.00	0.00
ATOM	35	Co	111	1	0.229	-3.691	0.437	1.00	0.00
ATOM	36	N	111	1	-0.584	-3.507	2.701	1.00	0.00
ATOM	37	S	111	1	-1.438	-2.010	3.079	1.00	0.00
ATOM	38	O	111	1	-2.763	-2.114	2.438	1.00	0.00
ATOM	39	O	111	1	-0.462	-0.957	2.709	1.00	0.00
ATOM	40	C	111	1	-1.676	-1.833	4.867	1.00	0.00
ATOM	41	C	111	1	-2.103	-1.369	7.582	1.00	0.00
ATOM	42	C	111	1	-0.626	-1.311	5.646	1.00	0.00
ATOM	43	C	111	1	-2.939	-2.110	5.416	1.00	0.00
ATOM	44	C	111	1	-3.146	-1.870	6.784	1.00	0.00
ATOM	45	C	111	1	-0.845	-1.092	7.015	1.00	0.00
ATOM	46	H	111	1	0.338	-1.059	5.177	1.00	0.00
ATOM	47	H	111	1	-3.744	-2.496	4.774	1.00	0.00
ATOM	48	H	111	1	-4.135	-2.074	7.227	1.00	0.00
ATOM	49	H	111	1	-0.033	-0.684	7.639	1.00	0.00
ATOM	50	H	111	1	-2.273	-1.183	8.655	1.00	0.00
ATOM	51	H	111	1	1.256	-4.452	3.390	1.00	0.00
ATOM	52	C	111	1	0.255	-4.146	3.738	1.00	0.00
ATOM	53	H	111	1	0.217	-3.702	4.750	1.00	0.00
ATOM	54	C	111	1	-0.972	-4.846	3.256	1.00	0.00
ATOM	55	H	111	1	-0.822	-5.602	2.464	1.00	0.00
ATOM	56	C	111	1	-2.179	-5.113	4.107	1.00	0.00
ATOM	57	C	111	1	-4.458	-5.791	5.633	1.00	0.00

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ATOM     58  C   111     1       -2.059  -5.407   5.481  1.00  0.00
ATOM     59  C   111     1       -3.453  -5.178   3.499  1.00  0.00
ATOM     60  C   111     1       -4.585  -5.505   4.261  1.00  0.00
ATOM     61  C   111     1       -3.192  -5.745   6.240  1.00  0.00
ATOM     62  H   111     1       -1.068  -5.381   5.962  1.00  0.00
ATOM     63  H   111     1       -3.552  -4.964   2.423  1.00  0.00
ATOM     64  H   111     1       -5.575  -5.548   3.776  1.00  0.00
ATOM     65  H   111     1       -3.083  -5.978   7.312  1.00  0.00
ATOM     66  H   111     1       -5.348  -6.058   6.227  1.00  0.00
ATOM     67  H   111     1       -3.968  -3.198  -1.159  1.00  0.00
ATOM     68  C   111     1        1.122   1.125  -0.377  1.00  0.00
ATOM     69  C   111     1        1.667   3.830  -0.972  1.00  0.00
ATOM     70  C   111     1        2.048   1.477  -1.380  1.00  0.00
ATOM     71  C   111     1        0.465   2.163   0.354  1.00  0.00
ATOM     72  C   111     1        0.747   3.515   0.038  1.00  0.00
ATOM     73  C   111     1        2.328   2.817  -1.686  1.00  0.00
ATOM     74  H   111     1        2.546   0.666  -1.937  1.00  0.00
ATOM     75  H   111     1        0.224   4.299   0.598  1.00  0.00
ATOM     76  H   111     1        3.051   3.065  -2.480  1.00  0.00
ATOM     77  H   111     1        1.869   4.890  -1.198  1.00  0.00
ATOM     78  N   111     1       -0.438   1.801   1.373  1.00  0.00
ATOM     79  H   111     1       -0.467   0.798   1.612  1.00  0.00
ATOM     80  C   111     1       -1.324   2.618   2.068  1.00  0.00
ATOM     81  O   111     1       -1.414   3.834   1.911  1.00  0.00
ATOM     82  C   111     1       -2.191   1.863   3.074  1.00  0.00
ATOM     83  H   111     1       -2.702   0.990   2.611  1.00  0.00
ATOM     84  H   111     1       -2.945   2.568   3.476  1.00  0.00
ATOM     85  H   111     1       -1.572   1.477   3.914  1.00  0.00
CONECT    1    2    7   16
CONECT    2    4   35
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8   15   67
CONECT    9   10   15   35
CONECT   10   11   24
CONECT   11   12   13
CONECT   13   14   15
CONECT   16   22   68
CONECT   17   18
CONECT   18   19   23
CONECT   19   21   33
CONECT   20   23
CONECT   21   22   35
CONECT   22   23
CONECT   24   25   30
CONECT   26   27
CONECT   27   28   32
CONECT   28   29   30
CONECT   30   31
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CONECT   33   34
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CONECT   40   42   43
CONECT   41   44   45   50
CONECT   42   45   46
CONECT   43   44   47
CONECT   44   48
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CONECT   45   49
CONECT   51   52
CONECT   52   53   54
CONECT   54   55   56
CONECT   56   58   59
CONECT   57   60   61   66
CONECT   58   61   62
CONECT   59   60   63
CONECT   60   64
CONECT   61   65
CONECT   68   70   71
CONECT   69   72   73   77
CONECT   70   73   74
CONECT   71   72   78
CONECT   72   75
CONECT   73   76
CONECT   78   79   80
CONECT   80   81   82
CONECT   82   83   84   85
END

4A_Co(por)
Xyz file
37
Energy =   -2370.629048901
C     0.7508865   0.5779703   0.5225386
N     0.4544062  -0.7630762   0.6703904
H    -0.5216741   2.4379784   0.2666988
C    -0.9230471  -0.8623824   0.6399738
C    -1.5140829   0.4512298   0.4689959
H    -2.5919638   0.6570008   0.4131910
C    -0.4716709   1.3479493   0.3955960
C    -1.6488986  -2.0590018   0.7567301
H    -2.7470757  -1.9818751   0.7138276
N     0.2410333  -3.6339218   0.9974460
C     0.3363625  -5.0024980   1.1583991
C    -0.9874733  -5.5948972   1.1850503
H    -1.1980331  -6.6670261   1.3012017
C    -1.8864785  -4.5621948   1.0386549
H    -2.9836095  -4.6158444   1.0114867
C    -1.1074781  -3.3443279   0.9219350
C     2.0460964   1.1204292   0.4984665
H     2.1275849   2.2120985   0.3742238
H     6.5677103   0.0166806   0.7647285
C     5.4705782  -0.0369650   0.7375945
C     4.6915783  -1.2548344   0.8542938
H     4.7821290   2.0678805   0.4751699
N     3.3430652  -0.9652342   0.7788366
C     3.2477344   0.4033483   0.6179398
C     4.5715707   0.9957464   0.5912760
C     1.5379990  -5.7195741   1.2779122
H     1.4565091  -6.8112378   1.4022021
H     6.1760663  -5.2561722   1.3629584
C     5.0981836  -5.0503946   1.3072113
C     4.0557690  -5.9471044   1.3806951
H     4.1057716  -7.0371304   1.5096186
C     2.8332105  -5.1771213   1.2537880
N     3.1296920  -3.8360804   1.1058901
C     4.5071475  -3.7367819   1.1362395
C     5.2330003  -2.5401669   1.0194443
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H      6.3311792  -2.6173003   1.0622919
Co     1.7920483  -2.2995783   0.8881424


Pdb file
HEADER B2Pdb
COMPND B2Pdb
ATOM      1  C   111     1       0.751   0.578   0.523  1.00  0.00
ATOM      2  N   111     1       0.454  -0.763   0.670  1.00  0.00
ATOM      3  H   111     1      -0.522   2.438   0.267  1.00  0.00
ATOM      4  C   111     1      -0.923  -0.862   0.640  1.00  0.00
ATOM      5  C   111     1      -1.514   0.451   0.469  1.00  0.00
ATOM      6  H   111     1      -2.592   0.657   0.413  1.00  0.00
ATOM      7  C   111     1      -0.472   1.348   0.396  1.00  0.00
ATOM      8  C   111     1      -1.649  -2.059   0.757  1.00  0.00
ATOM      9  H   111     1      -2.747  -1.982   0.714  1.00  0.00
ATOM     10  N   111     1       0.241  -3.634   0.997  1.00  0.00
ATOM     11  C   111     1       0.336  -5.002   1.158  1.00  0.00
ATOM     12  C   111     1      -0.987  -5.595   1.185  1.00  0.00
ATOM     13  H   111     1      -1.198  -6.667   1.301  1.00  0.00
ATOM     14  C   111     1      -1.886  -4.562   1.039  1.00  0.00
ATOM     15  H   111     1      -2.984  -4.616   1.011  1.00  0.00
ATOM     16  C   111     1      -1.107  -3.344   0.922  1.00  0.00
ATOM     17  C   111     1       2.046   1.120   0.498  1.00  0.00
ATOM     18  H   111     1       2.128   2.212   0.374  1.00  0.00
ATOM     19  H   111     1       6.568   0.017   0.765  1.00  0.00
ATOM     20  C   111     1       5.471  -0.037   0.738  1.00  0.00
ATOM     21  C   111     1       4.692  -1.255   0.854  1.00  0.00
ATOM     22  H   111     1       4.782   2.068   0.475  1.00  0.00
ATOM     23  N   111     1       3.343  -0.965   0.779  1.00  0.00
ATOM     24  C   111     1       3.248   0.403   0.618  1.00  0.00
ATOM     25  C   111     1       4.572   0.996   0.591  1.00  0.00
ATOM     26  C   111     1       1.538  -5.720   1.278  1.00  0.00
ATOM     27  H   111     1       1.457  -6.811   1.402  1.00  0.00
ATOM     28  H   111     1       6.176  -5.256   1.363  1.00  0.00
ATOM     29  C   111     1       5.098  -5.050   1.307  1.00  0.00
ATOM     30  C   111     1       4.056  -5.947   1.381  1.00  0.00
ATOM     31  H   111     1       4.106  -7.037   1.510  1.00  0.00
ATOM     32  C   111     1       2.833  -5.177   1.254  1.00  0.00
ATOM     33  N   111     1       3.130  -3.836   1.106  1.00  0.00
ATOM     34  C   111     1       4.507  -3.737   1.136  1.00  0.00
ATOM     35  C   111     1       5.233  -2.540   1.019  1.00  0.00
ATOM     36  H   111     1       6.331  -2.617   1.062  1.00  0.00
ATOM     37 Co   111     1       1.792  -2.300   0.888  1.00  0.00
CONECT    1    2    7   17
CONECT    2    4   37
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   37
CONECT   11   12   26
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   18   24
CONECT   19   20
CONECT   20   21   25
CONECT   21   23   35
CONECT   22   25
CONECT   23   24   37
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CONECT   24   25
CONECT   26   27   32
CONECT   28   29
CONECT   29   30   34
CONECT   30   31   32
CONECT   32   33
CONECT   33   34   37
CONECT   34   35
CONECT   35   36
END


4B_Co(por)
XYZ file
54
 Energy =   -3314.607239738
C     0.7932086   -0.0654984   -0.6975131
N     0.3360837   -1.3615641   -0.5684316
H     0.1297114    1.7077105   -1.9509604
C    -0.7388893   -1.4820082   -1.4216417
C    -0.9785118   -0.2209244   -2.1044013
H    -1.7737701   -0.0430298   -2.8416268
C    -0.0206138    0.6595227   -1.6579328
C    -1.4665051   -2.6644504   -1.6445750
H    -2.3032322   -2.6025628   -2.3589539
N    -0.1951853   -4.2091473   -0.1929693
C    -0.2445719   -5.5685620    0.0370055
C    -1.3126100   -6.1694172   -0.7420948
H    -1.5657606   -7.2385208   -0.7485224
C    -1.9109170   -5.1486683   -1.4428535
H    -2.7550391   -5.2089784   -2.1437923
C    -1.1992459   -3.9298180   -1.0952303
C     1.8857824    0.4723052    0.0034424
H     2.1364905    1.5265113   -0.1955358
H     5.1817715   -0.5603129    3.1373844
C     4.3219209   -0.6157006    2.4551887
C     3.5073719   -1.7987177    2.2312504
H     4.1701907    1.4067789    1.5283125
N     2.5179014   -1.5250598    1.3115588
C     2.6879307   -0.2076140    0.9364266
C     3.8144893    0.3738148    1.6451806
C     0.6104050   -6.2688752    0.9019761
H     0.4554348   -7.3564617    0.9855802
H     4.2248804   -5.7361226    3.8045850
C     3.3980777   -5.5464960    3.1055701
C     2.5247142   -6.4584455    2.5534584
H     2.4887650   -7.5456072    2.7097471
C     1.6438428   -5.7113220    1.6737771
N     1.9741600   -4.3708615    1.7010006
C     3.0478428   -4.2473921    2.5586037
C     3.7372377   -3.0516618    2.8263449
H     4.5772460   -3.1140693    3.5369807
Co    0.9750314   -2.8201786    0.7739796
N    -0.3354177   -2.1597655    2.3472307
S    -1.4960086   -3.1084451    3.4445542
O    -1.5620294   -4.4218982    2.7975661
O    -2.6632987   -2.2320808    3.6528352
C    -0.5523016   -3.2148907    4.9666406
C     0.8894603   -3.3862321    7.3337711
C    -0.8411434   -2.3080045    6.0014960
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C     0.4353584   -4.2077507    5.0837406
C     1.1576257   -4.2843573    6.2845746
C    -0.1067745   -2.4030868    7.1942667
H    -1.6353500   -1.5568023    5.8737843
H     0.6316715   -4.9066204    4.2559435
H     1.9364100   -5.0555051    6.3964274
H    -0.3193708   -1.7062365    8.0211453
H     1.4621182   -3.4548210    8.2732152
N    -0.4480983   -0.9251981    2.4990059
N    -0.4906686    0.2195448    2.5737991

Pdb file
HEADER B2Pdb
COMPND B2Pdb
ATOM      1  C   111     1       0.793  -0.065  -0.698  1.00  0.00
ATOM      2  N   111     1       0.336  -1.362  -0.568  1.00  0.00
ATOM      3  H   111     1       0.130   1.708  -1.951  1.00  0.00
ATOM      4  C   111     1      -0.739  -1.482  -1.422  1.00  0.00
ATOM      5  C   111     1      -0.979  -0.221  -2.104  1.00  0.00
ATOM      6  H   111     1      -1.774  -0.043  -2.842  1.00  0.00
ATOM      7  C   111     1      -0.021   0.660  -1.658  1.00  0.00
ATOM      8  C   111     1      -1.467  -2.664  -1.645  1.00  0.00
ATOM      9  H   111     1      -2.303  -2.603  -2.359  1.00  0.00
ATOM     10  N   111     1      -0.195  -4.209  -0.193  1.00  0.00
ATOM     11  C   111     1      -0.245  -5.569   0.037  1.00  0.00
ATOM     12  C   111     1      -1.313  -6.169  -0.742  1.00  0.00
ATOM     13  H   111     1      -1.566  -7.239  -0.749  1.00  0.00
ATOM     14  C   111     1      -1.911  -5.149  -1.443  1.00  0.00
ATOM     15  H   111     1      -2.755  -5.209  -2.144  1.00  0.00
ATOM     16  C   111     1      -1.199  -3.930  -1.095  1.00  0.00
ATOM     17  C   111     1       1.886   0.472   0.003  1.00  0.00
ATOM     18  H   111     1       2.136   1.527  -0.196  1.00  0.00
ATOM     19  H   111     1       5.182  -0.560   3.137  1.00  0.00
ATOM     20  C   111     1       4.322  -0.616   2.455  1.00  0.00
ATOM     21  C   111     1       3.507  -1.799   2.231  1.00  0.00
ATOM     22  H   111     1       4.170   1.407   1.528  1.00  0.00
ATOM     23  N   111     1       2.518  -1.525   1.312  1.00  0.00
ATOM     24  C   111     1       2.688  -0.208   0.936  1.00  0.00
ATOM     25  C   111     1       3.814   0.374   1.645  1.00  0.00
ATOM     26  C   111     1       0.610  -6.269   0.902  1.00  0.00
ATOM     27  H   111     1       0.455  -7.356   0.986  1.00  0.00
ATOM     28  H   111     1       4.225  -5.736   3.805  1.00  0.00
ATOM     29  C   111     1       3.398  -5.546   3.106  1.00  0.00
ATOM     30  C   111     1       2.525  -6.458   2.553  1.00  0.00
ATOM     31  H   111     1       2.489  -7.546   2.710  1.00  0.00
ATOM     32  C   111     1       1.644  -5.711   1.674  1.00  0.00
ATOM     33  N   111     1       1.974  -4.371   1.701  1.00  0.00
ATOM     34  C   111     1       3.048  -4.247   2.559  1.00  0.00
ATOM     35  C   111     1       3.737  -3.052   2.826  1.00  0.00
ATOM     36  H   111     1       4.577  -3.114   3.537  1.00  0.00
ATOM     37 Co   111     1       0.975  -2.820   0.774  1.00  0.00
ATOM     38  N   111     1      -0.335  -2.160   2.347  1.00  0.00
ATOM     39  S   111     1      -1.496  -3.108   3.445  1.00  0.00
ATOM     40  O   111     1      -1.562  -4.422   2.798  1.00  0.00
ATOM     41  O   111     1      -2.663  -2.232   3.653  1.00  0.00
ATOM     42  C   111     1      -0.552  -3.215   4.967  1.00  0.00
ATOM     43  C   111     1       0.889  -3.386   7.334  1.00  0.00
ATOM     44  C   111     1      -0.841  -2.308   6.001  1.00  0.00
ATOM     45  C   111     1       0.435  -4.208   5.084  1.00  0.00
ATOM     46  C   111     1       1.158  -4.284   6.285  1.00  0.00
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ATOM     47  C   111     1       -0.107  -2.403   7.194  1.00  0.00
ATOM     48  H   111     1       -1.635  -1.557   5.874  1.00  0.00
ATOM     49  H   111     1        0.632  -4.907   4.256  1.00  0.00
ATOM     50  H   111     1        1.936  -5.056   6.396  1.00  0.00
ATOM     51  H   111     1       -0.319  -1.706   8.021  1.00  0.00
ATOM     52  H   111     1        1.462  -3.455   8.273  1.00  0.00
ATOM     53  N   111     1       -0.448  -0.925   2.499  1.00  0.00
ATOM     54  N   111     1       -0.491   0.220   2.574  1.00  0.00
CONECT    1    2    7   17
CONECT    2    4   37
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   37
CONECT   11   12   26
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   18   24
CONECT   19   20
CONECT   20   21   25
CONECT   21   23   35
CONECT   22   25
CONECT   23   24   37
CONECT   24   25
CONECT   26   27   32
CONECT   28   29
CONECT   29   30   34
CONECT   30   31   32
CONECT   32   33
CONECT   33   34   37
CONECT   34   35
CONECT   35   36
CONECT   37   38
CONECT   38   39   53
CONECT   39   40   41   42
CONECT   42   44   45
CONECT   43   46   47   52
CONECT   44   47   48
CONECT   45   46   49
CONECT   46   50
CONECT   47   51
CONECT   53   54
END

4TS1_Co(por)
XYZ file
54
 Energy =   -3314.583455382
C     0.2216503    0.1206110    0.6344595
N     0.1914943   -1.2017390    0.2283591
H    -1.1405311    1.8922299    0.3171831
C    -0.9641675   -1.3344851   -0.5218832
C    -1.6531947   -0.0679976   -0.6168863
H    -2.5886948    0.0923352   -1.1690590
C    -0.9325307    0.8302169    0.1310695
C    -1.4529654   -2.5327289   -1.0370800
H    -2.3891251   -2.5050480   -1.6144161
N     0.2806505   -3.9845343   -0.0533471
C     0.4072152   -5.3559928    0.0636206
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C    -0.7082556   -6.0234060   -0.5730144
H    -0.8376342   -7.1130223   -0.6223398
C    -1.4987927   -5.0395211   -1.1133439
H    -2.4281617   -5.1430443   -1.6890644
C    -0.8889374   -3.7764879   -0.7606948
C     1.2724624    0.7244414    1.3227597
H     1.1694381    1.7847067    1.5982234
H     5.7865180    0.0360705    2.1441723
C     4.7232583   -0.1119722    1.9128730
C     4.1416664   -1.3681193    1.4947838
H     3.7318473    1.8563633    2.2606331
N     2.7841911   -1.2211888    1.2669103
C     2.4996786    0.1015130    1.5503795
C     3.6948385    0.7957541    1.9782086
C     1.5173292   -6.0171984    0.5893498
H     1.4989705   -7.1170890    0.6207683
H     5.9883666   -5.1924677    1.5241269
C     4.9136038   -5.0762451    1.3308111
C     3.9550683   -6.0504755    1.1914290
H     4.0748030   -7.1415981    1.2303945
C     2.7054589   -5.3701755    0.9325738
N     2.8884945   -3.9997078    0.9486277
C     4.2352075   -3.8064336    1.2071505
C     4.8438208   -2.5698823    1.4160677
H     5.9248591   -2.5522919    1.6193698
Co    1.4412622   -2.6324962    0.8339764
N     0.7400581   -2.8197527    2.6579732
S    -0.8460379   -2.4250362    3.1826131
O    -1.7493293   -2.9294881    2.1215837
O    -0.8944523   -1.0051593    3.6084928
C    -1.1107004   -3.4468098    4.6527501
C    -1.5790946   -5.0155229    6.9085435
C    -0.9472740   -2.8774147    5.9258703
C    -1.5113320   -4.7832003    4.4841410
C    -1.7434596   -5.5680677    5.6248703
C    -1.1847466   -3.6737825    7.0582727
H    -0.6486490   -1.8218203    6.0135013
H    -1.6486137   -5.1894905    3.4701468
H    -2.0618902   -6.6175956    5.5111782
H    -1.0631092   -3.2415313    8.0652039
H    -1.7649665   -5.6359585    7.8009004
N     2.7939465   -2.9082019    3.9104790
N     1.6517568   -2.6652685    3.9285822

Pdb file
HEADER B2Pdb
COMPND B2Pdb
ATOM      1  C   111     1       0.222   0.121   0.634  1.00  0.00
ATOM      2  N   111     1       0.191  -1.202   0.228  1.00  0.00
ATOM      3  H   111     1      -1.141   1.892   0.317  1.00  0.00
ATOM      4  C   111     1      -0.964  -1.334  -0.522  1.00  0.00
ATOM      5  C   111     1      -1.653  -0.068  -0.617  1.00  0.00
ATOM      6  H   111     1      -2.589   0.092  -1.169  1.00  0.00
ATOM      7  C   111     1      -0.933   0.830   0.131  1.00  0.00
ATOM      8  C   111     1      -1.453  -2.533  -1.037  1.00  0.00
ATOM      9  H   111     1      -2.389  -2.505  -1.614  1.00  0.00
ATOM     10  N   111     1       0.281  -3.985  -0.053  1.00  0.00
ATOM     11  C   111     1       0.407  -5.356   0.064  1.00  0.00
ATOM     12  C   111     1      -0.708  -6.023  -0.573  1.00  0.00
ATOM     13  H   111     1      -0.838  -7.113  -0.622  1.00  0.00
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ATOM     14  C   111     1       -1.499  -5.040  -1.113  1.00  0.00
ATOM     15  H   111     1       -2.428  -5.143  -1.689  1.00  0.00
ATOM     16  C   111     1       -0.889  -3.776  -0.761  1.00  0.00
ATOM     17  C   111     1        1.272   0.724   1.323  1.00  0.00
ATOM     18  H   111     1        1.169   1.785   1.598  1.00  0.00
ATOM     19  H   111     1        5.787   0.036   2.144  1.00  0.00
ATOM     20  C   111     1        4.723  -0.112   1.913  1.00  0.00
ATOM     21  C   111     1        4.142  -1.368   1.495  1.00  0.00
ATOM     22  H   111     1        3.732   1.856   2.261  1.00  0.00
ATOM     23  N   111     1        2.784  -1.221   1.267  1.00  0.00
ATOM     24  C   111     1        2.500   0.102   1.550  1.00  0.00
ATOM     25  C   111     1        3.695   0.796   1.978  1.00  0.00
ATOM     26  C   111     1        1.517  -6.017   0.589  1.00  0.00
ATOM     27  H   111     1        1.499  -7.117   0.621  1.00  0.00
ATOM     28  H   111     1        5.988  -5.192   1.524  1.00  0.00
ATOM     29  C   111     1        4.914  -5.076   1.331  1.00  0.00
ATOM     30  C   111     1        3.955  -6.050   1.191  1.00  0.00
ATOM     31  H   111     1        4.075  -7.142   1.230  1.00  0.00
ATOM     32  C   111     1        2.705  -5.370   0.933  1.00  0.00
ATOM     33  N   111     1        2.888  -4.000   0.949  1.00  0.00
ATOM     34  C   111     1        4.235  -3.806   1.207  1.00  0.00
ATOM     35  C   111     1        4.844  -2.570   1.416  1.00  0.00
ATOM     36  H   111     1        5.925  -2.552   1.619  1.00  0.00
ATOM     37 Co   111     1        1.441  -2.632   0.834  1.00  0.00
ATOM     38  N   111     1        0.740  -2.820   2.658  1.00  0.00
ATOM     39  S   111     1       -0.846  -2.425   3.183  1.00  0.00
ATOM     40  O   111     1       -1.749  -2.929   2.122  1.00  0.00
ATOM     41  O   111     1       -0.894  -1.005   3.608  1.00  0.00
ATOM     42  C   111     1       -1.111  -3.447   4.653  1.00  0.00
ATOM     43  C   111     1       -1.579  -5.016   6.909  1.00  0.00
ATOM     44  C   111     1       -0.947  -2.877   5.926  1.00  0.00
ATOM     45  C   111     1       -1.511  -4.783   4.484  1.00  0.00
ATOM     46  C   111     1       -1.743  -5.568   5.625  1.00  0.00
ATOM     47  C   111     1       -1.185  -3.674   7.058  1.00  0.00
ATOM     48  H   111     1       -0.649  -1.822   6.014  1.00  0.00
ATOM     49  H   111     1       -1.649  -5.189   3.470  1.00  0.00
ATOM     50  H   111     1       -2.062  -6.618   5.511  1.00  0.00
ATOM     51  H   111     1       -1.063  -3.242   8.065  1.00  0.00
ATOM     52  H   111     1       -1.765  -5.636   7.801  1.00  0.00
ATOM     53  N   111     1        2.794  -2.908   3.910  1.00  0.00
ATOM     54  N   111     1        1.652  -2.665   3.929  1.00  0.00
CONECT    1    2    7   17
CONECT    2    4   37
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   37
CONECT   11   12   26
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   18   24
CONECT   19   20
CONECT   20   21   25
CONECT   21   23   35
CONECT   22   25
CONECT   23   24   37
CONECT   24   25
CONECT   26   27   32
CONECT   28   29
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CONECT   29   30   34
CONECT   30   31   32
CONECT   32   33
CONECT   33   34   37
CONECT   34   35
CONECT   35   36
CONECT   37   38
CONECT   38   39   54
CONECT   39   40   41   42
CONECT   42   44   45
CONECT   43   46   47   52
CONECT   44   47   48
CONECT   45   46   49
CONECT   46   50
CONECT   47   51
CONECT   53   54
END



4C_Co(por)
XYZ file
52
 Energy =   -3207.0071099820
C     0.3424128   -0.2240022   -0.3064677
N     0.1013842   -1.5843737   -0.2614804
H    -0.7931396    1.5544704   -1.1101568
C    -1.1527298   -1.7511297   -0.8186640
C    -1.6882385   -0.4834745   -1.2632867
H    -2.6648087   -0.3558592   -1.7489147
C    -0.7542205    0.4696133   -0.9448534
C    -1.8299865   -2.9620710   -0.9304758
H    -2.8367183   -2.9505467   -1.3736613
N    -0.0654866   -4.3937767    0.0386769
C     0.0346625   -5.7615761    0.2217453
C    -1.1654687   -6.4272336   -0.2368892
H    -1.3230062   -7.5138117   -0.2099866
C    -2.0050555   -5.4466317   -0.6998172
H    -3.0067629   -5.5467804   -1.1383986
C    -1.3114515   -4.1890381   -0.5241504
C     1.4686205    0.4123131    0.2073510
H     1.5236891    1.5082051    0.1262268
H     5.5407625   -0.4451954    2.2524068
C     4.5441471   -0.5508057    1.8032230
C     3.8667543   -1.8132354    1.6004171
H     3.8694233    1.5098440    1.2768723
N     2.6374544   -1.6161354    0.9972235
C     2.5301149   -0.2491090    0.8199104
C     3.7109219    0.4238620    1.3163561
C     1.1417442   -6.4323977    0.7352108
H     1.0905040   -7.5291588    0.8096159
H     5.3822477   -5.6842266    2.4623124
C     4.3834056   -5.5519506    2.0252480
C     3.4591246   -6.5078419    1.6839677
H     3.5297815   -7.5996853    1.7790925
C     2.3121705   -5.8031327    1.1554647
N     2.5365004   -4.4393578    1.1497532
C     3.7932875   -4.2722693    1.7001678
C     4.4190528   -3.0483895    1.9311066
H     5.4175770   -3.0590559    2.3932402
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Co    1.1911031   -2.9866362    0.7312014
N     0.3953351   -2.7694460    2.3514833
S    -0.7970486   -1.9646353    3.1387010
O    -2.1123355   -2.4169196    2.6038706
O    -0.4696543   -0.5109907    3.1435692
C    -0.6721427   -2.5548144    4.8400810
C    -0.4479423   -3.4927718    7.4583675
C     0.1782201   -1.8854089    5.7375214
C    -1.4178707   -3.6804967    5.2311395
C    -1.3002826   -4.1472109    6.5499856
C     0.2872837   -2.3635220    7.0529406
H     0.7293064   -0.9937564    5.4002731
H    -2.0890666   -4.1653111    4.5050110
H    -1.8838442   -5.0252829    6.8736603
H     0.9467390   -1.8464392    7.7697431
H    -0.3606519   -3.8622363    8.4936855


Pdb file
HEADER B2Pdb
COMPND B2Pdb
ATOM      1  C   111     1       0.342  -0.224  -0.306  1.00  0.00
ATOM      2  N   111     1       0.101  -1.584  -0.261  1.00  0.00
ATOM      3  H   111     1      -0.793   1.554  -1.110  1.00  0.00
ATOM      4  C   111     1      -1.153  -1.751  -0.819  1.00  0.00
ATOM      5  C   111     1      -1.688  -0.483  -1.263  1.00  0.00
ATOM      6  H   111     1      -2.665  -0.356  -1.749  1.00  0.00
ATOM      7  C   111     1      -0.754   0.470  -0.945  1.00  0.00
ATOM      8  C   111     1      -1.830  -2.962  -0.930  1.00  0.00
ATOM      9  H   111     1      -2.837  -2.951  -1.374  1.00  0.00
ATOM     10  N   111     1      -0.065  -4.394   0.039  1.00  0.00
ATOM     11  C   111     1       0.035  -5.762   0.222  1.00  0.00
ATOM     12  C   111     1      -1.165  -6.427  -0.237  1.00  0.00
ATOM     13  H   111     1      -1.323  -7.514  -0.210  1.00  0.00
ATOM     14  C   111     1      -2.005  -5.447  -0.700  1.00  0.00
ATOM     15  H   111     1      -3.007  -5.547  -1.138  1.00  0.00
ATOM     16  C   111     1      -1.311  -4.189  -0.524  1.00  0.00
ATOM     17  C   111     1       1.469   0.412   0.207  1.00  0.00
ATOM     18  H   111     1       1.524   1.508   0.126  1.00  0.00
ATOM     19  H   111     1       5.541  -0.445   2.252  1.00  0.00
ATOM     20  C   111     1       4.544  -0.551   1.803  1.00  0.00
ATOM     21  C   111     1       3.867  -1.813   1.600  1.00  0.00
ATOM     22  H   111     1       3.869   1.510   1.277  1.00  0.00
ATOM     23  N   111     1       2.637  -1.616   0.997  1.00  0.00
ATOM     24  C   111     1       2.530  -0.249   0.820  1.00  0.00
ATOM     25  C   111     1       3.711   0.424   1.316  1.00  0.00
ATOM     26  C   111     1       1.142  -6.432   0.735  1.00  0.00
ATOM     27  H   111     1       1.091  -7.529   0.810  1.00  0.00
ATOM     28  H   111     1       5.382  -5.684   2.462  1.00  0.00
ATOM     29  C   111     1       4.383  -5.552   2.025  1.00  0.00
ATOM     30  C   111     1       3.459  -6.508   1.684  1.00  0.00
ATOM     31  H   111     1       3.530  -7.600   1.779  1.00  0.00
ATOM     32  C   111     1       2.312  -5.803   1.155  1.00  0.00
ATOM     33  N   111     1       2.537  -4.439   1.150  1.00  0.00
ATOM     34  C   111     1       3.793  -4.272   1.700  1.00  0.00
ATOM     35  C   111     1       4.419  -3.048   1.931  1.00  0.00
ATOM     36  H   111     1       5.418  -3.059   2.393  1.00  0.00
ATOM     37 Co   111     1       1.191  -2.987   0.731  1.00  0.00
ATOM     38  N   111     1       0.395  -2.769   2.351  1.00  0.00
ATOM     39  S   111     1      -0.797  -1.965   3.139  1.00  0.00
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ATOM     40  O   111     1       -2.112  -2.417   2.604  1.00  0.00
ATOM     41  O   111     1       -0.470  -0.511   3.144  1.00  0.00
ATOM     42  C   111     1       -0.672  -2.555   4.840  1.00  0.00
ATOM     43  C   111     1       -0.448  -3.493   7.458  1.00  0.00
ATOM     44  C   111     1        0.178  -1.885   5.738  1.00  0.00
ATOM     45  C   111     1       -1.418  -3.680   5.231  1.00  0.00
ATOM     46  C   111     1       -1.300  -4.147   6.550  1.00  0.00
ATOM     47  C   111     1        0.287  -2.364   7.053  1.00  0.00
ATOM     48  H   111     1        0.729  -0.994   5.400  1.00  0.00
ATOM     49  H   111     1       -2.089  -4.165   4.505  1.00  0.00
ATOM     50  H   111     1       -1.884  -5.025   6.874  1.00  0.00
ATOM     51  H   111     1        0.947  -1.846   7.770  1.00  0.00
ATOM     52  H   111     1       -0.361  -3.862   8.494  1.00  0.00
CONECT    1    2    7   17
CONECT    2    4   37
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   37
CONECT   11   12   26
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   18   24
CONECT   19   20
CONECT   20   21   25
CONECT   21   23   35
CONECT   22   25
CONECT   23   24   37
CONECT   24   25
CONECT   26   27   32
CONECT   28   29
CONECT   29   30   34
CONECT   30   31   32
CONECT   32   33
CONECT   33   34   37
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CONECT   37   38
CONECT   38   39
CONECT   39   40   41   42
CONECT   42   44   45
CONECT   43   46   47   52
CONECT   44   47   48
CONECT   45   46   49
CONECT   46   50
CONECT   47   51
END
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4TS2_Co(por)
Xyz file
68
 Energy =   -3516.7453726860
C    -0.4742377   -0.3018365    0.7192547
N    -0.3623410   -1.6748849    0.8189279
H    -2.0390173    1.0938659   -0.1212253
C    -1.5338802   -2.1813722    0.2866171
C    -2.3956959   -1.1076415   -0.1593457
H    -3.3825987   -1.2503350   -0.6194308
C    -1.7219580    0.0626676    0.0835873
C    -1.8069467   -3.5335307    0.0903364
H    -2.7796565   -3.8065618   -0.3456243
N     0.3873335   -4.3756083    0.8373312
C     1.0186313   -5.6001704    0.7134699
C     0.1495605   -6.5557736    0.0597307
H     0.4251902   -7.5935405   -0.1709357
C    -1.0364302   -5.9062629   -0.1827879
H    -1.9424283   -6.2900776   -0.6708632
C    -0.8683829   -4.5474675    0.2874717
C     0.4410255    0.6180604    1.2258204
H     4.1319846    0.8611658    4.0258850
C     3.3145058    0.4979945    3.3885854
C     3.0334787   -0.8988606    3.1264851
H     2.3006046    2.3133092    2.5812617
N     1.9500066   -1.0249865    2.2775146
C     1.5477482    0.2656621    1.9951122
C     2.4053929    1.2231224    2.6611302
C     2.2873136   -5.9080643    1.2062243
H     2.6719537   -6.9260176    1.0418523
H     5.5840623   -4.1829361    3.9835628
C     4.6946028   -4.3001797    3.3498205
C     4.3015835   -5.3930453    2.6158558
H     4.7905295   -6.3724888    2.5260573
C     3.0635295   -5.0287310    1.9620155
N     2.7237198   -3.7204819    2.2595416
C     3.7165264   -3.2627502    3.1052575
C     3.8331040   -1.9517404    3.5718314
H     4.6730129   -1.7150018    4.2424389
Co    1.0367468   -2.7319885    1.7885415
N     0.1037891   -2.9808775    3.4046829
S    -1.0477401   -2.0702801    4.1673685
O    -2.3981723   -2.6597787    3.9573708
O    -0.8303571   -0.6354168    3.8195941
C    -0.6687881   -2.1848918    5.9388512
C    -0.1529298   -2.1927797    8.6854945
C     0.6119108   -1.8293402    6.3997167
C    -1.6962135   -2.5335159    6.8292552
C    -1.4320097   -2.5318327    8.2106481
C     0.8673408   -1.8440514    7.7797592
H     1.3961899   -1.5455200    5.6799535
H    -2.6869468   -2.7971210    6.4277842
H    -2.2334549   -2.7958068    8.9209635
H     1.8688431   -1.5734752    8.1535365
H     0.0510873   -2.1959440    9.7692060
C    -1.0425707   -5.7610511    3.7837054
C     0.0608686   -5.0818390    4.2645888
H     1.0109138   -5.1357868    3.7166664
H     0.1248529   -4.7538051    5.3158562
H    -0.9999974   -6.1137710    2.7373736
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C    -2.2839873   -6.0597277    4.4822664
C    -4.7347639   -6.7413137    5.7604872
C    -3.3624167   -6.6357898    3.7554877
C    -2.4690688   -5.8488536    5.8768254
C    -3.6750508   -6.1831861    6.5023921
C    -4.5698596   -6.9674004    4.3816805
H    -3.2374274   -6.8120302    2.6736201
H    -1.6482134   -5.4277945    6.4781834
H    -3.7928311   -6.0126943    7.5857082
H    -5.3919416   -7.4056750    3.7914426
H    -5.6833582   -7.0035676    6.2576921
H     0.2331827    1.6886095    1.0797874
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Pdb file
HEADER B2Pdb
COMPND B2Pdb
ATOM      1  C   111     1      -0.474  -0.302   0.719  1.00  0.00
ATOM      2  N   111     1      -0.362  -1.675   0.819  1.00  0.00
ATOM      3  H   111     1      -2.039   1.094  -0.121  1.00  0.00
ATOM      4  C   111     1      -1.534  -2.181   0.287  1.00  0.00
ATOM      5  C   111     1      -2.396  -1.108  -0.159  1.00  0.00
ATOM      6  H   111     1      -3.383  -1.250  -0.619  1.00  0.00
ATOM      7  C   111     1      -1.722   0.063   0.084  1.00  0.00
ATOM      8  C   111     1      -1.807  -3.534   0.090  1.00  0.00
ATOM      9  H   111     1      -2.780  -3.807  -0.346  1.00  0.00
ATOM     10  N   111     1       0.387  -4.376   0.837  1.00  0.00
ATOM     11  C   111     1       1.019  -5.600   0.713  1.00  0.00
ATOM     12  C   111     1       0.150  -6.556   0.060  1.00  0.00
ATOM     13  H   111     1       0.425  -7.594  -0.171  1.00  0.00
ATOM     14  C   111     1      -1.036  -5.906  -0.183  1.00  0.00
ATOM     15  H   111     1      -1.942  -6.290  -0.671  1.00  0.00
ATOM     16  C   111     1      -0.868  -4.547   0.287  1.00  0.00
ATOM     17  C   111     1       0.441   0.618   1.226  1.00  0.00
ATOM     18  H   111     1       4.132   0.861   4.026  1.00  0.00
ATOM     19  C   111     1       3.315   0.498   3.389  1.00  0.00
ATOM     20  C   111     1       3.033  -0.899   3.126  1.00  0.00
ATOM     21  H   111     1       2.301   2.313   2.581  1.00  0.00
ATOM     22  N   111     1       1.950  -1.025   2.278  1.00  0.00
ATOM     23  C   111     1       1.548   0.266   1.995  1.00  0.00
ATOM     24  C   111     1       2.405   1.223   2.661  1.00  0.00
ATOM     25  C   111     1       2.287  -5.908   1.206  1.00  0.00
ATOM     26  H   111     1       2.672  -6.926   1.042  1.00  0.00
ATOM     27  H   111     1       5.584  -4.183   3.984  1.00  0.00
ATOM     28  C   111     1       4.695  -4.300   3.350  1.00  0.00
ATOM     29  C   111     1       4.302  -5.393   2.616  1.00  0.00
ATOM     30  H   111     1       4.791  -6.372   2.526  1.00  0.00
ATOM     31  C   111     1       3.064  -5.029   1.962  1.00  0.00
ATOM     32  N   111     1       2.724  -3.720   2.260  1.00  0.00
ATOM     33  C   111     1       3.717  -3.263   3.105  1.00  0.00
ATOM     34  C   111     1       3.833  -1.952   3.572  1.00  0.00
ATOM     35  H   111     1       4.673  -1.715   4.242  1.00  0.00
ATOM     36 Co   111     1       1.037  -2.732   1.789  1.00  0.00
ATOM     37  N   111     1       0.104  -2.981   3.405  1.00  0.00
ATOM     38  S   111     1      -1.048  -2.070   4.167  1.00  0.00
ATOM     39  O   111     1      -2.398  -2.660   3.957  1.00  0.00
ATOM     40  O   111     1      -0.830  -0.635   3.820  1.00  0.00
ATOM     41  C   111     1      -0.669  -2.185   5.939  1.00  0.00
ATOM     42  C   111     1      -0.153  -2.193   8.685  1.00  0.00
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ATOM     43  C   111     1       0.612  -1.829   6.400  1.00  0.00
ATOM     44  C   111     1      -1.696  -2.534   6.829  1.00  0.00
ATOM     45  C   111     1      -1.432  -2.532   8.211  1.00  0.00
ATOM     46  C   111     1       0.867  -1.844   7.780  1.00  0.00
ATOM     47  H   111     1       1.396  -1.546   5.680  1.00  0.00
ATOM     48  H   111     1      -2.687  -2.797   6.428  1.00  0.00
ATOM     49  H   111     1      -2.233  -2.796   8.921  1.00  0.00
ATOM     50  H   111     1       1.869  -1.573   8.154  1.00  0.00
ATOM     51  H   111     1       0.051  -2.196   9.769  1.00  0.00
ATOM     52  C   111     1      -1.043  -5.761   3.784  1.00  0.00
ATOM     53  C   111     1       0.061  -5.082   4.265  1.00  0.00
ATOM     54  H   111     1       1.011  -5.136   3.717  1.00  0.00
ATOM     55  H   111     1       0.125  -4.754   5.316  1.00  0.00
ATOM     56  H   111     1      -1.000  -6.114   2.737  1.00  0.00
ATOM     57  C   111     1      -2.284  -6.060   4.482  1.00  0.00
ATOM     58  C   111     1      -4.735  -6.741   5.760  1.00  0.00
ATOM     59  C   111     1      -3.362  -6.636   3.755  1.00  0.00
ATOM     60  C   111     1      -2.469  -5.849   5.877  1.00  0.00
ATOM     61  C   111     1      -3.675  -6.183   6.502  1.00  0.00
ATOM     62  C   111     1      -4.570  -6.967   4.382  1.00  0.00
ATOM     63  H   111     1      -3.237  -6.812   2.674  1.00  0.00
ATOM     64  H   111     1      -1.648  -5.428   6.478  1.00  0.00
ATOM     65  H   111     1      -3.793  -6.013   7.586  1.00  0.00
ATOM     66  H   111     1      -5.392  -7.406   3.791  1.00  0.00
ATOM     67  H   111     1      -5.683  -7.004   6.258  1.00  0.00
ATOM     68  H   111     1       0.233   1.689   1.080  1.00  0.00
CONECT    1    2    7   17
CONECT    2    4   36
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   36
CONECT   11   12   25
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   23   68
CONECT   18   19
CONECT   19   20   24
CONECT   20   22   34
CONECT   21   24
CONECT   22   23   36
CONECT   23   24
CONECT   25   26   31
CONECT   27   28
CONECT   28   29   33
CONECT   29   30   31
CONECT   31   32
CONECT   32   33   36
CONECT   33   34
CONECT   34   35
CONECT   36   37
CONECT   37   38
CONECT   38   39   40   41
CONECT   41   43   44
CONECT   42   45   46   51
CONECT   43   46   47
CONECT   44   45   48
CONECT   45   49
CONECT   46   50
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CONECT   52   53   56   57
CONECT   53   54   55
CONECT   57   59   60
CONECT   58   61   62   67
CONECT   59   62   63
CONECT   60   61   64
CONECT   61   65
CONECT   62   66
END

4D_Co(por)
Xyz file
68
 Energy =   -3516.7815291640
C     0.4136686   -1.0551759   -0.8891941
N    -0.2055825   -2.2215607   -0.4793197
H    -0.2317783    0.7188738   -2.1295496
C    -1.4868975   -2.1598497   -0.9936669
C    -1.6840460   -0.9242612   -1.7220539
H    -2.6193545   -0.6376209   -2.2210112
C    -0.4901678   -0.2500415   -1.6820327
C    -2.4175644   -3.1974350   -0.9570218
N    -0.9408651   -4.8614876    0.1064460
C    -1.0432916   -6.2287018    0.2956580
C    -2.2998885   -6.7217941   -0.2238587
H    -2.6139657   -7.7738629   -0.2037013
C    -2.9844976   -5.6296305   -0.6971264
H    -3.9784248   -5.5919307   -1.1627716
C    -2.1246305   -4.4828982   -0.5000976
C     1.7072555   -0.6697251   -0.5462770
H     5.0932038   -1.7450579    2.4345070
C     4.1846003   -1.7706159    1.8177263
C     3.1991841   -2.8313035    1.8469816
H     4.2488795    0.0584001    0.5413263
N     2.1807825   -2.5728245    0.9489793
C     2.5077131   -1.3677514    0.3556400
C     3.7672296   -0.8734363    0.8664886
C    -0.1103074   -7.0194753    0.9670012
H    -0.3135821   -8.0975855    1.0520738
H     3.6698400   -6.6495996    3.6385271
C     2.8300964   -6.4328608    2.9644269
C     1.9069352   -7.3025128    2.4370063
H     1.8150637   -8.3856640    2.5936841
C     1.0222967   -6.5143331    1.6067682
N     1.4165741   -5.1860804    1.6002353
C     2.5296539   -5.1267830    2.4190503
C     3.3361398   -4.0015454    2.5940877
H     4.1989860   -4.0841171    3.2729610
Co    0.4961305   -3.6196512    0.7550643
N    -0.4635581   -3.0747138    2.3940596
S    -0.8629529   -1.4562511    2.7303724
O    -2.2738203   -1.1921925    2.3317564
O     0.2174399   -0.6018188    2.1878482
C    -0.7841710   -1.3104367    4.5403515
C    -0.6488757   -1.0342254    7.3140311
C     0.4753210   -1.2348724    5.1609097
C    -1.9749497   -1.2384162    5.2805387
C    -1.9004836   -1.0998714    6.6773425
C     0.5362407   -1.0998722    6.5569231
H     1.3909803   -1.2691840    4.5497461
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H	-2.9412226	-1.2815547	4.7544052
H	-2.8278346	-1.0401499	7.2704991
H	1.5163393	-1.0375318	7.0583851
H	-0.5945795	-0.9260802	8.4099707
H	-0.6213969	-5.0357643	3.0423773
C	-1.1418747	-4.0669256	3.2286777
H	-0.9550724	-3.8508410	4.3144820
C	-2.6218240	-4.2172182	2.9856828
H	-3.0750843	-3.5610564	2.2266960
C	-3.4500956	-5.1424447	3.6797804
C	-5.1779171	-6.9746876	5.0333341
C	-2.9522394	-6.0351525	4.6870684
C	-4.8528600	-5.2120481	3.3828298
C	-5.6932931	-6.1070882	4.0456351
C	-3.8031423	-6.9281639	5.3443882
H	-1.8815755	-6.0195782	4.9476729
H	-5.2608181	-4.5364266	2.6122622
H	-6.7674156	-6.1355957	3.7955052
H	-3.3924860	-7.6032621	6.1144185
H	-5.8430055	-7.6815013	5.5563814
H	-3.4036089	-3.0234300	-1.4136947
H	2.0858809	0.2835475	-0.9439575

Pdb file
HEADER B2Pdb
COMPND B2Pdb

ATOM	1	C	111	1	0.414	-1.055	-0.889	1.00	0.00
ATOM	2	N	111	1	-0.206	-2.222	-0.479	1.00	0.00
ATOM	3	H	111	1	-0.232	0.719	-2.130	1.00	0.00
ATOM	4	C	111	1	-1.487	-2.160	-0.994	1.00	0.00
ATOM	5	C	111	1	-1.684	-0.924	-1.722	1.00	0.00
ATOM	6	H	111	1	-2.619	-0.638	-2.221	1.00	0.00
ATOM	7	C	111	1	-0.490	-0.250	-1.682	1.00	0.00
ATOM	8	C	111	1	-2.418	-3.197	-0.957	1.00	0.00
ATOM	9	N	111	1	-0.941	-4.861	0.106	1.00	0.00
ATOM	10	C	111	1	-1.043	-6.229	0.296	1.00	0.00
ATOM	11	C	111	1	-2.300	-6.722	-0.224	1.00	0.00
ATOM	12	H	111	1	-2.614	-7.774	-0.204	1.00	0.00
ATOM	13	C	111	1	-2.984	-5.630	-0.697	1.00	0.00
ATOM	14	H	111	1	-3.978	-5.592	-1.163	1.00	0.00
ATOM	15	C	111	1	-2.125	-4.483	-0.500	1.00	0.00
ATOM	16	C	111	1	1.707	-0.670	-0.546	1.00	0.00
ATOM	17	H	111	1	5.093	-1.745	2.435	1.00	0.00
ATOM	18	C	111	1	4.185	-1.771	1.818	1.00	0.00
ATOM	19	C	111	1	3.199	-2.831	1.847	1.00	0.00
ATOM	20	H	111	1	4.249	0.058	0.541	1.00	0.00
ATOM	21	N	111	1	2.181	-2.573	0.949	1.00	0.00
ATOM	22	C	111	1	2.508	-1.368	0.356	1.00	0.00
ATOM	23	C	111	1	3.767	-0.873	0.866	1.00	0.00
ATOM	24	C	111	1	-0.110	-7.019	0.967	1.00	0.00
ATOM	25	H	111	1	-0.314	-8.098	1.052	1.00	0.00
ATOM	26	H	111	1	3.670	-6.650	3.639	1.00	0.00
ATOM	27	C	111	1	2.830	-6.433	2.964	1.00	0.00
ATOM	28	C	111	1	1.907	-7.303	2.437	1.00	0.00
ATOM	29	H	111	1	1.815	-8.386	2.594	1.00	0.00
ATOM	30	C	111	1	1.022	-6.514	1.607	1.00	0.00
ATOM	31	N	111	1	1.417	-5.186	1.600	1.00	0.00
ATOM	32	C	111	1	2.530	-5.127	2.419	1.00	0.00

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ATOM     33  C   111     1       3.336  -4.002   2.594  1.00  0.00
ATOM     34  H   111     1       4.199  -4.084   3.273  1.00  0.00
ATOM     35 Co   111     1       0.496  -3.620   0.755  1.00  0.00
ATOM     36  N   111     1      -0.464  -3.075   2.394  1.00  0.00
ATOM     37  S   111     1      -0.863  -1.456   2.730  1.00  0.00
ATOM     38  O   111     1      -2.274  -1.192   2.332  1.00  0.00
ATOM     39  O   111     1       0.217  -0.602   2.188  1.00  0.00
ATOM     40  C   111     1      -0.784  -1.310   4.540  1.00  0.00
ATOM     41  C   111     1      -0.649  -1.034   7.314  1.00  0.00
ATOM     42  C   111     1       0.475  -1.235   5.161  1.00  0.00
ATOM     43  C   111     1      -1.975  -1.238   5.281  1.00  0.00
ATOM     44  C   111     1      -1.900  -1.100   6.677  1.00  0.00
ATOM     45  C   111     1       0.536  -1.100   6.557  1.00  0.00
ATOM     46  H   111     1       1.391  -1.269   4.550  1.00  0.00
ATOM     47  H   111     1      -2.941  -1.282   4.754  1.00  0.00
ATOM     48  H   111     1      -2.828  -1.040   7.270  1.00  0.00
ATOM     49  H   111     1       1.516  -1.038   7.058  1.00  0.00
ATOM     50  H   111     1      -0.595  -0.926   8.410  1.00  0.00
ATOM     51  H   111     1      -0.621  -5.036   3.042  1.00  0.00
ATOM     52  C   111     1      -1.142  -4.067   3.229  1.00  0.00
ATOM     53  H   111     1      -0.955  -3.851   4.314  1.00  0.00
ATOM     54  C   111     1      -2.622  -4.217   2.986  1.00  0.00
ATOM     55  H   111     1      -3.075  -3.561   2.227  1.00  0.00
ATOM     56  C   111     1      -3.450  -5.142   3.680  1.00  0.00
ATOM     57  C   111     1      -5.178  -6.975   5.033  1.00  0.00
ATOM     58  C   111     1      -2.952  -6.035   4.687  1.00  0.00
ATOM     59  C   111     1      -4.853  -5.212   3.383  1.00  0.00
ATOM     60  C   111     1      -5.693  -6.107   4.046  1.00  0.00
ATOM     61  C   111     1      -3.803  -6.928   5.344  1.00  0.00
ATOM     62  H   111     1      -1.882  -6.020   4.948  1.00  0.00
ATOM     63  H   111     1      -5.261  -4.536   2.612  1.00  0.00
ATOM     64  H   111     1      -6.767  -6.136   3.796  1.00  0.00
ATOM     65  H   111     1      -3.392  -7.603   6.114  1.00  0.00
ATOM     66  H   111     1      -5.843  -7.682   5.556  1.00  0.00
ATOM     67  H   111     1      -3.404  -3.023  -1.414  1.00  0.00
ATOM     68  H   111     1       2.086   0.284  -0.944  1.00  0.00
CONECT    1    2    7   16
CONECT    2    4   35
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8   15   67
CONECT    9   10   15   35
CONECT   10   11   24
CONECT   11   12   13
CONECT   13   14   15
CONECT   16   22   68
CONECT   17   18
CONECT   18   19   23
CONECT   19   21   33
CONECT   20   23
CONECT   21   22   35
CONECT   22   23
CONECT   24   25   30
CONECT   26   27
CONECT   27   28   32
CONECT   28   29   30
CONECT   30   31
CONECT   31   32   35
CONECT   32   33
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CONECT   33   34
CONECT   35   36
CONECT   36   37   52
CONECT   37   38   39   40
CONECT   40   42   43
CONECT   41   44   45   50
CONECT   42   45   46
CONECT   43   44   47
CONECT   44   48
CONECT   45   49
CONECT   51   52
CONECT   52   53   54
CONECT   54   55   56
CONECT   56   58   59
CONECT   57   60   61   66
CONECT   58   61   62
CONECT   59   60   63
CONECT   60   64
CONECT   61   65
END


4C_Co(PorAmide)
Xyz file
69
 Energy =   -3646.2507762640
C     0.2500399   -0.3861130   -0.1506673
N     0.0876707   -1.7608672   -0.2119433
H    -0.9379840    1.3692005   -0.9271910
C    -1.1200353   -1.9593329   -0.8603507
C    -1.6963242   -0.6984960   -1.2623584
H    -2.6414533   -0.5916778   -1.8108915
C    -0.8481700    0.2821931   -0.8169326
C    -1.7423619   -3.1862674   -1.0690353
N    -0.0105313   -4.5951800   -0.0232662
C     0.0836158   -5.9572952    0.2016464
C    -1.0975528   -6.6372465   -0.2831638
H    -1.2562042   -7.7227907   -0.2303904
C    -1.9115207   -5.6731961   -0.8223351
H    -2.8903993   -5.7889534   -1.3061745
C    -1.2294905   -4.4098643   -0.6461321
C     1.3268339    0.2965896    0.4414743
H     5.5475645   -0.5992266    2.1668363
C     4.5299201   -0.7043022    1.7678318
C     3.8969020   -1.9657936    1.4629815
H     3.7225532    1.3621256    1.5742284
N     2.6212279   -1.7638550    0.9622636
C     2.4402218   -0.3897010    0.9552425
C     3.6183132    0.2758003    1.4729444
C     1.1903824   -6.6130568    0.7346543
H     1.1425022   -7.7071714    0.8414433
H     5.5577081   -5.8239565    2.0892903
C     4.5211895   -5.7009563    1.7476198
C     3.5678977   -6.6631186    1.5229288
H     3.6499882   -7.7526418    1.6330259
C     2.3774524   -5.9711408    1.0820487
N     2.5962804   -4.6068002    1.0315930
C     3.8969259   -4.4287881    1.4620969
C     4.5155953   -3.1970282    1.6626779
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H	5.5500920	-3.1948893	2.0372699
Co	1.2119311	-3.1659235	0.7010226
N	0.4653853	-3.0133490	2.3521707
S	-0.4625644	-2.0397688	3.2669204
O	-1.8563815	-2.0087489	2.7363133
O	0.2477019	-0.7265376	3.4472359
C	-0.4973980	-2.8342753	4.8834483
C	-0.5297033	-4.1187195	7.3592554
C	0.5567183	-2.6068347	5.7869607
C	-1.5686281	-3.6888087	5.1973638
C	-1.5786377	-4.3313092	6.4459793
C	0.5338492	-3.2573062	7.0305484
H	1.3716819	-1.9188638	5.5140047
H	-2.3833761	-3.8289459	4.4702948
H	-2.4151109	-4.9992218	6.7100048
H	1.3501424	-3.0861657	7.7514973
H	-0.5431400	-4.6252558	8.3384756
H	-2.7186775	-3.1850405	-1.5761536
C	1.3220110	1.7950525	0.4298987
C	1.3047518	4.6076702	0.2289086
C	0.4427713	2.5584944	1.2600123
C	2.1838866	2.4664144	-0.4645428
C	2.1862121	3.8641056	-0.5738357
C	0.4441672	3.9715808	1.1331034
H	2.8498335	1.8610758	-1.1014834
H	2.8613255	4.3645442	-1.2867596
H	-0.2520838	4.5474036	1.7544575
H	1.2837656	5.7081075	0.1562180
N	-0.3859107	1.8923115	2.1805371
H	-0.1463541	0.9088830	2.3997056
C	-1.4765380	2.4174654	2.8751102
O	-1.8736823	3.5742386	2.7533785
C	-2.1421942	1.4238393	3.8208223
H	-2.3848566	0.4622008	3.3191757
H	-3.0652135	1.8919835	4.2149875
H	-1.4625291	1.1802965	4.6670165

Pdb file

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HEADER B2Pdb
COMPND B2Pdb
ATOM      1  C   111     1       0.250  -0.386  -0.151  1.00  0.00
ATOM      2  N   111     1       0.088  -1.761  -0.212  1.00  0.00
ATOM      3  H   111     1      -0.938   1.369  -0.927  1.00  0.00
ATOM      4  C   111     1      -1.120  -1.959  -0.860  1.00  0.00
ATOM      5  C   111     1      -1.696  -0.698  -1.262  1.00  0.00
ATOM      6  H   111     1      -2.641  -0.592  -1.811  1.00  0.00
ATOM      7  C   111     1      -0.848   0.282  -0.817  1.00  0.00
ATOM      8  C   111     1      -1.742  -3.186  -1.069  1.00  0.00
ATOM      9  N   111     1      -0.011  -4.595  -0.023  1.00  0.00
ATOM     10  C   111     1       0.084  -5.957   0.202  1.00  0.00
ATOM     11  C   111     1      -1.098  -6.637  -0.283  1.00  0.00
ATOM     12  H   111     1      -1.256  -7.723  -0.230  1.00  0.00
ATOM     13  C   111     1      -1.912  -5.673  -0.822  1.00  0.00
ATOM     14  H   111     1      -2.890  -5.789  -1.306  1.00  0.00
ATOM     15  C   111     1      -1.229  -4.410  -0.646  1.00  0.00
ATOM     16  C   111     1       1.327   0.297   0.441  1.00  0.00
ATOM     17  H   111     1       5.548  -0.599   2.167  1.00  0.00
ATOM     18  C   111     1       4.530  -0.704   1.768  1.00  0.00
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ATOM     19  C   111     1       3.897  -1.966   1.463  1.00  0.00
ATOM     20  H   111     1       3.723   1.362   1.574  1.00  0.00
ATOM     21  N   111     1       2.621  -1.764   0.962  1.00  0.00
ATOM     22  C   111     1       2.440  -0.390   0.955  1.00  0.00
ATOM     23  C   111     1       3.618   0.276   1.473  1.00  0.00
ATOM     24  C   111     1       1.190  -6.613   0.735  1.00  0.00
ATOM     25  H   111     1       1.143  -7.707   0.841  1.00  0.00
ATOM     26  H   111     1       5.558  -5.824   2.089  1.00  0.00
ATOM     27  C   111     1       4.521  -5.701   1.748  1.00  0.00
ATOM     28  C   111     1       3.568  -6.663   1.523  1.00  0.00
ATOM     29  H   111     1       3.650  -7.753   1.633  1.00  0.00
ATOM     30  C   111     1       2.377  -5.971   1.082  1.00  0.00
ATOM     31  N   111     1       2.596  -4.607   1.032  1.00  0.00
ATOM     32  C   111     1       3.897  -4.429   1.462  1.00  0.00
ATOM     33  C   111     1       4.516  -3.197   1.663  1.00  0.00
ATOM     34  H   111     1       5.550  -3.195   2.037  1.00  0.00
ATOM     35 Co   111     1       1.212  -3.166   0.701  1.00  0.00
ATOM     36  N   111     1       0.465  -3.013   2.352  1.00  0.00
ATOM     37  S   111     1      -0.463  -2.040   3.267  1.00  0.00
ATOM     38  O   111     1      -1.856  -2.009   2.736  1.00  0.00
ATOM     39  O   111     1       0.248  -0.727   3.447  1.00  0.00
ATOM     40  C   111     1      -0.497  -2.834   4.883  1.00  0.00
ATOM     41  C   111     1      -0.530  -4.119   7.359  1.00  0.00
ATOM     42  C   111     1       0.557  -2.607   5.787  1.00  0.00
ATOM     43  C   111     1      -1.569  -3.689   5.197  1.00  0.00
ATOM     44  C   111     1      -1.579  -4.331   6.446  1.00  0.00
ATOM     45  C   111     1       0.534  -3.257   7.031  1.00  0.00
ATOM     46  H   111     1       1.372  -1.919   5.514  1.00  0.00
ATOM     47  H   111     1      -2.383  -3.829   4.470  1.00  0.00
ATOM     48  H   111     1      -2.415  -4.999   6.710  1.00  0.00
ATOM     49  H   111     1       1.350  -3.086   7.751  1.00  0.00
ATOM     50  H   111     1      -0.543  -4.625   8.338  1.00  0.00
ATOM     51  H   111     1      -2.719  -3.185  -1.576  1.00  0.00
ATOM     52  C   111     1       1.322   1.795   0.430  1.00  0.00
ATOM     53  C   111     1       1.305   4.608   0.229  1.00  0.00
ATOM     54  C   111     1       0.443   2.558   1.260  1.00  0.00
ATOM     55  C   111     1       2.184   2.466  -0.465  1.00  0.00
ATOM     56  C   111     1       2.186   3.864  -0.574  1.00  0.00
ATOM     57  C   111     1       0.444   3.972   1.133  1.00  0.00
ATOM     58  H   111     1       2.850   1.861  -1.101  1.00  0.00
ATOM     59  H   111     1       2.861   4.365  -1.287  1.00  0.00
ATOM     60  H   111     1      -0.252   4.547   1.754  1.00  0.00
ATOM     61  H   111     1       1.284   5.708   0.156  1.00  0.00
ATOM     62  N   111     1      -0.386   1.892   2.181  1.00  0.00
ATOM     63  H   111     1      -0.146   0.909   2.400  1.00  0.00
ATOM     64  C   111     1      -1.477   2.417   2.875  1.00  0.00
ATOM     65  O   111     1      -1.874   3.574   2.753  1.00  0.00
ATOM     66  C   111     1      -2.142   1.424   3.821  1.00  0.00
ATOM     67  H   111     1      -2.385   0.462   3.319  1.00  0.00
ATOM     68  H   111     1      -3.065   1.892   4.215  1.00  0.00
ATOM     69  H   111     1      -1.463   1.180   4.667  1.00  0.00
CONECT    1    2    7   16
CONECT    2    4   35
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8   15   51
CONECT    9   10   15   35
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CONECT   13   14   15
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CONECT   17   18
CONECT   18   19   23
CONECT   19   21   33
CONECT   20   23
CONECT   21   22   35
CONECT   22   23
CONECT   24   25   30
CONECT   26   27
CONECT   27   28   32
CONECT   28   29   30
CONECT   30   31
CONECT   31   32   35
CONECT   32   33
CONECT   33   34
CONECT   35   36
CONECT   36   37
CONECT   37   38   39   40
CONECT   40   42   43
CONECT   41   44   45   50
CONECT   42   45   46
CONECT   43   44   47
CONECT   44   48
CONECT   45   49
CONECT   52   54   55
CONECT   53   56   57   61
CONECT   54   57   62
CONECT   55   56   58
CONECT   56   59
CONECT   57   60
CONECT   62   63   64
CONECT   64   65   66
CONECT   66   67   68   69
END

4TS2_Co(PorAmide)
Xyz file
85
 Energy =   -3955.9904745100
C    -0.4100593   -0.3064681    0.6642833
N    -0.2795758   -1.6810660    0.7681249
H    -1.9598861    1.0554081   -0.2550933
C    -1.4311702   -2.2052305    0.2055491
C    -2.2899520   -1.1474119   -0.2741346
H    -3.2563328   -1.3053618   -0.7709976
C    -1.6414645    0.0332900   -0.0187309
C    -1.7005799   -3.5578532    0.0141649
H    -2.6647036   -3.8293581   -0.4413666
N     0.4742626   -4.3983358    0.8068688
C     1.1007306   -5.6286442    0.7072144
C     0.2335305   -6.5911139    0.0627933
H     0.5069889   -7.6337835   -0.1472014
C    -0.9453983   -5.9395964   -0.2062904
H    -1.8472010   -6.3263688   -0.6996616
C    -0.7742630   -4.5746163    0.2423894
C     0.4699097    0.6479660    1.2013503
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H	4.1691943	0.8547578	4.0063154
C	3.3567677	0.4956955	3.3604438
C	3.0952943	-0.8957736	3.0659773
H	2.3123510	2.3142688	2.6086066
N	2.0157555	-1.0184343	2.2091733
C	1.5907577	0.2747831	1.9611575
C	2.4343084	1.2259733	2.6577462
C	2.3680666	-5.9316782	1.2046440
H	2.7518710	-6.9524190	1.0570927
H	5.6777868	-4.1529795	3.9299644
C	4.7842540	-4.2832185	3.3046353
C	4.3887009	-5.3886012	2.5910612
H	4.8797173	-6.3679018	2.5120316
C	3.1453507	-5.0379624	1.9409728
N	2.8031306	-3.7254778	2.2199278
C	3.8003654	-3.2542510	3.0520909
C	3.9065086	-1.9399530	3.5079313
H	4.7436660	-1.6914849	4.1776654
Co	1.1132694	-2.7328446	1.7443012
N	0.1750076	-2.9551011	3.3666867
S	-0.9410476	-1.9943542	4.0932508
O	-2.3305054	-2.4032958	3.7402656
O	-0.5676546	-0.5557388	3.8620282
C	-0.7222364	-2.2255691	5.8772235
C	-0.4295518	-2.4280564	8.6469154
C	0.5393829	-1.9890058	6.4536913
C	-1.8381553	-2.5548020	6.6612085
C	-1.6852845	-2.6494153	8.0562302
C	0.6814967	-2.1009361	7.8451553
H	1.3959929	-1.7199012	5.8155225
H	-2.8086089	-2.7298229	6.1723418
H	-2.5566723	-2.8992220	8.6839468
H	1.6652879	-1.9231696	8.3104040
H	-0.3132904	-2.5069769	9.7405921
C	-1.1579565	-5.6287019	3.7640437
C	0.0355565	-5.0593918	4.1713652
H	0.9270793	-5.1583964	3.5388508
H	0.2172239	-4.7912759	5.2262495
H	-1.2435892	-5.9072289	2.6983718
C	-2.3405115	-5.8933147	4.5699525
C	-4.6860892	-6.5095553	6.0595489
C	-3.5482566	-6.2767998	3.9223643
C	-2.3425488	-5.8417174	5.9921845
C	-3.4972736	-6.1456219	6.7222526
C	-4.7041805	-6.5741535	4.6535722
H	-3.5662606	-6.3265281	2.8207723
H	-1.4177894	-5.5801890	6.5299451
H	-3.4708755	-6.1072896	7.8240853
H	-5.6293825	-6.8595075	4.1258255
H	-5.5931844	-6.7493069	6.6385823
C	0.1561155	2.1027164	1.0277626
C	-0.4150466	4.8281313	0.6023010
C	0.9073108	2.8651889	0.1098288
C	-0.8963033	2.7286178	1.7671899
C	-1.1725604	4.0991584	1.5295064
C	0.6330086	4.2232204	-0.1114927
H	1.7152080	2.3640751	-0.4488129
H	-1.9949848	4.5648633	2.0857333
H	1.2275800	4.7986119	-0.8394782
H	-0.6516747	5.8933611	0.4408395

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N    -1.6143187    1.9662621    2.7064043
H    -1.2280155    1.0340007    2.9434151
C    -2.7851496    2.3185779    3.3751800
O    -3.3674359    3.3909099    3.2252630
C    -3.2848253    1.2518191    4.3447800
H    -2.6691269    1.2669490    5.2720943
H    -3.2219704    0.2243133    3.9281646
H    -4.3325831    1.4941719    4.6113211
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Pdb file
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COMPND B2Pdb
ATOM      1  C   111     1      -0.410  -0.306   0.664  1.00  0.00
ATOM      2  N   111     1      -0.280  -1.681   0.768  1.00  0.00
ATOM      3  H   111     1      -1.960   1.055  -0.255  1.00  0.00
ATOM      4  C   111     1      -1.431  -2.205   0.206  1.00  0.00
ATOM      5  C   111     1      -2.290  -1.147  -0.274  1.00  0.00
ATOM      6  H   111     1      -3.256  -1.305  -0.771  1.00  0.00
ATOM      7  C   111     1      -1.641   0.033  -0.019  1.00  0.00
ATOM      8  C   111     1      -1.701  -3.558   0.014  1.00  0.00
ATOM      9  H   111     1      -2.665  -3.829  -0.441  1.00  0.00
ATOM     10  N   111     1       0.474  -4.398   0.807  1.00  0.00
ATOM     11  C   111     1       1.101  -5.629   0.707  1.00  0.00
ATOM     12  C   111     1       0.234  -6.591   0.063  1.00  0.00
ATOM     13  H   111     1       0.507  -7.634  -0.147  1.00  0.00
ATOM     14  C   111     1      -0.945  -5.940  -0.206  1.00  0.00
ATOM     15  H   111     1      -1.847  -6.326  -0.700  1.00  0.00
ATOM     16  C   111     1      -0.774  -4.575   0.242  1.00  0.00
ATOM     17  C   111     1       0.470   0.648   1.201  1.00  0.00
ATOM     18  H   111     1       4.169   0.855   4.006  1.00  0.00
ATOM     19  C   111     1       3.357   0.496   3.360  1.00  0.00
ATOM     20  C   111     1       3.095  -0.896   3.066  1.00  0.00
ATOM     21  H   111     1       2.312   2.314   2.609  1.00  0.00
ATOM     22  N   111     1       2.016  -1.018   2.209  1.00  0.00
ATOM     23  C   111     1       1.591   0.275   1.961  1.00  0.00
ATOM     24  C   111     1       2.434   1.226   2.658  1.00  0.00
ATOM     25  C   111     1       2.368  -5.932   1.205  1.00  0.00
ATOM     26  H   111     1       2.752  -6.952   1.057  1.00  0.00
ATOM     27  H   111     1       5.678  -4.153   3.930  1.00  0.00
ATOM     28  C   111     1       4.784  -4.283   3.305  1.00  0.00
ATOM     29  C   111     1       4.389  -5.389   2.591  1.00  0.00
ATOM     30  H   111     1       4.880  -6.368   2.512  1.00  0.00
ATOM     31  C   111     1       3.145  -5.038   1.941  1.00  0.00
ATOM     32  N   111     1       2.803  -3.725   2.220  1.00  0.00
ATOM     33  C   111     1       3.800  -3.254   3.052  1.00  0.00
ATOM     34  C   111     1       3.907  -1.940   3.508  1.00  0.00
ATOM     35  H   111     1       4.744  -1.691   4.178  1.00  0.00
ATOM     36 Co   111     1       1.113  -2.733   1.744  1.00  0.00
ATOM     37  N   111     1       0.175  -2.955   3.367  1.00  0.00
ATOM     38  S   111     1      -0.941  -1.994   4.093  1.00  0.00
ATOM     39  O   111     1      -2.331  -2.403   3.740  1.00  0.00
ATOM     40  O   111     1      -0.568  -0.556   3.862  1.00  0.00
ATOM     41  C   111     1      -0.722  -2.226   5.877  1.00  0.00
ATOM     42  C   111     1      -0.430  -2.428   8.647  1.00  0.00
ATOM     43  C   111     1       0.539  -1.989   6.454  1.00  0.00
ATOM     44  C   111     1      -1.838  -2.555   6.661  1.00  0.00
ATOM     45  C   111     1      -1.685  -2.649   8.056  1.00  0.00
ATOM     46  C   111     1       0.681  -2.101   7.845  1.00  0.00
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ATOM     47  H   111     1       1.396  -1.720   5.816  1.00  0.00
ATOM     48  H   111     1      -2.809  -2.730   6.172  1.00  0.00
ATOM     49  H   111     1      -2.557  -2.899   8.684  1.00  0.00
ATOM     50  H   111     1       1.665  -1.923   8.310  1.00  0.00
ATOM     51  H   111     1      -0.313  -2.507   9.741  1.00  0.00
ATOM     52  C   111     1      -1.158  -5.629   3.764  1.00  0.00
ATOM     53  C   111     1       0.036  -5.059   4.171  1.00  0.00
ATOM     54  H   111     1       0.927  -5.158   3.539  1.00  0.00
ATOM     55  H   111     1       0.217  -4.791   5.226  1.00  0.00
ATOM     56  H   111     1      -1.244  -5.907   2.698  1.00  0.00
ATOM     57  C   111     1      -2.341  -5.893   4.570  1.00  0.00
ATOM     58  C   111     1      -4.686  -6.510   6.060  1.00  0.00
ATOM     59  C   111     1      -3.548  -6.277   3.922  1.00  0.00
ATOM     60  C   111     1      -2.343  -5.842   5.992  1.00  0.00
ATOM     61  C   111     1      -3.497  -6.146   6.722  1.00  0.00
ATOM     62  C   111     1      -4.704  -6.574   4.654  1.00  0.00
ATOM     63  H   111     1      -3.566  -6.327   2.821  1.00  0.00
ATOM     64  H   111     1      -1.418  -5.580   6.530  1.00  0.00
ATOM     65  H   111     1      -3.471  -6.107   7.824  1.00  0.00
ATOM     66  H   111     1      -5.629  -6.860   4.126  1.00  0.00
ATOM     67  H   111     1      -5.593  -6.749   6.639  1.00  0.00
ATOM     68  C   111     1       0.156   2.103   1.028  1.00  0.00
ATOM     69  C   111     1      -0.415   4.828   0.602  1.00  0.00
ATOM     70  C   111     1       0.907   2.865   0.110  1.00  0.00
ATOM     71  C   111     1      -0.896   2.729   1.767  1.00  0.00
ATOM     72  C   111     1      -1.173   4.099   1.530  1.00  0.00
ATOM     73  C   111     1       0.633   4.223  -0.111  1.00  0.00
ATOM     74  H   111     1       1.715   2.364  -0.449  1.00  0.00
ATOM     75  H   111     1      -1.995   4.565   2.086  1.00  0.00
ATOM     76  H   111     1       1.228   4.799  -0.839  1.00  0.00
ATOM     77  H   111     1      -0.652   5.893   0.441  1.00  0.00
ATOM     78  N   111     1      -1.614   1.966   2.706  1.00  0.00
ATOM     79  H   111     1      -1.228   1.034   2.943  1.00  0.00
ATOM     80  C   111     1      -2.785   2.319   3.375  1.00  0.00
ATOM     81  O   111     1      -3.367   3.391   3.225  1.00  0.00
ATOM     82  C   111     1      -3.285   1.252   4.345  1.00  0.00
ATOM     83  H   111     1      -2.669   1.267   5.272  1.00  0.00
ATOM     84  H   111     1      -3.222   0.224   3.928  1.00  0.00
ATOM     85  H   111     1      -4.333   1.494   4.611  1.00  0.00
CONECT    1    2    7   17
CONECT    2    4   36
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   36
CONECT   11   12   25
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   23   68
CONECT   18   19
CONECT   19   20   24
CONECT   20   22   34
CONECT   21   24
CONECT   22   23   36
CONECT   23   24
CONECT   25   26   31
CONECT   27   28
CONECT   28   29   33
CONECT   29   30   31
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CONECT   32   33   36
CONECT   33   34
CONECT   34   35
CONECT   36   37
CONECT   37   38
CONECT   38   39   40   41
CONECT   41   43   44
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CONECT   45   49
CONECT   46   50
CONECT   52   53   56   57
CONECT   53   54   55
CONECT   57   59   60
CONECT   58   61   62   67
CONECT   59   62   63
CONECT   60   61   64
CONECT   61   65
CONECT   62   66
CONECT   68   70   71
CONECT   69   72   73   77
CONECT   70   73   74
CONECT   71   72   78
CONECT   72   75
CONECT   73   76
CONECT   78   79   80
CONECT   80   81   82
CONECT   82   83   84   85
END

4D_Co(PorAmide)
Xyz file
85
 Energy =   -3956.0180032490
C    -0.8774835   -1.2913240   -0.4105216
N    -0.8015633   -2.6615440   -0.2062078
H    -2.4182183    0.0633138   -1.3549990
C    -1.9467921   -3.1869160   -0.7792863
C    -2.7542661   -2.1393801   -1.3541904
H    -3.7091555   -2.3005804   -1.8717855
C    -2.1092024   -0.9550543   -1.0932071
C    -2.3235727   -4.5294772   -0.7680210
N    -0.5418041   -5.3226892    0.7372861
C    -0.3027045   -6.5440606    1.3428784
C    -1.2779933   -7.5270084    0.9207059
H    -1.2925806   -8.5735307    1.2534228
C    -2.1141382   -6.8943513    0.0355526
H    -2.9752233   -7.3021778   -0.5100388
C    -1.6606040   -5.5231281   -0.0531962
C     0.1436307   -0.3631743   -0.1267171
H     4.6125460   -0.3868365    1.1413410
C     3.5700875   -0.6754472    0.9528072
C     3.0165678   -1.9822207    1.2311830
H     2.5727733    1.1184031    0.0890492
N     1.6898993   -2.0479857    0.8453850
C     1.3861308   -0.7825882    0.3785387
C     2.5518377    0.0776551    0.4333724
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C	0.7594660	-6.8160520	2.2035806
H	0.8183220	-7.8174147	2.6558686
H	4.9311415	-5.1416442	3.3330544
C	3.8987936	-5.2392008	2.9708966
C	3.0300231	-6.2937335	3.1206711
H	3.1955222	-7.2545894	3.6261134
C	1.8173685	-5.9336664	2.4226141
N	1.9216908	-4.6604298	1.8865443
C	3.1957949	-4.2300772	2.2134980
C	3.7323676	-2.9908773	1.8692122
H	4.7751661	-2.7817422	2.1522245
Co	0.4342110	-3.5857857	1.0658503
N	-0.6093978	-3.1100996	2.7086487
S	-0.3721456	-1.7852356	3.7335804
O	-1.6738174	-1.1092858	4.0019154
O	0.7561321	-0.9643923	3.2171963
C	0.1779211	-2.5114960	5.2994226
C	1.0283575	-3.6101055	7.7202784
C	1.4762436	-3.0446881	5.3919625
C	-0.6987113	-2.5124619	6.3975300
C	-0.2640084	-3.0677623	7.6137019
C	1.8961508	-3.5965783	6.6116889
H	2.1476996	-3.0185687	4.5198129
H	-1.6989550	-2.0643343	6.2929171
H	-0.9400746	-3.0711059	8.4844775
H	2.9114580	-4.0169889	6.6979021
H	1.3653178	-4.0439239	8.6762293
H	-1.7072553	-4.8844451	2.7518947
C	-1.8443463	-3.8279965	3.0698299
H	-1.9504902	-3.8809741	4.1869803
C	-3.1010730	-3.2553370	2.4693640
H	-3.0301358	-2.2610394	2.0025892
C	-4.3735137	-3.8876117	2.5334320
C	-6.9651658	-5.0918504	2.6332372
C	-4.5816946	-5.1660173	3.1515492
C	-5.5245763	-3.2418520	1.9685777
C	-6.7876224	-3.8327571	2.0189021
C	-5.8515659	-5.7482608	3.1966934
H	-3.7284414	-5.6998403	3.6001414
H	-5.3942880	-2.2553286	1.4922245
H	-7.6534247	-3.3090964	1.5793486
H	-5.9814783	-6.7313431	3.6806236
H	-7.9643978	-5.5556162	2.6745866
H	-3.2402796	-4.8084925	-1.3087978
C	-0.0419214	1.0753344	-0.4962915
C	-0.3766272	3.7512878	-1.3252466
C	-0.1206922	1.4133188	-1.8658092
C	-0.1255925	2.1145942	0.4852597
C	-0.2987342	3.4518057	0.0406827
C	-0.2848324	2.7377973	-2.2933436
H	-0.0343365	0.6013756	-2.6067784
H	-0.3715564	4.2393423	0.8001705
H	-0.3353231	2.9729673	-3.3687920
H	-0.5091353	4.8021956	-1.6326941
N	-0.0455755	1.7925429	1.8529198
H	0.1110147	0.8000275	2.0920401
C	-0.1349223	2.6616798	2.9451283
O	-0.2981028	3.8755090	2.8444673

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C    -0.0177493    1.9700210    4.2970394
H    -0.8284623    1.2210494    4.4337496
H    -0.0846612    2.7465112    5.0837847
H     0.9429136    1.4190756    4.3870863

Pdb file
HEADER B2Pdb
COMPND B2Pdb
ATOM      1  C   111     1      -0.877  -1.291  -0.411  1.00  0.00
ATOM      2  N   111     1      -0.802  -2.662  -0.206  1.00  0.00
ATOM      3  H   111     1      -2.418   0.063  -1.355  1.00  0.00
ATOM      4  C   111     1      -1.947  -3.187  -0.779  1.00  0.00
ATOM      5  C   111     1      -2.754  -2.139  -1.354  1.00  0.00
ATOM      6  H   111     1      -3.709  -2.301  -1.872  1.00  0.00
ATOM      7  C   111     1      -2.109  -0.955  -1.093  1.00  0.00
ATOM      8  C   111     1      -2.324  -4.529  -0.768  1.00  0.00
ATOM      9  N   111     1      -0.542  -5.323   0.737  1.00  0.00
ATOM     10  C   111     1      -0.303  -6.544   1.343  1.00  0.00
ATOM     11  C   111     1      -1.278  -7.527   0.921  1.00  0.00
ATOM     12  H   111     1      -1.293  -8.574   1.253  1.00  0.00
ATOM     13  C   111     1      -2.114  -6.894   0.036  1.00  0.00
ATOM     14  H   111     1      -2.975  -7.302  -0.510  1.00  0.00
ATOM     15  C   111     1      -1.661  -5.523  -0.053  1.00  0.00
ATOM     16  C   111     1       0.144  -0.363  -0.127  1.00  0.00
ATOM     17  H   111     1       4.613  -0.387   1.141  1.00  0.00
ATOM     18  C   111     1       3.570  -0.675   0.953  1.00  0.00
ATOM     19  C   111     1       3.017  -1.982   1.231  1.00  0.00
ATOM     20  H   111     1       2.573   1.118   0.089  1.00  0.00
ATOM     21  N   111     1       1.690  -2.048   0.845  1.00  0.00
ATOM     22  C   111     1       1.386  -0.783   0.379  1.00  0.00
ATOM     23  C   111     1       2.552   0.078   0.433  1.00  0.00
ATOM     24  C   111     1       0.759  -6.816   2.204  1.00  0.00
ATOM     25  H   111     1       0.818  -7.817   2.656  1.00  0.00
ATOM     26  H   111     1       4.931  -5.142   3.333  1.00  0.00
ATOM     27  C   111     1       3.899  -5.239   2.971  1.00  0.00
ATOM     28  C   111     1       3.030  -6.294   3.121  1.00  0.00
ATOM     29  H   111     1       3.196  -7.255   3.626  1.00  0.00
ATOM     30  C   111     1       1.817  -5.934   2.423  1.00  0.00
ATOM     31  N   111     1       1.922  -4.660   1.887  1.00  0.00
ATOM     32  C   111     1       3.196  -4.230   2.213  1.00  0.00
ATOM     33  C   111     1       3.732  -2.991   1.869  1.00  0.00
ATOM     34  H   111     1       4.775  -2.782   2.152  1.00  0.00
ATOM     35 Co   111     1       0.434  -3.586   1.066  1.00  0.00
ATOM     36  N   111     1      -0.609  -3.110   2.709  1.00  0.00
ATOM     37  S   111     1      -0.372  -1.785   3.734  1.00  0.00
ATOM     38  O   111     1      -1.674  -1.109   4.002  1.00  0.00
ATOM     39  O   111     1       0.756  -0.964   3.217  1.00  0.00
ATOM     40  C   111     1       0.178  -2.511   5.299  1.00  0.00
ATOM     41  C   111     1       1.028  -3.610   7.720  1.00  0.00
ATOM     42  C   111     1       1.476  -3.045   5.392  1.00  0.00
ATOM     43  C   111     1      -0.699  -2.512   6.398  1.00  0.00
ATOM     44  C   111     1      -0.264  -3.068   7.614  1.00  0.00
ATOM     45  C   111     1       1.896  -3.597   6.612  1.00  0.00
ATOM     46  H   111     1       2.148  -3.019   4.520  1.00  0.00
ATOM     47  H   111     1      -1.699  -2.064   6.293  1.00  0.00
ATOM     48  H   111     1      -0.940  -3.071   8.484  1.00  0.00
ATOM     49  H   111     1       2.911  -4.017   6.698  1.00  0.00
ATOM     50  H   111     1       1.365  -4.044   8.676  1.00  0.00
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ATOM     51  H   111     1       -1.707  -4.884   2.752  1.00  0.00
ATOM     52  C   111     1       -1.844  -3.828   3.070  1.00  0.00
ATOM     53  H   111     1       -1.950  -3.881   4.187  1.00  0.00
ATOM     54  C   111     1       -3.101  -3.255   2.469  1.00  0.00
ATOM     55  H   111     1       -3.030  -2.261   2.003  1.00  0.00
ATOM     56  C   111     1       -4.374  -3.888   2.533  1.00  0.00
ATOM     57  C   111     1       -6.965  -5.092   2.633  1.00  0.00
ATOM     58  C   111     1       -4.582  -5.166   3.152  1.00  0.00
ATOM     59  C   111     1       -5.525  -3.242   1.969  1.00  0.00
ATOM     60  C   111     1       -6.788  -3.833   2.019  1.00  0.00
ATOM     61  C   111     1       -5.852  -5.748   3.197  1.00  0.00
ATOM     62  H   111     1       -3.728  -5.700   3.600  1.00  0.00
ATOM     63  H   111     1       -5.394  -2.255   1.492  1.00  0.00
ATOM     64  H   111     1       -7.653  -3.309   1.579  1.00  0.00
ATOM     65  H   111     1       -5.981  -6.731   3.681  1.00  0.00
ATOM     66  H   111     1       -7.964  -5.556   2.675  1.00  0.00
ATOM     67  H   111     1       -3.240  -4.808  -1.309  1.00  0.00
ATOM     68  C   111     1       -0.042   1.075  -0.496  1.00  0.00
ATOM     69  C   111     1       -0.377   3.751  -1.325  1.00  0.00
ATOM     70  C   111     1       -0.121   1.413  -1.866  1.00  0.00
ATOM     71  C   111     1       -0.126   2.115   0.485  1.00  0.00
ATOM     72  C   111     1       -0.299   3.452   0.041  1.00  0.00
ATOM     73  C   111     1       -0.285   2.738  -2.293  1.00  0.00
ATOM     74  H   111     1       -0.034   0.601  -2.607  1.00  0.00
ATOM     75  H   111     1       -0.372   4.239   0.800  1.00  0.00
ATOM     76  H   111     1       -0.335   2.973  -3.369  1.00  0.00
ATOM     77  H   111     1       -0.509   4.802  -1.633  1.00  0.00
ATOM     78  N   111     1       -0.046   1.793   1.853  1.00  0.00
ATOM     79  H   111     1        0.111   0.800   2.092  1.00  0.00
ATOM     80  C   111     1       -0.135   2.662   2.945  1.00  0.00
ATOM     81  O   111     1       -0.298   3.876   2.844  1.00  0.00
ATOM     82  C   111     1       -0.018   1.970   4.297  1.00  0.00
ATOM     83  H   111     1       -0.828   1.221   4.434  1.00  0.00
ATOM     84  H   111     1       -0.085   2.747   5.084  1.00  0.00
ATOM     85  H   111     1        0.943   1.419   4.387  1.00  0.00
CONECT    1    2    7   16
CONECT    2    4   35
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8   15   67
CONECT    9   10   15   35
CONECT   10   11   24
CONECT   11   12   13
CONECT   13   14   15
CONECT   16   22   68
CONECT   17   18
CONECT   18   19   23
CONECT   19   21   33
CONECT   20   23
CONECT   21   22   35
CONECT   22   23
CONECT   24   25   30
CONECT   26   27
CONECT   27   28   32
CONECT   28   29   30
CONECT   30   31
CONECT   31   32   35
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CONECT   32   33
CONECT   33   34
CONECT   35   36
CONECT   36   37   52
CONECT   37   38   39   40
CONECT   40   42   43
CONECT   41   44   45   50
CONECT   42   45   46
CONECT   43   44   47
CONECT   44   48
CONECT   45   49
CONECT   51   52
CONECT   52   53   54
CONECT   54   55   56
CONECT   56   58   59
CONECT   57   60   61   66
CONECT   58   61   62
CONECT   59   60   63
CONECT   60   64
CONECT   61   65
CONECT   68   70   71
CONECT   69   72   73   77
CONECT   70   73   74
CONECT   71   72   78
CONECT   72   75
CONECT   73   76
CONECT   78   79   80
CONECT   80   81   82
CONECT   82   83   84   85
END

(bis) (bridge) nitrene
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Xyz file
52
 Energy =   -3207.0028852960
C     0.1246631   -0.3438446   -0.1300505
N    -0.3446818   -1.6644491   -0.1428432
H    -0.5989583    1.5507374   -1.1341574
C    -1.4388075   -1.6745467   -0.9916904
C    -1.7126444   -0.3403644   -1.4873544
H    -2.5344546   -0.0792509   -2.1675587
C    -0.7421680    0.4741987   -0.9690236
C    -2.1423410   -2.8203568   -1.3901878
H    -3.0072402   -2.6711767   -2.0554286
N    -0.7439192   -4.4731558   -0.2396105
C    -0.7721721   -5.8431593   -0.0868362
C    -1.8847514   -6.3975525   -0.8371340
H    -2.1363316   -7.4653165   -0.8929330
C    -2.5355066   -5.3374710   -1.4249228
H    -3.4304145   -5.3576539   -2.0615387
C    -1.8179831   -4.1369576   -1.0356273
C     1.2888519    0.2441027    0.4188109
H     1.4577937    1.2854117    0.0992871
H     5.4448834   -1.1667988    2.0954060
C     4.3649662   -1.0590392    1.9304248
C     3.3841809   -2.0722917    2.2157789
H     4.1862782    0.9081656    0.8908460
N     2.1658967   -1.5296639    1.8439683
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C     2.3220997   -0.3214655    1.1844788
C     3.7178023    0.0070785    1.3075466
C     0.1434919   -6.5617848    0.6950524
H     0.0454564   -7.6586315    0.7138377
H     4.0099647   -6.0676694    3.2213673
C     3.0925216   -5.8658552    2.6517404
C     2.1964342   -6.7695306    2.1446907
H     2.2186885   -7.8657363    2.2105661
C     1.1896758   -6.0004721    1.4420707
N     1.4418373   -4.6432466    1.5612408
C     2.6405510   -4.5293534    2.2834042
C     3.4939965   -3.4317770    2.5629824
H     4.4600356   -3.7240194    3.0068842
Co    0.2989397   -3.2510001    0.7909451
N     0.9928288   -2.1419961    2.1106819
S    -0.0714298   -1.5547787    3.2662206
O    -1.3010920   -2.3187924    2.9184475
O    -0.0517265   -0.0753993    3.3673873
C     0.5290075   -2.1813311    4.8542435
C     1.4833731   -3.1650061    7.2874756
C     0.2899962   -3.5252724    5.1927660
C     1.2264554   -1.3194077    5.7168504
C     1.7066679   -1.8214924    6.9387000
C     0.7726876   -4.0129462    6.4168071
H    -0.2772512   -4.1697313    4.5039250
H     1.3706380   -0.2664855    5.4302766
H     2.2527370   -1.1543500    7.6262080
H     0.5878489   -5.0634583    6.6958719
H     1.8586241   -3.5536554    8.2487064



Pdb file
HEADER B2Pdb
COMPND B2Pdb
ATOM      1  C   111     1       0.125  -0.344  -0.130  1.00  0.00
ATOM      2  N   111     1      -0.345  -1.664  -0.143  1.00  0.00
ATOM      3  H   111     1      -0.599   1.551  -1.134  1.00  0.00
ATOM      4  C   111     1      -1.439  -1.675  -0.992  1.00  0.00
ATOM      5  C   111     1      -1.713  -0.340  -1.487  1.00  0.00
ATOM      6  H   111     1      -2.534  -0.079  -2.168  1.00  0.00
ATOM      7  C   111     1      -0.742   0.474  -0.969  1.00  0.00
ATOM      8  C   111     1      -2.142  -2.820  -1.390  1.00  0.00
ATOM      9  H   111     1      -3.007  -2.671  -2.055  1.00  0.00
ATOM     10  N   111     1      -0.744  -4.473  -0.240  1.00  0.00
ATOM     11  C   111     1      -0.772  -5.843  -0.087  1.00  0.00
ATOM     12  C   111     1      -1.885  -6.398  -0.837  1.00  0.00
ATOM     13  H   111     1      -2.136  -7.465  -0.893  1.00  0.00
ATOM     14  C   111     1      -2.536  -5.337  -1.425  1.00  0.00
ATOM     15  H   111     1      -3.430  -5.358  -2.062  1.00  0.00
ATOM     16  C   111     1      -1.818  -4.137  -1.036  1.00  0.00
ATOM     17  C   111     1       1.289   0.244   0.419  1.00  0.00
ATOM     18  H   111     1       1.458   1.285   0.099  1.00  0.00
ATOM     19  H   111     1       5.445  -1.167   2.095  1.00  0.00
ATOM     20  C   111     1       4.365  -1.059   1.930  1.00  0.00
ATOM     21  C   111     1       3.384  -2.072   2.216  1.00  0.00
ATOM     22  H   111     1       4.186   0.908   0.891  1.00  0.00
ATOM     23  N   111     1       2.166  -1.530   1.844  1.00  0.00
ATOM     24  C   111     1       2.322  -0.321   1.184  1.00  0.00
ATOM     25  C   111     1       3.718   0.007   1.308  1.00  0.00
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ATOM     26  C   111     1        0.143  -6.562   0.695  1.00  0.00
ATOM     27  H   111     1        0.045  -7.659   0.714  1.00  0.00
ATOM     28  H   111     1        4.010  -6.068   3.221  1.00  0.00
ATOM     29  C   111     1        3.093  -5.866   2.652  1.00  0.00
ATOM     30  C   111     1        2.196  -6.770   2.145  1.00  0.00
ATOM     31  H   111     1        2.219  -7.866   2.211  1.00  0.00
ATOM     32  C   111     1        1.190  -6.000   1.442  1.00  0.00
ATOM     33  N   111     1        1.442  -4.643   1.561  1.00  0.00
ATOM     34  C   111     1        2.641  -4.529   2.283  1.00  0.00
ATOM     35  C   111     1        3.494  -3.432   2.563  1.00  0.00
ATOM     36  H   111     1        4.460  -3.724   3.007  1.00  0.00
ATOM     37 Co   111     1        0.299  -3.251   0.791  1.00  0.00
ATOM     38  N   111     1        0.993  -2.142   2.111  1.00  0.00
ATOM     39  S   111     1       -0.071  -1.555   3.266  1.00  0.00
ATOM     40  O   111     1       -1.301  -2.319   2.918  1.00  0.00
ATOM     41  O   111     1       -0.052  -0.075   3.367  1.00  0.00
ATOM     42  C   111     1        0.529  -2.181   4.854  1.00  0.00
ATOM     43  C   111     1        1.483  -3.165   7.287  1.00  0.00
ATOM     44  C   111     1        0.290  -3.525   5.193  1.00  0.00
ATOM     45  C   111     1        1.226  -1.319   5.717  1.00  0.00
ATOM     46  C   111     1        1.707  -1.821   6.939  1.00  0.00
ATOM     47  C   111     1        0.773  -4.013   6.417  1.00  0.00
ATOM     48  H   111     1       -0.277  -4.170   4.504  1.00  0.00
ATOM     49  H   111     1        1.371  -0.266   5.430  1.00  0.00
ATOM     50  H   111     1        2.253  -1.154   7.626  1.00  0.00
ATOM     51  H   111     1        0.588  -5.063   6.696  1.00  0.00
ATOM     52  H   111     1        1.859  -3.554   8.249  1.00  0.00
CONECT    1    2    7   17
CONECT    2    4   37
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   37
CONECT   11   12   26
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   18   24
CONECT   19   20
CONECT   20   21   25
CONECT   21   23   35
CONECT   22   25
CONECT   23   24   38
CONECT   24   25
CONECT   26   27   32
CONECT   28   29
CONECT   29   30   34
CONECT   30   31   32
CONECT   32   33
CONECT   33   34   37
CONECT   34   35
CONECT   35   36
CONECT   37   38
CONECT   38   39
CONECT   39   40   41   42
CONECT   42   44   45
CONECT   43   46   47   52
CONECT   44   47   48
CONECT   45   46   49
CONECT   46   50
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CONECT   47   51
END

II
Xyz file
69
 Energy =   -4151.6970253710
C    -0.1190190    0.4627086   -0.4797732
N    -0.0805768   -0.9137380   -0.5026496
H    -1.2331905    2.0042363   -1.7156415
C    -0.9069459   -1.3213572   -1.5254076
C    -1.5013253   -0.1623886   -2.1682427
H    -2.2062735   -0.2016292   -3.0098066
C    -1.0141502    0.9465194   -1.5163149
C    -1.1224912   -2.6632547   -1.8644276
H    -1.7894743   -2.8708031   -2.7157150
N     0.2290521   -3.7238538   -0.0760919
C     0.4447730   -5.0464323    0.3146644
C    -0.2423864   -5.9333395   -0.6130234
H    -0.2445979   -7.0288445   -0.5299137
C    -0.8941505   -5.1489790   -1.5305117
H    -1.5396833   -5.4608908   -2.3625814
C    -0.5992899   -3.7730502   -1.1844558
C     0.6249920    1.2462289    0.4145463
H     0.5397066    2.3404332    0.3256380
H     3.5039387    0.9918204    4.0562636
C     2.8518154    0.7361733    3.2099235
C     2.5049065   -0.6263525    2.8286731
H     2.2004063    2.6841328    2.3478859
N     1.6719977   -0.5871007    1.7109998
C     1.4592118    0.7520256    1.4278448
C     2.1965390    1.5858090    2.3572658
C     1.2055608   -5.5890129    1.3758312
H     1.3144651   -6.6850875    1.3491596
H     4.5491381   -4.1815279    4.3285658
C     3.6096692   -4.2314887    3.7624952
C     3.0664190   -5.3506862    3.1440850
H     3.4872967   -6.3642938    3.1265936
C     1.9175143   -4.9343428    2.3869636
N     1.7330582   -3.5861163    2.6772413
C     2.8026300   -3.0905566    3.4200355
C     3.0383209   -1.7170138    3.5586476
H     3.8131404   -1.4395133    4.2917288
Co    0.9215108   -2.0825508    0.6983763
N     0.6133002   -2.8614099    2.4009183
S    -0.8477822   -3.2857406    3.1533711
O    -0.7888511   -4.6838874    3.6497633
O    -1.9045184   -2.8095563    2.2371103
C    -0.8969716   -2.2231551    4.6194062
C    -0.9787156   -0.5801855    6.8766645
C    -1.2405749   -0.8677028    4.4699866
C    -0.6023309   -2.7713195    5.8783918
C    -0.6444261   -1.9389429    7.0104213
C    -1.2772101   -0.0475745    5.6079398
H    -1.4839261   -0.4719091    3.4719409
H    -0.3594696   -3.8420485    5.9582087
H    -0.4213890   -2.3590263    8.0053699
H    -1.5473089    1.0164351    5.5046700
H    -1.0136980    0.0685480    7.7676190
N     2.6199576   -1.9788112   -0.7591058
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S      4.0620116   -3.0845939   -0.8770634
O      5.2648589   -2.2330685   -0.9092218
O      3.7975433   -4.0689166    0.1793541
C      3.8293714   -3.8329857   -2.4933339
C      3.4775437   -4.9825861   -4.9988149
C      4.6247881   -3.3848637   -3.5619040
C      2.8631036   -4.8428657   -2.6438334
C      2.6930030   -5.4155055   -3.9135049
C      4.4406662   -3.9729613   -4.8240828
H      5.3775981   -2.5995680   -3.3961278
H      2.2570576   -5.1737574   -1.7856192
H      1.9395331   -6.2072012   -4.0528844
H      5.0568271   -3.6401035   -5.6750098
H      3.3370654   -5.4389058   -5.9925173
N      2.7590808   -0.9412822   -1.4414082
N      2.7483036    0.0566488   -2.0156044
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Pdb file
HEADER B2Pdb
COMPND B2Pdb
ATOM      1  C   111     1      -0.119   0.463  -0.480  1.00  0.00
ATOM      2  N   111     1      -0.081  -0.914  -0.503  1.00  0.00
ATOM      3  H   111     1      -1.233   2.004  -1.716  1.00  0.00
ATOM      4  C   111     1      -0.907  -1.321  -1.525  1.00  0.00
ATOM      5  C   111     1      -1.501  -0.162  -2.168  1.00  0.00
ATOM      6  H   111     1      -2.206  -0.202  -3.010  1.00  0.00
ATOM      7  C   111     1      -1.014   0.947  -1.516  1.00  0.00
ATOM      8  C   111     1      -1.122  -2.663  -1.864  1.00  0.00
ATOM      9  H   111     1      -1.789  -2.871  -2.716  1.00  0.00
ATOM     10  N   111     1       0.229  -3.724  -0.076  1.00  0.00
ATOM     11  C   111     1       0.445  -5.046   0.315  1.00  0.00
ATOM     12  C   111     1      -0.242  -5.933  -0.613  1.00  0.00
ATOM     13  H   111     1      -0.245  -7.029  -0.530  1.00  0.00
ATOM     14  C   111     1      -0.894  -5.149  -1.531  1.00  0.00
ATOM     15  H   111     1      -1.540  -5.461  -2.363  1.00  0.00
ATOM     16  C   111     1      -0.599  -3.773  -1.184  1.00  0.00
ATOM     17  C   111     1       0.625   1.246   0.415  1.00  0.00
ATOM     18  H   111     1       0.540   2.340   0.326  1.00  0.00
ATOM     19  H   111     1       3.504   0.992   4.056  1.00  0.00
ATOM     20  C   111     1       2.852   0.736   3.210  1.00  0.00
ATOM     21  C   111     1       2.505  -0.626   2.829  1.00  0.00
ATOM     22  H   111     1       2.200   2.684   2.348  1.00  0.00
ATOM     23  N   111     1       1.672  -0.587   1.711  1.00  0.00
ATOM     24  C   111     1       1.459   0.752   1.428  1.00  0.00
ATOM     25  C   111     1       2.197   1.586   2.357  1.00  0.00
ATOM     26  C   111     1       1.206  -5.589   1.376  1.00  0.00
ATOM     27  H   111     1       1.314  -6.685   1.349  1.00  0.00
ATOM     28  H   111     1       4.549  -4.182   4.329  1.00  0.00
ATOM     29  C   111     1       3.610  -4.231   3.762  1.00  0.00
ATOM     30  C   111     1       3.066  -5.351   3.144  1.00  0.00
ATOM     31  H   111     1       3.487  -6.364   3.127  1.00  0.00
ATOM     32  C   111     1       1.918  -4.934   2.387  1.00  0.00
ATOM     33  N   111     1       1.733  -3.586   2.677  1.00  0.00
ATOM     34  C   111     1       2.803  -3.091   3.420  1.00  0.00
ATOM     35  C   111     1       3.038  -1.717   3.559  1.00  0.00
ATOM     36  H   111     1       3.813  -1.440   4.292  1.00  0.00
ATOM     37 Co   111     1       0.922  -2.083   0.698  1.00  0.00
ATOM     38  N   111     1       0.613  -2.861   2.401  1.00  0.00
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ATOM     39  S   111     1       -0.848  -3.286   3.153  1.00  0.00
ATOM     40  O   111     1       -0.789  -4.684   3.650  1.00  0.00
ATOM     41  O   111     1       -1.905  -2.810   2.237  1.00  0.00
ATOM     42  C   111     1       -0.897  -2.223   4.619  1.00  0.00
ATOM     43  C   111     1       -0.979  -0.580   6.877  1.00  0.00
ATOM     44  C   111     1       -1.241  -0.868   4.470  1.00  0.00
ATOM     45  C   111     1       -0.602  -2.771   5.878  1.00  0.00
ATOM     46  C   111     1       -0.644  -1.939   7.010  1.00  0.00
ATOM     47  C   111     1       -1.277  -0.048   5.608  1.00  0.00
ATOM     48  H   111     1       -1.484  -0.472   3.472  1.00  0.00
ATOM     49  H   111     1       -0.359  -3.842   5.958  1.00  0.00
ATOM     50  H   111     1       -0.421  -2.359   8.005  1.00  0.00
ATOM     51  H   111     1       -1.547   1.016   5.505  1.00  0.00
ATOM     52  H   111     1       -1.014   0.069   7.768  1.00  0.00
ATOM     53  N   111     1        2.620  -1.979  -0.759  1.00  0.00
ATOM     54  S   111     1        4.062  -3.085  -0.877  1.00  0.00
ATOM     55  O   111     1        5.265  -2.233  -0.909  1.00  0.00
ATOM     56  O   111     1        3.798  -4.069   0.179  1.00  0.00
ATOM     57  C   111     1        3.829  -3.833  -2.493  1.00  0.00
ATOM     58  C   111     1        3.478  -4.983  -4.999  1.00  0.00
ATOM     59  C   111     1        4.625  -3.385  -3.562  1.00  0.00
ATOM     60  C   111     1        2.863  -4.843  -2.644  1.00  0.00
ATOM     61  C   111     1        2.693  -5.416  -3.914  1.00  0.00
ATOM     62  C   111     1        4.441  -3.973  -4.824  1.00  0.00
ATOM     63  H   111     1        5.378  -2.600  -3.396  1.00  0.00
ATOM     64  H   111     1        2.257  -5.174  -1.786  1.00  0.00
ATOM     65  H   111     1        1.940  -6.207  -4.053  1.00  0.00
ATOM     66  H   111     1        5.057  -3.640  -5.675  1.00  0.00
ATOM     67  H   111     1        3.337  -5.439  -5.993  1.00  0.00
ATOM     68  N   111     1        2.759  -0.941  -1.441  1.00  0.00
ATOM     69  N   111     1        2.748   0.057  -2.016  1.00  0.00
CONECT    1    2    7   17
CONECT    2    4   37
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   37
CONECT   11   12   26
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   18   24
CONECT   19   20
CONECT   20   21   25
CONECT   21   23   35
CONECT   22   25
CONECT   23   24   37
CONECT   24   25
CONECT   26   27   32
CONECT   28   29
CONECT   29   30   34
CONECT   30   31   32
CONECT   32   33
CONECT   33   34   38
CONECT   34   35
CONECT   35   36
CONECT   37   38
CONECT   38   39
CONECT   39   40   41   42
CONECT   42   44   45
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CONECT   43   46   47   52
CONECT   44   47   48
CONECT   45   46   49
CONECT   46   50
CONECT   47   51
CONECT   53   54   68
CONECT   54   55   56   57
CONECT   57   59   60
CONECT   58   61   62   67
CONECT   59   62   63
CONECT   60   61   64
CONECT   61   65
CONECT   62   66
CONECT   68   69
END


III
Xyz file
69
 Energy =   -4151.7226911900
C     0.4022529    0.7936280   -0.3972921
N     0.0070564   -0.5262986   -0.2917570
H    -0.5098700    2.6358786   -1.3344041
C    -1.2436159   -0.5902859   -0.8796302
C    -1.6345270    0.7092512   -1.3803763
H    -2.5797361    0.9186075   -1.8987834
C    -0.5973310    1.5654402   -1.1049185
C    -1.9802974   -1.7587762   -1.0648567
H    -2.9618503   -1.6821286   -1.5554575
N    -0.2996039   -3.2951603   -0.1189586
C    -0.1768438   -4.6748128   -0.1217088
C    -1.3046956   -5.2814637   -0.7925039
H    -1.4371748   -6.3625733   -0.9324837
C    -2.1429811   -4.2587751   -1.1594207
H    -3.1085610   -4.3137187   -1.6791887
C    -1.5012629   -3.0292215   -0.7543093
C     1.5518473    1.3416045    0.1727279
H     1.7526693    2.4095952   -0.0016394
H     4.7196709    0.4114050    3.4320409
C     3.9235684    0.3249667    2.6803732
C     3.2004812   -0.8945959    2.3824608
H     3.7371411    2.3375065    1.7365439
N     2.2754644   -0.6780889    1.3835299
C     2.3902716    0.6545524    1.0507359
C     3.4390127    1.2845573    1.8289095
C     0.8426871   -5.3924277    0.4982564
H     0.8185130   -6.4899727    0.4256067
H     4.1661381   -4.8181544    3.6859824
C     3.3995214   -4.6424665    2.9191834
C     2.7134866   -5.5615873    2.1624163
H     2.7772930   -6.6578242    2.1877850
C     1.8061169   -4.8119580    1.3216224
N     1.9739617   -3.4558146    1.5215074
C     2.9390869   -3.3353348    2.5033336
C     3.4818034   -2.1331086    2.9561732
H     4.2456009   -2.1767783    3.7474266
Co    0.9218539   -1.9854751    0.7234506
N    -0.0533785   -1.6562538    2.2065290
S    -1.1886262   -2.7551187    2.8023181
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O    -0.6672772   -4.1327553    3.0330880
O    -2.4893784   -2.5849025    2.0902918
C    -1.3902794   -1.9889328    4.4384219
C    -1.7458784   -0.8523921    6.9623094
C    -2.2587108   -0.8933981    4.5807421
C    -0.7014990   -2.5294657    5.5360298
C    -0.8856368   -1.9541321    6.8043774
C    -2.4318116   -0.3244245    5.8524761
H    -2.7954091   -0.5071699    3.7005728
H    -0.0435133   -3.3990565    5.3852003
H    -0.3567435   -2.3720133    7.6772522
H    -3.1115192    0.5345894    5.9798105
H    -1.8865187   -0.4035220    7.9597600
N     2.2894850   -2.2437089   -1.2768900
S     4.0961785   -2.1998716   -1.5727314
O     4.3167318   -1.2725416   -2.6972676
O     4.6591262   -2.0006860   -0.2342090
C     4.4163853   -3.8805788   -2.1204492
C     4.9430094   -6.4733512   -2.9703096
C     4.5283532   -4.1318758   -3.4988004
C     4.5659782   -4.8907564   -1.1545420
C     4.8316200   -6.1965694   -1.5953006
C     4.7938359   -5.4455997   -3.9185124
H     4.4250200   -3.3079257   -4.2211660
H     4.4823670   -4.6571791   -0.0817374
H     4.9548227   -7.0035101   -0.8550112
H     4.8906749   -5.6641367   -4.9943506
H     5.1530336   -7.5018954   -3.3066078
N     1.6376604   -2.1621312   -2.3343309
N     0.9617378   -2.0919262   -3.2593401
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Pdb file
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COMPND B2Pdb
ATOM      1  C   111     1       0.402   0.794  -0.397  1.00  0.00
ATOM      2  N   111     1       0.007  -0.526  -0.292  1.00  0.00
ATOM      3  H   111     1      -0.510   2.636  -1.334  1.00  0.00
ATOM      4  C   111     1      -1.244  -0.590  -0.880  1.00  0.00
ATOM      5  C   111     1      -1.635   0.709  -1.380  1.00  0.00
ATOM      6  H   111     1      -2.580   0.919  -1.899  1.00  0.00
ATOM      7  C   111     1      -0.597   1.565  -1.105  1.00  0.00
ATOM      8  C   111     1      -1.980  -1.759  -1.065  1.00  0.00
ATOM      9  H   111     1      -2.962  -1.682  -1.555  1.00  0.00
ATOM     10  N   111     1      -0.300  -3.295  -0.119  1.00  0.00
ATOM     11  C   111     1      -0.177  -4.675  -0.122  1.00  0.00
ATOM     12  C   111     1      -1.305  -5.281  -0.793  1.00  0.00
ATOM     13  H   111     1      -1.437  -6.363  -0.932  1.00  0.00
ATOM     14  C   111     1      -2.143  -4.259  -1.159  1.00  0.00
ATOM     15  H   111     1      -3.109  -4.314  -1.679  1.00  0.00
ATOM     16  C   111     1      -1.501  -3.029  -0.754  1.00  0.00
ATOM     17  C   111     1       1.552   1.342   0.173  1.00  0.00
ATOM     18  H   111     1       1.753   2.410  -0.002  1.00  0.00
ATOM     19  H   111     1       4.720   0.411   3.432  1.00  0.00
ATOM     20  C   111     1       3.924   0.325   2.680  1.00  0.00
ATOM     21  C   111     1       3.200  -0.895   2.382  1.00  0.00
ATOM     22  H   111     1       3.737   2.338   1.737  1.00  0.00
ATOM     23  N   111     1       2.275  -0.678   1.384  1.00  0.00
ATOM     24  C   111     1       2.390   0.655   1.051  1.00  0.00
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ATOM     25  C   111     1        3.439   1.285   1.829  1.00  0.00
ATOM     26  C   111     1        0.843  -5.392   0.498  1.00  0.00
ATOM     27  H   111     1        0.819  -6.490   0.426  1.00  0.00
ATOM     28  H   111     1        4.166  -4.818   3.686  1.00  0.00
ATOM     29  C   111     1        3.400  -4.642   2.919  1.00  0.00
ATOM     30  C   111     1        2.713  -5.562   2.162  1.00  0.00
ATOM     31  H   111     1        2.777  -6.658   2.188  1.00  0.00
ATOM     32  C   111     1        1.806  -4.812   1.322  1.00  0.00
ATOM     33  N   111     1        1.974  -3.456   1.522  1.00  0.00
ATOM     34  C   111     1        2.939  -3.335   2.503  1.00  0.00
ATOM     35  C   111     1        3.482  -2.133   2.956  1.00  0.00
ATOM     36  H   111     1        4.246  -2.177   3.747  1.00  0.00
ATOM     37 Co   111     1        0.922  -1.985   0.723  1.00  0.00
ATOM     38  N   111     1       -0.053  -1.656   2.207  1.00  0.00
ATOM     39  S   111     1       -1.189  -2.755   2.802  1.00  0.00
ATOM     40  O   111     1       -0.667  -4.133   3.033  1.00  0.00
ATOM     41  O   111     1       -2.489  -2.585   2.090  1.00  0.00
ATOM     42  C   111     1       -1.390  -1.989   4.438  1.00  0.00
ATOM     43  C   111     1       -1.746  -0.852   6.962  1.00  0.00
ATOM     44  C   111     1       -2.259  -0.893   4.581  1.00  0.00
ATOM     45  C   111     1       -0.701  -2.529   5.536  1.00  0.00
ATOM     46  C   111     1       -0.886  -1.954   6.804  1.00  0.00
ATOM     47  C   111     1       -2.432  -0.324   5.852  1.00  0.00
ATOM     48  H   111     1       -2.795  -0.507   3.701  1.00  0.00
ATOM     49  H   111     1       -0.044  -3.399   5.385  1.00  0.00
ATOM     50  H   111     1       -0.357  -2.372   7.677  1.00  0.00
ATOM     51  H   111     1       -3.112   0.535   5.980  1.00  0.00
ATOM     52  H   111     1       -1.887  -0.404   7.960  1.00  0.00
ATOM     53  N   111     1        2.289  -2.244  -1.277  1.00  0.00
ATOM     54  S   111     1        4.096  -2.200  -1.573  1.00  0.00
ATOM     55  O   111     1        4.317  -1.273  -2.697  1.00  0.00
ATOM     56  O   111     1        4.659  -2.001  -0.234  1.00  0.00
ATOM     57  C   111     1        4.416  -3.881  -2.120  1.00  0.00
ATOM     58  C   111     1        4.943  -6.473  -2.970  1.00  0.00
ATOM     59  C   111     1        4.528  -4.132  -3.499  1.00  0.00
ATOM     60  C   111     1        4.566  -4.891  -1.155  1.00  0.00
ATOM     61  C   111     1        4.832  -6.197  -1.595  1.00  0.00
ATOM     62  C   111     1        4.794  -5.446  -3.919  1.00  0.00
ATOM     63  H   111     1        4.425  -3.308  -4.221  1.00  0.00
ATOM     64  H   111     1        4.482  -4.657  -0.082  1.00  0.00
ATOM     65  H   111     1        4.955  -7.004  -0.855  1.00  0.00
ATOM     66  H   111     1        4.891  -5.664  -4.994  1.00  0.00
ATOM     67  H   111     1        5.153  -7.502  -3.307  1.00  0.00
ATOM     68  N   111     1        1.638  -2.162  -2.334  1.00  0.00
ATOM     69  N   111     1        0.962  -2.092  -3.259  1.00  0.00
CONECT    1    2    7   17
CONECT    2    4   37
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   37
CONECT   11   12   26
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   18   24
CONECT   19   20
CONECT   20   21   25
CONECT   21   23   35
CONECT   22   25
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CONECT   23   24   37
CONECT   24   25
CONECT   26   27   32
CONECT   28   29
CONECT   29   30   34
CONECT   30   31   32
CONECT   32   33
CONECT   33   34   37
CONECT   34   35
CONECT   35   36
CONECT   37   38
CONECT   38   39
CONECT   39   40   41   42
CONECT   42   44   45
CONECT   43   46   47   52
CONECT   44   47   48
CONECT   45   46   49
CONECT   46   50
CONECT   47   51
CONECT   53   54   68
CONECT   54   55   56   57
CONECT   57   59   60
CONECT   58   61   62   67
CONECT   59   62   63
CONECT   60   61   64
CONECT   61   65
CONECT   62   66
CONECT   68   69
END



IV
Xyz file
67
 Energy =   -4042.1388527510
C    -0.0239677    1.0531156   -0.3091792
N    -0.3391482   -0.2843804   -0.2735161
H    -1.0330045    2.8820112   -1.1755608
C    -1.5251339   -0.4157485   -0.9577175
C    -1.9916577    0.8799025   -1.4086319
H    -2.9195507    1.0459617   -1.9719934
C    -1.0485273    1.7958190   -1.0144971
C    -2.1638731   -1.6194352   -1.2597049
H    -3.1044234   -1.5690265   -1.8285519
N    -0.5372635   -3.1379904   -0.1986960
C    -0.4190344   -4.5086548   -0.1364846
C    -1.5067587   -5.1374038   -0.8544062
H    -1.6440790   -6.2226635   -0.9478623
C    -2.2948385   -4.1249381   -1.3412572
H    -3.2202632   -4.1940851   -1.9281431
C    -1.6750741   -2.8825929   -0.9334383
C     1.1137161    1.6270047    0.2613547
H     1.2516526    2.7130956    0.1476913
H     4.6739432    0.6529249    3.0721015
C     3.7980816    0.5742129    2.4145540
C     3.0965778   -0.6587214    2.1291150
H     3.3955505    2.6338069    1.6568860
N     2.0448938   -0.4258939    1.2692199
C     2.0618427    0.9291479    1.0094843
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C	3.1638045	1.5613958	1.7040687
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C	3.3172586	-4.4050230	2.7410908
C	2.5203186	-5.3353278	2.1242498
H	2.5498651	-6.4298392	2.2039264
C	1.5759084	-4.6010402	1.3113080
N	1.8096978	-3.2465134	1.4125682
C	2.8688728	-3.1078305	2.2828863
C	3.4644433	-1.9007833	2.6436696
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O	-1.2936579	-3.9229065	2.9385137
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C	-1.7787898	-1.6953921	4.3086751
C	-2.0425463	-0.4717692	6.8011654
C	-2.5136274	-0.5006669	4.4112572
C	-1.1793238	-2.2922601	5.4311248
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C	-2.6407763	0.1106042	5.6681922
H	-2.9848265	-0.0725429	3.5130850
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H	-0.8578896	-2.1300891	7.5743881
H	-3.2157827	1.0461358	5.7656083
H	-2.1471910	0.0115037	7.7866917
N	1.5748300	-1.9339210	-1.1026119
S	3.0695773	-2.6350338	-1.3451178
O	4.1480559	-1.9991303	-0.5352580
O	2.9416742	-4.1214861	-1.3551613
C	3.3410011	-2.1125527	-3.0606754
C	3.7788926	-1.3190495	-5.6994431
C	4.0401672	-0.9199827	-3.3102287
C	2.8617356	-2.9189512	-4.1067335
C	3.0860746	-2.5145210	-5.4322335
C	4.2568627	-0.5256753	-4.6405998
H	4.4166031	-0.3244043	-2.4644162
H	2.3330060	-3.8558977	-3.8727028
H	2.7211475	-3.1398739	-6.2638421
H	4.8078549	0.4057372	-4.8520747
H	3.9517915	-1.0056355	-6.7424326

Pdb file

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HEADER B2Pdb
COMPND B2Pdb
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ATOM      3  H   111     1      -1.033   2.882  -1.176  1.00  0.00
ATOM      4  C   111     1      -1.525  -0.416  -0.958  1.00  0.00
ATOM      5  C   111     1      -1.992   0.880  -1.409  1.00  0.00
ATOM      6  H   111     1      -2.920   1.046  -1.972  1.00  0.00
ATOM      7  C   111     1      -1.049   1.796  -1.014  1.00  0.00
ATOM      8  C   111     1      -2.164  -1.619  -1.260  1.00  0.00
ATOM      9  H   111     1      -3.104  -1.569  -1.829  1.00  0.00
ATOM     10  N   111     1      -0.537  -3.138  -0.199  1.00  0.00
ATOM     11  C   111     1      -0.419  -4.509  -0.136  1.00  0.00
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ATOM     12  C   111     1       -1.507  -5.137  -0.854  1.00  0.00
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ATOM     14  C   111     1       -2.295  -4.125  -1.341  1.00  0.00
ATOM     15  H   111     1       -3.220  -4.194  -1.928  1.00  0.00
ATOM     16  C   111     1       -1.675  -2.883  -0.933  1.00  0.00
ATOM     17  C   111     1        1.114   1.627   0.261  1.00  0.00
ATOM     18  H   111     1        1.252   2.713   0.148  1.00  0.00
ATOM     19  H   111     1        4.674   0.653   3.072  1.00  0.00
ATOM     20  C   111     1        3.798   0.574   2.415  1.00  0.00
ATOM     21  C   111     1        3.097  -0.659   2.129  1.00  0.00
ATOM     22  H   111     1        3.396   2.634   1.657  1.00  0.00
ATOM     23  N   111     1        2.045  -0.426   1.269  1.00  0.00
ATOM     24  C   111     1        2.062   0.929   1.009  1.00  0.00
ATOM     25  C   111     1        3.164   1.561   1.704  1.00  0.00
ATOM     26  C   111     1        0.566  -5.202   0.564  1.00  0.00
ATOM     27  H   111     1        0.522  -6.301   0.556  1.00  0.00
ATOM     28  H   111     1        4.153  -4.565   3.435  1.00  0.00
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ATOM     30  C   111     1        2.520  -5.335   2.124  1.00  0.00
ATOM     31  H   111     1        2.550  -6.430   2.204  1.00  0.00
ATOM     32  C   111     1        1.576  -4.601   1.311  1.00  0.00
ATOM     33  N   111     1        1.810  -3.247   1.413  1.00  0.00
ATOM     34  C   111     1        2.869  -3.108   2.283  1.00  0.00
ATOM     35  C   111     1        3.464  -1.901   2.644  1.00  0.00
ATOM     36  H   111     1        4.316  -1.936   3.340  1.00  0.00
ATOM     37 Co   111     1        0.757  -1.764   0.561  1.00  0.00
ATOM     38  N   111     1       -0.297  -1.675   2.102  1.00  0.00
ATOM     39  S   111     1       -1.612  -2.489   2.694  1.00  0.00
ATOM     40  O   111     1       -1.294  -3.923   2.939  1.00  0.00
ATOM     41  O   111     1       -2.821  -2.126   1.902  1.00  0.00
ATOM     42  C   111     1       -1.779  -1.695   4.309  1.00  0.00
ATOM     43  C   111     1       -2.043  -0.472   6.801  1.00  0.00
ATOM     44  C   111     1       -2.514  -0.501   4.411  1.00  0.00
ATOM     45  C   111     1       -1.179  -2.292   5.431  1.00  0.00
ATOM     46  C   111     1       -1.317  -1.671   6.683  1.00  0.00
ATOM     47  C   111     1       -2.641   0.111   5.668  1.00  0.00
ATOM     48  H   111     1       -2.985  -0.073   3.513  1.00  0.00
ATOM     49  H   111     1       -0.627  -3.237   5.313  1.00  0.00
ATOM     50  H   111     1       -0.858  -2.130   7.574  1.00  0.00
ATOM     51  H   111     1       -3.216   1.046   5.766  1.00  0.00
ATOM     52  H   111     1       -2.147   0.012   7.787  1.00  0.00
ATOM     53  N   111     1        1.575  -1.934  -1.103  1.00  0.00
ATOM     54  S   111     1        3.070  -2.635  -1.345  1.00  0.00
ATOM     55  O   111     1        4.148  -1.999  -0.535  1.00  0.00
ATOM     56  O   111     1        2.942  -4.121  -1.355  1.00  0.00
ATOM     57  C   111     1        3.341  -2.113  -3.061  1.00  0.00
ATOM     58  C   111     1        3.779  -1.319  -5.699  1.00  0.00
ATOM     59  C   111     1        4.040  -0.920  -3.310  1.00  0.00
ATOM     60  C   111     1        2.862  -2.919  -4.107  1.00  0.00
ATOM     61  C   111     1        3.086  -2.515  -5.432  1.00  0.00
ATOM     62  C   111     1        4.257  -0.526  -4.641  1.00  0.00
ATOM     63  H   111     1        4.417  -0.324  -2.464  1.00  0.00
ATOM     64  H   111     1        2.333  -3.856  -3.873  1.00  0.00
ATOM     65  H   111     1        2.721  -3.140  -6.264  1.00  0.00
ATOM     66  H   111     1        4.808   0.406  -4.852  1.00  0.00
ATOM     67  H   111     1        3.952  -1.006  -6.742  1.00  0.00
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CONECT    2    4   37
CONECT    3    7
CONECT    4    5    8
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CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   37
CONECT   11   12   26
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   18   24
CONECT   19   20
CONECT   20   21   25
CONECT   21   23   35
CONECT   22   25
CONECT   23   24   37
CONECT   24   25
CONECT   26   27   32
CONECT   28   29
CONECT   29   30   34
CONECT   30   31   32
CONECT   32   33
CONECT   33   34   37
CONECT   34   35
CONECT   35   36
CONECT   37   38   53
CONECT   38   39
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CONECT   42   44   45
CONECT   43   46   47   52
CONECT   44   47   48
CONECT   45   46   49
CONECT   46   50
CONECT   47   51
CONECT   53   54
CONECT   54   55   56   57
CONECT   57   59   60
CONECT   58   61   62   67
CONECT   59   62   63
CONECT   60   61   64
CONECT   61   65
CONECT   62   66
END



V
Xyz file
67
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C    -1.9131738   -0.1914903   -1.2700712
C    -1.7520100    1.1267034   -1.8359014
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C    -0.9256283    1.8671309   -0.9925445
C    -2.3459389   -1.4049367   -1.8354263
H    -2.9712221   -1.2955563   -2.7369172
N    -1.1095113   -3.3271530   -0.6502524
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C    -2.0549815   -5.0034763   -1.9426809
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C    -2.6163515   -3.8165786   -2.3354121
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H	-3.3837539	-3.6498276	-3.1033809
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H	0.8613555	2.1338871	1.2418506
H	3.7381664	-0.6321162	3.8651277
C	2.8929546	-0.5699009	3.1670504
C	2.2792080	-1.7025082	2.5052168
H	2.4450756	1.5973230	2.9658320
N	1.2330752	-1.2758398	1.7160273
C	1.1961834	0.1231759	1.7916968
C	2.2400658	0.5478123	2.7142551
C	-0.1807376	-5.5937281	-0.3497271
H	-0.2983281	-6.6504063	-0.6362582
H	3.3367597	-5.8806415	2.7099880
C	2.5555665	-5.5078001	2.0341348
C	1.7380203	-6.2320509	1.1973592
H	1.7113640	-7.3198532	1.0487818
C	0.8585131	-5.2828210	0.5389169
N	1.1672044	-4.0101276	0.9638859
C	2.1800200	-4.1137510	1.8910240
C	2.7115749	-3.0338126	2.6071806
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O	3.4519055	-2.5460446	-0.4817426
C	2.6537964	-1.6449137	-2.8619333
C	2.7760919	-1.8987485	-5.6376030
C	2.3751928	-0.5263042	-3.6648329
C	3.0014461	-2.8854489	-3.4213278
C	3.0610549	-3.0070866	-4.8191316
C	2.4381209	-0.6603155	-5.0609380
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H	3.2311732	-3.7328357	-2.7571051
H	3.3343686	-3.9740392	-5.2732093
H	2.2270111	0.2097464	-5.7046895
H	2.8227311	-1.9996314	-6.7347284
S	-2.3605634	-1.7865484	1.8150517
C	-2.5425742	-0.6532003	3.2058152
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H	-0.9411024	0.2911613	6.0739795
H	-2.9195586	1.8324000	6.1751479
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Pdb file
HEADER B2Pdb
COMPND B2Pdb

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ATOM	2	N	111	1	-1.313	-0.117	-0.031	1.00	0.00
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ATOM	4	C	111	1	-1.913	-0.191	-1.270	1.00	0.00
ATOM	5	C	111	1	-1.752	1.127	-1.836	1.00	0.00
ATOM	6	H	111	1	-2.140	1.438	-2.815	1.00	0.00
ATOM	7	C	111	1	-0.926	1.867	-0.993	1.00	0.00
ATOM	8	C	111	1	-2.346	-1.405	-1.835	1.00	0.00
ATOM	9	H	111	1	-2.971	-1.296	-2.737	1.00	0.00
ATOM	10	N	111	1	-1.110	-3.327	-0.650	1.00	0.00
ATOM	11	C	111	1	-1.081	-4.677	-0.918	1.00	0.00
ATOM	12	C	111	1	-2.055	-5.003	-1.943	1.00	0.00
ATOM	13	H	111	1	-2.255	-6.014	-2.324	1.00	0.00
ATOM	14	C	111	1	-2.616	-3.817	-2.335	1.00	0.00
ATOM	15	H	111	1	-3.384	-3.650	-3.103	1.00	0.00
ATOM	16	C	111	1	-2.018	-2.753	-1.537	1.00	0.00
ATOM	17	C	111	1	0.462	1.118	1.089	1.00	0.00
ATOM	18	H	111	1	0.861	2.134	1.242	1.00	0.00
ATOM	19	H	111	1	3.738	-0.632	3.865	1.00	0.00
ATOM	20	C	111	1	2.893	-0.570	3.167	1.00	0.00
ATOM	21	C	111	1	2.279	-1.703	2.505	1.00	0.00
ATOM	22	H	111	1	2.445	1.597	2.966	1.00	0.00
ATOM	23	N	111	1	1.233	-1.276	1.716	1.00	0.00
ATOM	24	C	111	1	1.196	0.123	1.792	1.00	0.00
ATOM	25	C	111	1	2.240	0.548	2.714	1.00	0.00
ATOM	26	C	111	1	-0.181	-5.594	-0.350	1.00	0.00
ATOM	27	H	111	1	-0.298	-6.650	-0.636	1.00	0.00
ATOM	28	H	111	1	3.337	-5.881	2.710	1.00	0.00
ATOM	29	C	111	1	2.556	-5.508	2.034	1.00	0.00
ATOM	30	C	111	1	1.738	-6.232	1.197	1.00	0.00
ATOM	31	H	111	1	1.711	-7.320	1.049	1.00	0.00
ATOM	32	C	111	1	0.859	-5.283	0.539	1.00	0.00
ATOM	33	N	111	1	1.167	-4.010	0.964	1.00	0.00
ATOM	34	C	111	1	2.180	-4.114	1.891	1.00	0.00
ATOM	35	C	111	1	2.712	-3.034	2.607	1.00	0.00
ATOM	36	H	111	1	3.543	-3.242	3.297	1.00	0.00
ATOM	37	Co	111	1	0.171	-2.443	0.567	1.00	0.00
ATOM	38	N	111	1	-1.161	-1.154	0.852	1.00	0.00
ATOM	39	N	111	1	0.920	-1.749	-0.907	1.00	0.00
ATOM	40	S	111	1	2.584	-1.480	-1.054	1.00	0.00
ATOM	41	O	111	1	2.889	-0.054	-0.739	1.00	0.00
ATOM	42	O	111	1	3.452	-2.546	-0.482	1.00	0.00
ATOM	43	C	111	1	2.654	-1.645	-2.862	1.00	0.00
ATOM	44	C	111	1	2.776	-1.899	-5.638	1.00	0.00
ATOM	45	C	111	1	2.375	-0.526	-3.665	1.00	0.00
ATOM	46	C	111	1	3.001	-2.885	-3.421	1.00	0.00
ATOM	47	C	111	1	3.061	-3.007	-4.819	1.00	0.00
ATOM	48	C	111	1	2.438	-0.660	-5.061	1.00	0.00
ATOM	49	H	111	1	2.125	0.434	-3.188	1.00	0.00
ATOM	50	H	111	1	3.231	-3.733	-2.757	1.00	0.00
ATOM	51	H	111	1	3.334	-3.974	-5.273	1.00	0.00
ATOM	52	H	111	1	2.227	0.210	-5.705	1.00	0.00
ATOM	53	H	111	1	2.823	-2.000	-6.735	1.00	0.00
ATOM	54	S	111	1	-2.361	-1.787	1.815	1.00	0.00
ATOM	55	C	111	1	-2.543	-0.653	3.206	1.00	0.00
ATOM	56	C	111	1	-2.814	1.127	5.334	1.00	0.00
ATOM	57	C	111	1	-1.558	-0.633	4.209	1.00	0.00

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ATOM     58  C   111     1       -3.664    0.192    3.252  1.00  0.00
ATOM     59  C   111     1       -3.792    1.089    4.325  1.00  0.00
ATOM     60  C   111     1       -1.702    0.265    5.277  1.00  0.00
ATOM     61  H   111     1       -0.701   -1.321    4.151  1.00  0.00
ATOM     62  H   111     1       -4.424    0.129    2.459  1.00  0.00
ATOM     63  H   111     1       -4.667    1.758    4.375  1.00  0.00
ATOM     64  H   111     1       -0.941    0.291    6.074  1.00  0.00
ATOM     65  H   111     1       -2.920    1.832    6.175  1.00  0.00
ATOM     66  O   111     1       -1.602   -2.993    2.287  1.00  0.00
ATOM     67  O   111     1       -3.697   -1.902    1.188  1.00  0.00
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CONECT    2    4   38
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   37
CONECT   11   12   26
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   18   24
CONECT   19   20
CONECT   20   21   25
CONECT   21   23   35
CONECT   22   25
CONECT   23   24   37
CONECT   24   25
CONECT   26   27   32
CONECT   28   29
CONECT   29   30   34
CONECT   30   31   32
CONECT   32   33
CONECT   33   34   37
CONECT   34   35
CONECT   35   36
CONECT   37   38   39
CONECT   38   54
CONECT   39   40
CONECT   40   41   42   43
CONECT   43   45   46
CONECT   44   47   48   53
CONECT   45   48   49
CONECT   46   47   50
CONECT   47   51
CONECT   48   52
CONECT   54   55   66   67
CONECT   55   57   58
CONECT   56   59   60   65
CONECT   57   60   61
CONECT   58   59   62
CONECT   59   63
CONECT   60   64
END



VI
Xyz file
67
 Energy =   -4042.1359362610
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C	-0.9594126	1.4978486	0.2604366
N	-1.5002469	0.2366971	0.0119849
H	-1.2738657	3.4391764	-0.8258787
C	-2.2369234	0.2421022	-1.1718795
C	-2.3020395	1.6106527	-1.5924238
H	-2.8035174	1.9581744	-2.5050932
C	-1.5196071	2.3740300	-0.7251422
C	-2.6174462	-0.9354920	-1.8458583
H	-3.3768477	-0.8071243	-2.6340098
N	-0.9808412	-2.6753622	-1.0161441
C	-0.8065993	-4.0212992	-1.3274266
C	-1.8352457	-4.4318459	-2.2795617
H	-1.9346669	-5.4481432	-2.6841574
C	-2.5993522	-3.3333915	-2.5529009
H	-3.4625443	-3.2531752	-3.2269656
C	-2.0758574	-2.2322660	-1.7495917
C	0.0882720	1.6925414	1.1835595
H	0.2960135	2.7409733	1.4536927
H	3.6633513	-0.0075934	3.6060875
C	2.8008603	0.0714823	2.9309433
C	2.2746643	-1.0318508	2.1328682
H	2.1420292	2.1887083	3.0515672
N	1.1833597	-0.5887489	1.3938098
C	1.0101774	0.7581683	1.7015099
C	2.0399674	1.1707872	2.6515316
C	0.1119525	-4.9574579	-0.8071924
H	-0.0949145	-6.0052308	-1.0806084
H	2.9712618	-5.2224536	2.9070217
C	2.4793291	-4.8761527	1.9886593
C	1.7015812	-5.6397654	1.1170119
H	1.4519591	-6.7040404	1.2175392
C	1.1525724	-4.7646761	0.1247925
N	1.6948195	-3.5042033	0.3737964
C	2.4227450	-3.5084616	1.5641411
C	2.8070701	-2.3313574	2.2370338
H	3.5640107	-2.4615466	3.0271835
Co	0.1023900	-1.6335356	0.1889372
N	-1.4128726	-0.7985262	0.9050584
N	1.6148623	-2.4762741	-0.5283512
S	3.0205178	-1.9387244	-1.3006597
O	2.7015698	-0.5503860	-1.6982601
O	4.2327420	-2.2894472	-0.5166191
C	3.0938523	-2.9310987	-2.8145260
C	3.1884816	-4.4618911	-5.1493503
C	2.3139454	-2.5476017	-3.9196815
C	3.9286433	-4.0602136	-2.8622081
C	3.9688675	-4.8282000	-4.0387752
C	2.3651571	-3.3214773	-5.0893147
H	1.6882729	-1.6440738	-3.8561695
H	4.5482581	-4.3156308	-1.9886387
H	4.6233191	-5.7143067	-4.0903709
H	1.7622825	-3.0281212	-5.9648002
H	3.2274090	-5.0636469	-6.0724807
S	-2.8082088	-1.3261808	1.7024260
C	-2.7716365	-0.4299919	3.2762445
C	-2.6560041	0.9765286	5.6874914
C	-2.0264246	-0.9580348	4.3449388
C	-3.4736530	0.7809242	3.3994475
C	-3.4075742	1.4857106	4.6134112
C	-1.9718726	-0.2461160	5.5535598

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H    -1.5097550   -1.9225463    4.2232829
H    -4.0733999    1.1494411    2.5531912
H    -3.9547149    2.4368592    4.7225512
H    -1.3941625   -0.6519895    6.4006681
H    -2.6085941    1.5320942    6.6386741
O    -2.5453973   -2.7495886    2.0066500
O    -4.0256012   -0.8683878    0.9845230
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Pdb file
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COMPND B2Pdb
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ATOM      2  N   111     1      -1.500   0.237   0.012  1.00  0.00
ATOM      3  H   111     1      -1.274   3.439  -0.826  1.00  0.00
ATOM      4  C   111     1      -2.237   0.242  -1.172  1.00  0.00
ATOM      5  C   111     1      -2.302   1.611  -1.592  1.00  0.00
ATOM      6  H   111     1      -2.804   1.958  -2.505  1.00  0.00
ATOM      7  C   111     1      -1.520   2.374  -0.725  1.00  0.00
ATOM      8  C   111     1      -2.617  -0.935  -1.846  1.00  0.00
ATOM      9  H   111     1      -3.377  -0.807  -2.634  1.00  0.00
ATOM     10  N   111     1      -0.981  -2.675  -1.016  1.00  0.00
ATOM     11  C   111     1      -0.807  -4.021  -1.327  1.00  0.00
ATOM     12  C   111     1      -1.835  -4.432  -2.280  1.00  0.00
ATOM     13  H   111     1      -1.935  -5.448  -2.684  1.00  0.00
ATOM     14  C   111     1      -2.599  -3.333  -2.553  1.00  0.00
ATOM     15  H   111     1      -3.463  -3.253  -3.227  1.00  0.00
ATOM     16  C   111     1      -2.076  -2.232  -1.750  1.00  0.00
ATOM     17  C   111     1       0.088   1.693   1.184  1.00  0.00
ATOM     18  H   111     1       0.296   2.741   1.454  1.00  0.00
ATOM     19  H   111     1       3.663  -0.008   3.606  1.00  0.00
ATOM     20  C   111     1       2.801   0.071   2.931  1.00  0.00
ATOM     21  C   111     1       2.275  -1.032   2.133  1.00  0.00
ATOM     22  H   111     1       2.142   2.189   3.052  1.00  0.00
ATOM     23  N   111     1       1.183  -0.589   1.394  1.00  0.00
ATOM     24  C   111     1       1.010   0.758   1.702  1.00  0.00
ATOM     25  C   111     1       2.040   1.171   2.652  1.00  0.00
ATOM     26  C   111     1       0.112  -4.957  -0.807  1.00  0.00
ATOM     27  H   111     1      -0.095  -6.005  -1.081  1.00  0.00
ATOM     28  H   111     1       2.971  -5.222   2.907  1.00  0.00
ATOM     29  C   111     1       2.479  -4.876   1.989  1.00  0.00
ATOM     30  C   111     1       1.702  -5.640   1.117  1.00  0.00
ATOM     31  H   111     1       1.452  -6.704   1.218  1.00  0.00
ATOM     32  C   111     1       1.153  -4.765   0.125  1.00  0.00
ATOM     33  N   111     1       1.695  -3.504   0.374  1.00  0.00
ATOM     34  C   111     1       2.423  -3.508   1.564  1.00  0.00
ATOM     35  C   111     1       2.807  -2.331   2.237  1.00  0.00
ATOM     36  H   111     1       3.564  -2.462   3.027  1.00  0.00
ATOM     37 Co   111     1       0.102  -1.634   0.189  1.00  0.00
ATOM     38  N   111     1      -1.413  -0.799   0.905  1.00  0.00
ATOM     39  N   111     1       1.615  -2.476  -0.528  1.00  0.00
ATOM     40  S   111     1       3.021  -1.939  -1.301  1.00  0.00
ATOM     41  O   111     1       2.702  -0.550  -1.698  1.00  0.00
ATOM     42  O   111     1       4.233  -2.289  -0.517  1.00  0.00
ATOM     43  C   111     1       3.094  -2.931  -2.815  1.00  0.00
ATOM     44  C   111     1       3.188  -4.462  -5.149  1.00  0.00
ATOM     45  C   111     1       2.314  -2.548  -3.920  1.00  0.00
ATOM     46  C   111     1       3.929  -4.060  -2.862  1.00  0.00
ATOM     47  C   111     1       3.969  -4.828  -4.039  1.00  0.00
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ATOM     49  H   111     1       1.688  -1.644  -3.856  1.00  0.00
ATOM     50  H   111     1       4.548  -4.316  -1.989  1.00  0.00
ATOM     51  H   111     1       4.623  -5.714  -4.090  1.00  0.00
ATOM     52  H   111     1       1.762  -3.028  -5.965  1.00  0.00
ATOM     53  H   111     1       3.227  -5.064  -6.072  1.00  0.00
ATOM     54  S   111     1      -2.808  -1.326   1.702  1.00  0.00
ATOM     55  C   111     1      -2.772  -0.430   3.276  1.00  0.00
ATOM     56  C   111     1      -2.656   0.977   5.687  1.00  0.00
ATOM     57  C   111     1      -2.026  -0.958   4.345  1.00  0.00
ATOM     58  C   111     1      -3.474   0.781   3.399  1.00  0.00
ATOM     59  C   111     1      -3.408   1.486   4.613  1.00  0.00
ATOM     60  C   111     1      -1.972  -0.246   5.554  1.00  0.00
ATOM     61  H   111     1      -1.510  -1.923   4.223  1.00  0.00
ATOM     62  H   111     1      -4.073   1.149   2.553  1.00  0.00
ATOM     63  H   111     1      -3.955   2.437   4.723  1.00  0.00
ATOM     64  H   111     1      -1.394  -0.652   6.401  1.00  0.00
ATOM     65  H   111     1      -2.609   1.532   6.639  1.00  0.00
ATOM     66  O   111     1      -2.545  -2.750   2.007  1.00  0.00
ATOM     67  O   111     1      -4.026  -0.868   0.985  1.00  0.00
CONECT    1    2    7   17
CONECT    2    4   38
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8    9   16
CONECT   10   11   16   37
CONECT   11   12   26
CONECT   12   13   14
CONECT   14   15   16
CONECT   17   18   24
CONECT   19   20
CONECT   20   21   25
CONECT   21   23   35
CONECT   22   25
CONECT   23   24   37
CONECT   24   25
CONECT   26   27   32
CONECT   28   29
CONECT   29   30   34
CONECT   30   31   32
CONECT   32   33
CONECT   33   34   39
CONECT   34   35
CONECT   35   36
CONECT   37   38   39
CONECT   38   54
CONECT   39   40
CONECT   40   41   42   43
CONECT   43   45   46
CONECT   44   47   48   53
CONECT   45   48   49
CONECT   46   47   50
CONECT   47   51
CONECT   48   52
CONECT   54   55   66   67
CONECT   55   57   58
CONECT   56   59   60   65
CONECT   57   60   61
CONECT   58   59   62
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CONECT   59   63
CONECT   60   64
END
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