Electronic Supplementary Material (ESI) for CrystEngComm
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Three cobalt(II) coordination polymers based on V-shaped aromatic polycarboxylates and rigid bis(imidazole) ligand: Syntheses, crystal structures, physical properties and theoretical studies

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Supporting Information

Section-1.

Section-2. Computational Outputs

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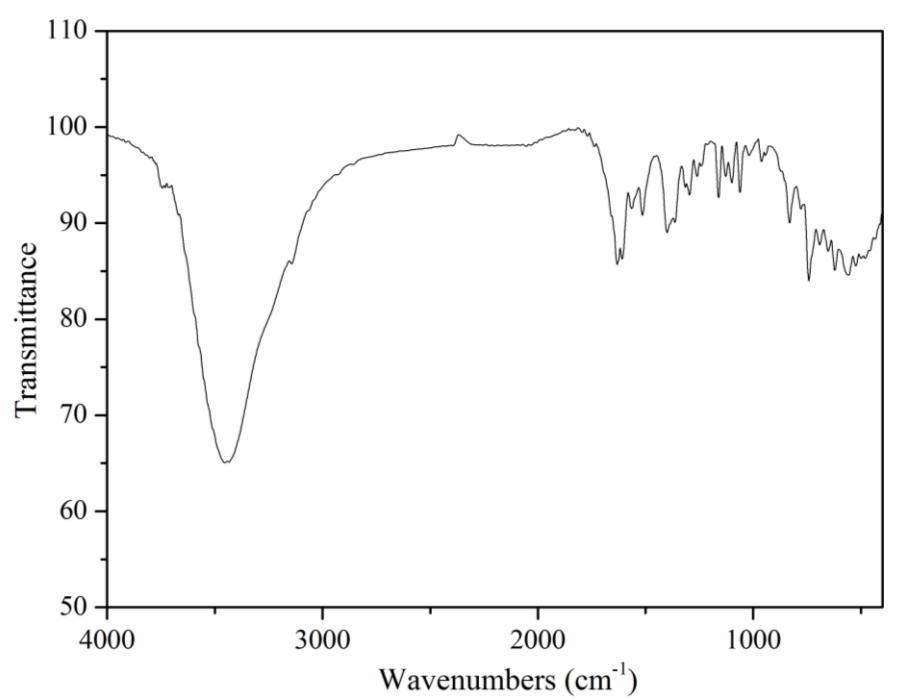
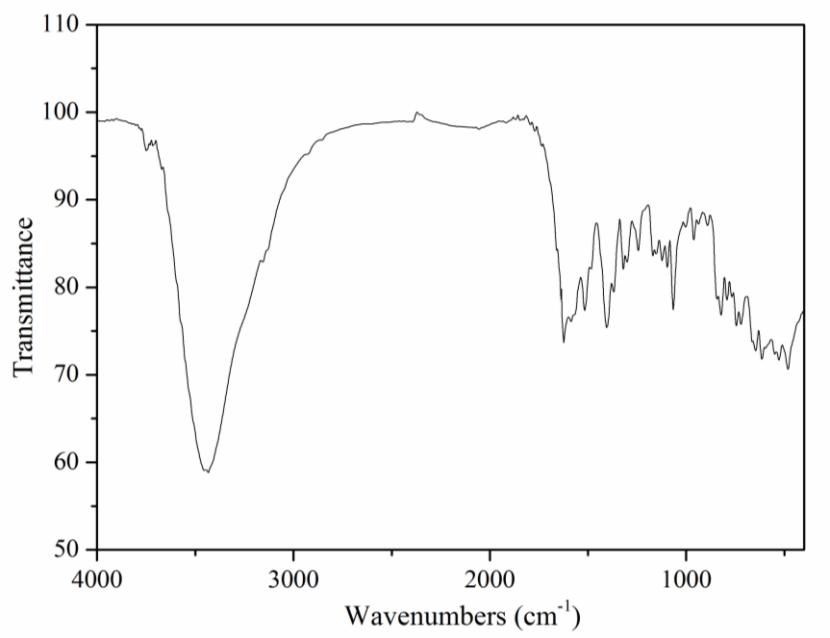
Section-1.



(a)



(b)

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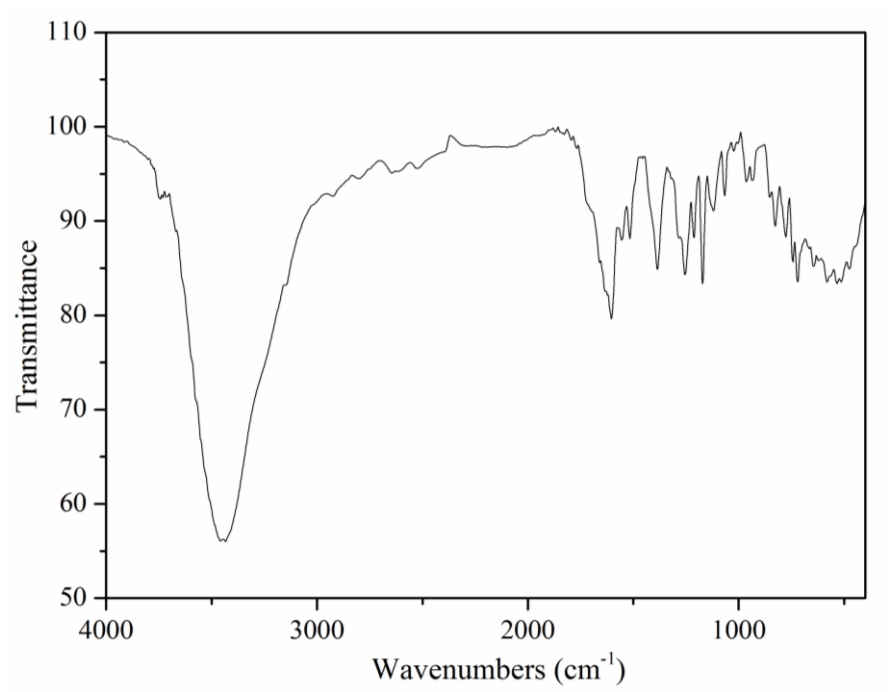

(c)

Figure S1. Infrared spectra of complexes **1** – **3**.

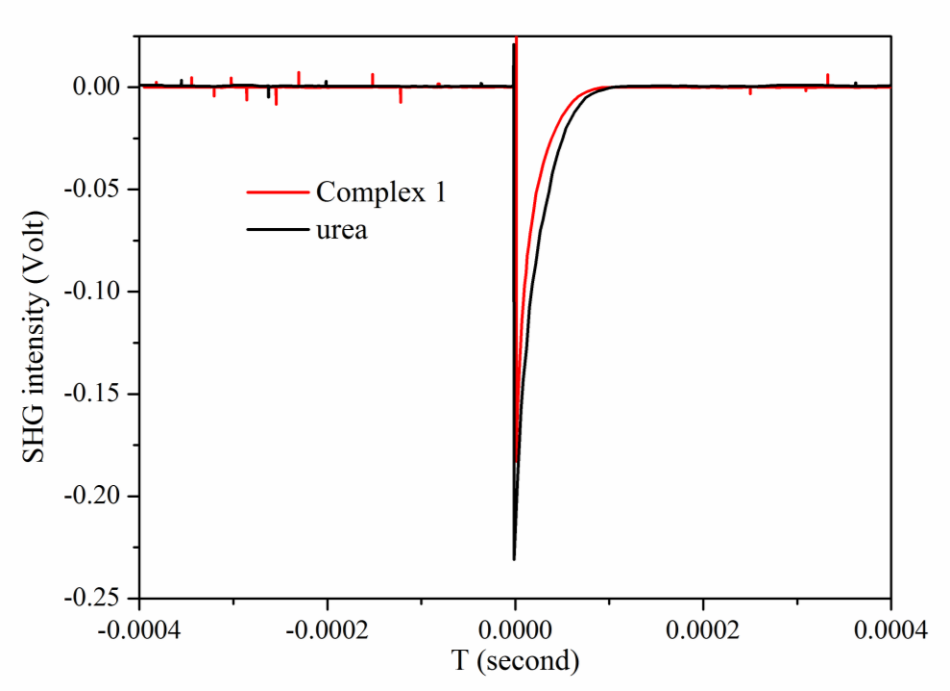

Figure S2. Oscilloscope traces of the SHG signals for the powders of Co(SDBA)(BIMB) (**1**) and urea.

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Section-2. Computational Outputs

Complex 1 BIMB opt

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opt freq b3lyp/6-311++g geom=connectivity

Stoichiometry C18H14N4

Framework group C1[X(C18H14N4)]

Deg. of freedom 102

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-7.034264	0.614092	-0.387739
2	7	0	-4.949647	-0.000548	-0.099902
3	7	0	4.960804	-0.050493	0.002653
4	7	0	6.877614	-0.766613	-0.780698
5	6	0	-5.796708	1.029979	-0.260493
6	1	0	-5.538070	1.923607	-0.278525
7	6	0	-6.978916	-0.750166	-0.307678
8	1	0	-7.711608	-1.320005	-0.367758
9	6	0	-5.715236	-1.140384	-0.129441
10	1	0	-5.411325	-2.015005	-0.042771
11	6	0	-3.516491	0.049322	0.028661
12	6	0	-2.866165	1.239176	0.271331
13	1	0	-3.347728	2.031505	0.350840
14	6	0	-1.498853	1.243288	0.394484
15	1	0	-1.064571	2.049702	0.553441
16	6	0	-0.736667	0.072593	0.289231
17	6	0	-1.423259	-1.100760	0.056726
18	1	0	-0.951616	-1.898534	-0.019472

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19	6	0	-2.788861	-1.112393	-0.063339
20	1	0	-3.229098	-1.918200	-0.209358
21	6	0	5.621404	-1.069071	-0.565409
22	1	0	5.235640	-1.887866	-0.780638
23	6	0	7.040077	0.505251	-0.302736
24	1	0	7.836814	0.985346	-0.310243
25	6	0	5.848501	0.958634	0.185654
26	1	0	5.680163	1.789822	0.566457
27	6	0	3.535017	0.010902	0.207799
28	6	0	2.846765	-1.074497	0.704639
29	1	0	3.309488	-1.829137	0.989933
30	6	0	1.477435	-1.038143	0.777312
31	1	0	1.020733	-1.775176	1.113264
32	6	0	0.751586	0.081858	0.357052
33	6	0	1.479952	1.191527	-0.096025
34	1	0	1.031145	1.968862	-0.337609
35	6	0	2.858794	1.143650	-0.189172
36	1	0	3.328224	1.875403	-0.519349

Rotational constants (GHZ): 1.7817952 0.0827816 0.0800392

SCF Done: E(RB3LYP) = -720.9155202325 A.U. after 16 cycles

Convg = 0.4468D-08 -V/T = 1.9980

Electronic spatial extent (au): <R**2> = 12306.9444

Charge = 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 0.0009 Y= 0.0006 Z= 1.1667 Tot= 1.1667

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -205.3391 YY= -115.2250 ZZ= -134.3105

XY= 23.3861 XZ= -0.0112 YZ= 0.0005

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= -53.7142 YY= 36.3999 ZZ= 17.3143

XY= 23.3861 XZ= -0.0112 YZ= 0.0005

Octapole moment (field-independent basis, Debye-Ang**2):

XXX = 0.0380	YYY = 0.0058	ZZZ = -1.5775	XYY = 0.0079
XXY = 0.0350	XXZ = 87.2963	XZZ = -0.0065	YZZ = -0.0018
YYZ = 2.0691	XYZ = 5.2659		

Hexadecapole moment (field-independent basis, Debye-Ang**3):

XXXX = -21949.1781	YYYY = -798.4690	ZZZZ = -277.1209	XXXY = 1671.9456
XXXZ = -0.5465	YYYX = 17.5129	YYYZ = -0.0007	ZZZX = -0.0185
ZZZY = -0.0035	XXYY = -2782.1019	XXZZ = -2925.5086	YYZZ = -179.8737
XXYZ = 0.0306	YYXZ = -0.0254	ZZXY = -1.7442	

N-N= 1.497489721633D+03 E-N=-5.115089149787D+03 KE= 9.100449486227D+02

Zero-point correction= 0.284228 (Hartree/Particle)

Thermal correction to Energy= 0.300748

Thermal correction to Enthalpy= 0.301692

Thermal correction to Gibbs Free Energy= 0.237398

Sum of electronic and zero-point Energies= -723.014145

Sum of electronic and thermal Energies= -722.997625

Sum of electronic and thermal Enthalpies= -722.996681

Sum of electronic and thermal Free Energies= -723.060975

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Complex 2 BIMB-1 opt

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opt freq b3lyp/6-311++g geom=connectivity

Stoichiometry C18H14N4

Framework group C1[X(C18H14N4)]

Deg. of freedom 102

Full point group C1 NOp 1

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Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	7.033968	-0.835987	-0.164125
2	7	0	4.981270	-0.020503	0.039267
3	7	0	-5.005248	0.001998	0.071701
4	7	0	-7.008848	-0.653348	0.654912
5	6	0	5.758249	-1.063542	-0.346226
6	1	0	5.421470	-1.854548	-0.702009
7	6	0	7.083173	0.424736	0.368448
8	1	0	7.862178	0.867821	0.617206
9	6	0	5.807221	0.939536	0.480700
10	1	0	5.568657	1.780675	0.797425
11	6	0	3.550011	0.032920	-0.025735
12	6	0	2.891512	1.225454	0.021166
13	1	0	3.375470	2.015953	0.092656
14	6	0	1.498307	1.271068	-0.037014
15	1	0	1.067564	2.095525	-0.008431
16	6	0	0.747492	0.118640	-0.135091
17	6	0	1.447530	-1.064103	-0.175602
18	1	0	0.971684	-1.859506	-0.247555
19	6	0	2.819367	-1.123170	-0.114838
20	1	0	3.251088	-1.946364	-0.131833
21	6	0	-5.715008	-0.765204	0.896888
22	1	0	-5.347691	-1.308466	1.556850
23	6	0	-7.093929	0.223371	-0.370127
24	1	0	-7.883671	0.505633	-0.771115
25	6	0	-5.840261	0.628541	-0.724004
26	1	0	-5.621095	1.232041	-1.396699
27	6	0	-3.544738	0.065398	0.012057
28	6	0	-2.868066	1.233869	0.006717
29	1	0	-3.337945	2.034958	0.053910

30	6	0	-1.491445	1.261471	-0.066896
31	1	0	-1.059192	2.085081	-0.084698
32	6	0	-0.747706	0.131206	-0.112475
33	6	0	-1.457509	-1.034772	-0.187363
34	1	0	-0.997503	-1.833808	-0.308119
35	6	0	-2.843122	-1.067875	-0.088462
36	1	0	-3.285475	-1.885391	-0.092730

Rotational constants (GHZ): 1.9047656 0.0837698 0.0812239

SCF Done: E(RB3LYP) = -721.24715788 A.U. after 16 cycles

Convg = 0.3335D-08 -V/T = 1.9975

Electronic spatial extent (au): <R**2>= 12119.4993

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 0.7239 Y= 2.7885 Z= -0.8755 Tot= 3.0110

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -206.8705 YY= -115.8763 ZZ= -131.8034

XY= 2.8234 XZ= 15.0181 YZ= 0.9555

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= -55.3538 YY= 35.6404 ZZ= 19.7133

XY= 2.8234 XZ= 15.0181 YZ= 0.9555

Octapole moment (field-independent basis, Debye-Ang**2):

XXX = 34.0589 YYY = 5.0588 ZZZ = -0.0051 XYY = 9.1506

XXY = 193.2464 XXZ = -53.6991 XZZ = -4.7024 YZZ = 0.4242

YYZ = -1.0606 XYZ = 14.5423

Hexadecapole moment (field-independent basis, Debye-Ang**3):

XXXX = -21637.0612 YYYY = -717.3247 ZZZZ = -260.0028 XXXY = 213.4167

XXXZ = 1041.0023 YYYX = 9.2696 YYYZ = 10.0583 ZZZX = 2.6992

ZZZY = -6.9801 XXYY = -2827.7296 XXZZ = -2810.4488 YYZZ = -173.3556

XXYZ = 35.4291 YYXZ = 18.2226 ZZXY = -8.6304

N-N= 1.529664586312D+03 E-N=-5.182409005879D+03 KE= 9.153211016914D+02

Zero-point correction= 0.273832 (Hartree/Particle)

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Thermal correction to Energy= 0.297642

Thermal correction to Enthalpy= 0.2987532

Thermal correction to Gibbs Free Energy= 0.2189321

Sum of electronic and zero-point Energies= -721.027536

Sum of electronic and thermal Energies= -720.894264

Sum of electronic and thermal Enthalpies= -720.896683

Sum of electronic and thermal Free Energies= -721.057403

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Complex 2 BIMB-2 opt

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opt freq b3lyp/6-311++g geom=connectivity

Stoichiometry C18H14N4

Framework group C1[X(C18H14N4)]

Deg. of freedom 102

Full point group CI NOp 2

Largest Abelian subgroup CI NOp 2

Largest concise Abelian subgroup CI NOp 2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	6.962198	-0.734435	0.382384
2	7	0	4.952749	0.049574	-0.033529
3	6	0	5.678945	-0.966834	0.432720
4	1	0	5.309793	-1.756461	0.757344
5	6	0	7.063707	0.494638	-0.168786
6	1	0	7.862576	0.938937	-0.339463
7	6	0	5.852555	0.975624	-0.431380

8	1	0	5.658816	1.798162	-0.818287
9	6	0	3.520164	0.061649	-0.078848
10	6	0	2.829808	1.219216	0.174030
11	1	0	3.282344	2.019426	0.315980
12	6	0	1.457754	1.175631	0.214031
13	1	0	0.990334	1.956848	0.400076
14	6	0	0.745582	0.007647	-0.014286
15	6	0	1.478115	-1.141265	-0.308765
16	1	0	1.030955	-1.939570	-0.477426
17	6	0	2.850467	-1.108393	-0.353345
18	1	0	3.327490	-1.876276	-0.569347
19	7	0	-6.962670	0.734284	-0.382671
20	7	0	-4.953249	-0.049506	0.033276
21	6	0	-5.678129	0.966570	-0.432369
22	1	0	-5.310243	1.756443	-0.757589
23	6	0	-7.063377	-0.494159	0.168934
24	1	0	-7.862240	-0.938563	0.339707
25	6	0	-5.852270	-0.975164	0.431616
26	1	0	-5.658882	-1.799000	0.818060
27	6	0	-3.519320	-0.062133	0.079166
28	6	0	-2.830308	-1.219147	-0.174283
29	1	0	-3.282670	-2.019482	-0.316170
30	6	0	-1.458226	-1.175534	-0.214149
31	1	0	-0.989970	-1.956445	-0.399698
32	6	0	-0.746032	-0.007664	0.014040
33	6	0	-1.477293	1.140896	0.309211
34	1	0	-1.031382	1.939686	0.477221
35	6	0	-2.850967	1.108461	0.353092
36	1	0	-3.327154	1.876650	0.569591

Rotational constants (GHZ): 1.8966639 0.0848095 0.0818475

SCF Done: E(RB3LYP) = -721.0030685 A.U. after 16 cycles

Convg = 0.1489D-08 -V/T = 1.9974

Electronic spatial extent (au): <R**2>= 12008.5714

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 0.0194 Y= -0.0010 Z= 0.0006 Tot = 0.0194

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -203.5160 YY= -114.0399 ZZ= -132.9577

XY= 26.2488 XZ= -13.7339 YZ= 1.3373

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= -53.3448 YY= 36.1313 ZZ= 17.2135

XY= 26.2488 XZ= -13.7339 YZ= 1.3373

Octapole moment (field-independent basis, Debye-Ang**2):

XXX = 1.3277 YYY = 0.0050 ZZZ = -0.0047 XYY = 0.0103

XXY = -0.0527 XXZ = 0.0316 XZZ = 0.0384 YZZ = 0.0000

YYZ = 0.0020 XYZ = -0.0286

Hexadecapole moment (field-independent basis, Debye-Ang**3):

XXXX = -21084.8889 YYYY = -748.8693 ZZZZ = -228.9878 XXXY = 1731.2580

XXXZ = -840.6860 YYYX = 45.4392 YYYZ = 3.7797 ZZZX = -2.2505

ZZZY = 0.1492 XXYY = -2733.4857 XXZZ = -2820.2044 YYZZ = -173.2308

XXYZ = -3.7152 YYXZ = -29.5609 ZZXY = 6.8936

N-N= 1.532213427619D+03 E-N=-5.187682806955D+03 KE= 9.153675711404D+02

Zero-point correction= 0.265439 (Hartree/Particle)

Thermal correction to Energy= 0.2731245

Thermal correction to Enthalpy= 0.275682

Thermal correction to Gibbs Free Energy= 0.214732

Sum of electronic and zero-point Energies= -721.061358

Sum of electronic and thermal Energies= -720.084597

Sum of electronic and thermal Enthalpies= -720.087646

Sum of electronic and thermal Free Energies= -721.0669821

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Complex 3 BIMB opt

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opt freq b3lyp/6-311++g geom=connectivity

Stoichiometry C18H14N4

Framework group C1[X(C18H14N4)]

Deg. of freedom 102

Full point group CI NOp 2

Largest Abelian subgroup CI NOp 2

Largest concise Abelian subgroup CI NOp 2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	7.071667	0.410372	0.517721
2	7	0	4.964146	-0.022691	0.079489
3	6	0	5.824888	0.498961	0.949645
4	1	0	5.580651	0.879230	1.762247
5	6	0	6.989394	-0.281210	-0.661466
6	1	0	7.714867	-0.519742	-1.191635
7	6	0	5.713298	-0.560759	-0.935262
8	1	0	5.393628	-1.029484	-1.672409
9	6	0	3.534954	-0.013948	0.101838
10	6	0	2.835876	-1.180971	0.385668
11	1	0	3.298408	-1.959339	0.600404
12	6	0	1.446205	-1.186034	0.348980
13	1	0	1.021302	-1.989674	0.546003
14	6	0	0.755541	-0.024118	0.028519
15	6	0	1.453741	1.144024	-0.255754
16	1	0	1.033803	1.944615	-0.474024
17	6	0	2.843411	1.149087	-0.219067
18	1	0	3.310830	1.930531	-0.409280
19	7	0	-7.071469	-0.410866	-0.517105
20	7	0	-4.963972	0.022757	-0.080097
21	6	0	-5.825356	-0.499282	-0.949755

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22	1	0	-5.580514	-0.878430	-1.762509
23	6	0	-6.989890	0.280668	0.661330
24	1	0	-7.715376	0.520095	1.191998
25	6	0	-5.712632	0.561361	0.935708
26	1	0	-5.393628	1.030259	1.672129
27	6	0	-3.533976	0.013867	-0.101703
28	6	0	-2.835826	1.181877	-0.385962
29	1	0	-3.298814	1.958940	-0.600313
30	6	0	-1.446227	1.186898	-0.349219
31	1	0	-1.021687	1.989186	-0.545953
32	6	0	-0.756019	0.023676	-0.028372
33	6	0	-1.454076	-1.144380	0.255790
34	1	0	-1.032896	-1.944738	0.474215
35	6	0	-2.843725	-1.149532	0.219062
36	1	0	-3.310669	-1.929570	0.409172

Rotational constants (GHZ): 1.8525071 0.0836826 0.0823395

SCF Done: E(RB3LYP) = -721.0438121 A.U. after 16 cycles

Convg = 0.3385D-08 -V/T = 1.9981

Electronic spatial extent (au): <R**2>= 12056.2705

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= -0.0016 Y= 0.0012 Z= -0.0029 Tot= 0.0036

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -215.8740 YY= -117.6729 ZZ= -126.2153

XY= -14.6757 XZ= -18.9910 YZ= -0.5499

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= -62.6199 YY= 35.5811 ZZ= 27.0388

XY= -14.6757 XZ= -18.9910 YZ= -0.5499

Octapole moment (field-independent basis, Debye-Ang**2):

XXX= -0.1552 YYY= 0.0070 ZZZ= -0.0207 XYY= 0.0059

XXY= 0.0663 XXZ= -0.1572 XZZ= -0.0137 YZZ= 0.0070

YYZ= 0.0022 XYZ= -0.0022

Hexadecapole moment (field-independent basis, Debye-Ang**3):

XXXX= -22429.9741 YYYY= -615.0838 ZZZZ= -380.0252 XXXY= -957.8237

XXXZ= -1408.3410 YYYX= -5.3428 YYYZ= -22.1888 ZZZX= -5.9182

ZZZY= 21.0554 XXYY= -2802.9937 XXZZ= -2633.3697 YYZZ= -170.4930

XXYZ= 63.1761 YYXZ= -7.0767 ZZXY= -19.8814

N-N= 1.523477660357D+03 E-N=-5.169931198646D+03 KE= 9.147036850957D+02

Zero-point correction= 0.275345 (Hartree/Particle)

Thermal correction to Energy= 0.294834

Thermal correction to Enthalpy= 0.286739

Thermal correction to Gibbs Free Energy= 0.216783

Sum of electronic and zero-point Energies= -720.012456

Sum of electronic and thermal Energies= -720.942178

Sum of electronic and thermal Enthalpies= -720.943867

Sum of electronic and thermal Free Energies= -721.059612