

ДОПОЛНИТЕЛЬНЫЕ МАТЕРИАЛЫ К СТАТЬЕ
**СТРОЕНИЕ И ТЕРМИЧЕСКИЕ СВОЙСТВА НОВЫХ ПОЛИМОРФНЫХ
МОДИФИКАЦИЙ БИС-(ДИПИВАЛОИЛМЕТАНО)
(N,N,N',N'-ТЕТРАМЕТИЛЭТИЛЕНДИАМИН)МАГНИЯ**

**Г.С. Евсеев, А.С. Сухих, К.В. Жерикова, А.М. Макаренко,
И.В. Корольков, Д.П. Пищур, Н.Б. Морозова, Е.С. Викулова**

Институт неорганической химии им. А.В. Николаева СО РАН, Новосибирск
E-mail: lazorevka@mail.ru

Table S1

Total electronic energies E_0 and number of formula units in the periodic unit cell Z .
Theory level: PBEsol/SSSP Precision

Polymorph	I $P2_1/n$	II $C2/c$	III $P-1$	Isolated molecule
Z	4	2	2	1
E_0 , Ry	-3607.218488	-1803.610682	-1803.612927	-901.7036424

Table S2

Experimental and optimized unit cell parameters (in Å) for the studied polymorphic modifications.
Theory level: PBEsol/SSSP Precision

Polymorphic modification	I $P2_1/n$ (193 K)		II $C2/c$		III $P-1 P\bar{1}$	
	Exp.	Calc.	Exp.	*Calc.	Exp.	Calc.
a , Å	10.091(4)	9.728	10.3585(8)	9.399	9.6863(5)	9.369
b , Å	19.133(5)	18.973	17.0505(16)	9.399	10.0069(5)	9.539
c , Å	17.021(5)	16.677	19.0407(17)	18.738	19.1822(9)	18.913
α , °	90	90	90	89.563	87.995(2)	89.893
β , °	93.250(5)	94.907	91.303(4)	89.563	89.177(2)	89.922
γ , °	90	90	90	115.317	62.910(2)	62.848
V , Å ³	3281.0(18)	3066.7	3362.1(5)	1496.2	1654.33(14)	1504.1
Z	4	4	4	2	2	2
V/Z , Å ³	820.3	766.7	840.5	748.1	827.17	752.1
Density, g/cm ³	1.026	1.098	1.002	1.125	1.018	1.120

* The experimental cell was symmetrized prior to optimization: the c vector, number of formula units Z , and volume V were halved.

Table S3

Parameter comparison of the experimental and optimized molecular geometries. Theory level: PBEsol/SSSP Precision

Parameter	Isolated molecule, calc.	I $P2_1/n$ (193 K)		II $C2/c$ (250 K)		III $P-1 P\bar{1}$ (200 K)	
		Exp.	Calc.	Exp.	Calc.	Exp.	Calc.
$\langle d \rangle(\text{M—N})$, Å	2.286	2.277	2.270	2.274	2.268	2.278	2.277
$\langle d \rangle(\text{M—O})$, Å	2.020	2.006	2.023	2.017	2.032	2.020	2.034
$\langle d \rangle(\text{C—O})$, Å	1.271	1.258	1.270	1.260	1.270	1.260	1.270
$\varphi(\text{NMN})$, °	79.4	79.2	80.4	81.0	80.8	79.8	80.6
$\langle \varphi \rangle(\text{OMO})$, °	87.0	86.4	87.0	85.8	87.4	86.4	87.1
$\langle \varphi \rangle(\text{O...O})$, °	164.3	161.8	162.8	163.0	161.6	165.1	163.8

Table S4

Optimized geometries of periodic structures (fractional coordinates). Theory level: PBEsol/SSSP Precision

I $P2_1/n$							
Mg	0.2164642035	0.1149632579	0.2938486069	N	0.1645838101	0.5547521182	0.1068027351
Mg	0.2835366894	0.6149632862	0.2061513272	N	0.6645835038	0.9452474754	0.6068035201
Mg	0.7835357965	0.8850367421	0.7061513931	N	0.8354161899	0.4452478818	0.8931972649
Mg	0.7164633106	0.3850367138	0.7938486728	N	0.4184472892	0.1775585434	0.3024981220
N	0.3354154962	0.0547525246	0.3931964799	N	0.0815537773	0.6775584353	0.1975015128
				N	0.5815517108	0.8224414566	0.6975018780

N	0.9184472227	0.3224415647	0.8024984872	H	0.5681430171	0.2159237753	0.2267578260
C	0.4449642023	0.1032026746	0.4235765896	H	0.4318569829	0.7840762247	0.7732421740
C	0.0550346376	0.6032009578	0.0764221592	H	0.3912905484	0.2153827387	0.1844640910
C	0.5550357977	0.8967973254	0.5764234104	H	0.1087083692	0.7153836408	0.3155351342
C	0.9449653624	0.3967990422	0.9235778408	H	0.6087094516	0.7846172613	0.8155359090
H	0.3962812916	0.1442393768	0.4586157486	H	0.8912916308	0.2846163592	0.6844648658
H	0.1037197023	0.6442384611	0.0413852318	H	0.4835506933	0.1343819816	0.1959831671
H	0.6037187084	0.8557606232	0.5413842514	H	0.0164487143	0.6343822911	0.3040157059
H	0.8962802977	0.3557615389	0.9586147682	H	0.5164493067	0.8656180184	0.8040168329
H	0.5225431423	0.0759097005	0.4655064514	H	0.9835512857	0.3656177089	0.6959842941
H	-0.0225463748	0.5759089426	0.0344914954	C	0.3934470754	0.2468892545	0.3366342998
H	0.4774578577	0.9240902996	0.5344935486	C	0.1065525186	0.7468894621	0.1633650065
H	1.0225463748	0.4240910574	0.9655085046	C	0.6065529246	0.7531107455	0.6633657002
C	0.5160673580	0.1368479305	0.3559193238	C	0.8934474814	0.2531105379	0.8366349935
C	-0.0160651639	0.6368462455	0.1440806974	H	0.4895615249	0.2787742217	0.3423858541
C	0.4839326420	0.8631520695	0.6440806762	H	0.0104393553	0.7787754964	0.1576138723
C	1.0160651639	0.3631537545	0.8559193026	H	0.5104394751	0.7212257783	0.6576141459
H	0.5618662944	0.0958872171	0.3196343506	H	0.9895606447	0.2212245036	0.8423861277
H	0.4381337056	0.9041127829	0.6803656494	H	0.3535398615	0.2415105066	0.3960304595
H	0.6027336920	0.1703688488	0.3813188682	H	0.1464608564	0.7415097326	0.1039692740
H	0.3972653080	0.8296311512	0.6186811318	H	0.6464601385	0.7584894934	0.6039695405
C	0.2470867078	0.0370301749	0.4568901601	H	0.8535391436	0.2584902674	0.8960307260
C	0.2529147305	0.5370299062	0.0431096799	H	0.3146528254	0.2747008590	0.2973257911
C	0.7529132922	0.9629698251	0.5431098399	H	0.1853464782	0.7747014726	0.2026734156
C	0.7470862695	0.4629700938	0.9568903201	H	0.6853471746	0.7252991410	0.7026742089
H	0.3052438918	0.0084546685	0.5070071235	H	0.8146535218	0.2252985274	0.7973265844
H	0.1947547755	0.5084546516	-0.0070065733	O	0.2816258745	0.0513404146	0.2066473745
H	0.6947561082	0.9915453315	0.4929928765	O	0.2183771663	0.5513386876	0.2933517692
H	0.8052452245	0.4915453484	1.0070065733	O	0.7183741255	0.9486595854	0.7933526255
H	0.1612873357	0.0037607655	0.4318263307	O	0.7816228337	0.4486613124	0.7066482308
H	0.3387134447	0.5037614193	0.0681741678	O	0.0504959751	0.0514433924	0.2944929867
H	0.8387116643	0.9962382345	0.5681736693	O	0.4495033915	0.5514440314	0.2055089776
H	0.6612865553	0.4962385807	0.9318258322	O	0.9495030249	0.9485566076	0.7055070133
H	0.2035417472	0.0857724610	0.4798620973	O	0.5504966085	0.4485559686	0.7944910224
H	0.2964596535	0.5857721708	0.0201376013	O	0.1358214470	0.1744586050	0.3804256962
H	0.7964582528	0.9142275390	0.5201379027	O	0.3641845584	0.6744596874	0.1195787261
H	0.7035403465	0.4142278292	0.9798623987	O	0.8641785530	0.8255413950	0.6195743038
C	0.1086847480	0.4901036182	0.1386094292	O	0.6358164416	0.3255403126	0.8804212739
C	0.8913142520	0.5098963818	0.8613905708	O	0.1394907324	0.1866641697	0.2143810013
H	0.0456555094	0.4607811371	0.0910299284	O	0.3605123385	0.6866640344	0.2856165544
H	0.9543434906	0.5392188629	0.9089700716	O	0.8605092676	0.8133358303	0.7856189987
H	0.0455968812	0.5015642519	0.1886333072	O	0.6394876615	0.3133359656	0.7143834456
H	0.9544031188	0.4984357481	0.8113666928	C	0.2191013243	0.4776415814	0.4085245288
H	0.1945791182	0.4564199262	0.1625993695	C	0.7808986757	0.5223584186	0.5914754712
H	0.8054208818	0.5435800738	0.8374006305	C	0.2101577917	0.0074987524	0.1628930593
C	0.4692035925	0.1863720429	0.2231958266	C	0.2898444799	0.5074976213	0.3371072579
C	0.0307967261	0.6863723648	0.2768034640	C	0.7898422083	0.9925012476	0.8371069407
C	0.5307964075	0.8136279571	0.7768041734	C	0.7101555201	0.4925023787	0.6628927421
C	0.9692042739	0.3136276352	0.7231965360	C	0.4241851415	0.4857706008	0.3239635115

C	0.5758148585	0.5142293992	0.6760364885	C	0.6725280713	0.4742986871	0.1666915880
H	0.4749651791	0.4485420688	0.3663339288	C	0.3274709287	0.5257013129	0.8333084120
H	0.5250348209	0.5514569312	0.6336660712	H	0.6171803917	0.4269564455	0.1429795257
C	0.0024476510	0.0093256588	0.2401094505	H	0.3828196083	0.5730435546	0.8570204743
C	0.4975526035	0.5093256186	0.2598915923	H	0.7833280037	0.4661383362	0.1605901285
C	0.9975513490	0.9906743412	0.7598905495	H	0.2166729963	0.5338616638	0.8394098715
C	0.5024483965	0.4906743814	0.7401084077	H	0.6360497753	0.5196803736	0.1297523569
C	0.6482722488	0.4870440527	0.2548314022	H	0.3639492247	0.4803196265	0.8702476431
C	0.3517277512	0.5129559473	0.7451685978	C	0.5457621614	0.7284511854	0.0554561056
C	0.1778302121	0.5402568734	0.4591727567	C	0.4542378386	0.2715488146	0.9445438944
C	0.8221697879	0.4597431267	0.5408272433	C	0.0309720806	0.2143684812	0.3693675005
H	0.1099558114	0.5765974247	0.4227997007	C	0.4690333163	0.7143699284	0.1306346399
H	0.8900441886	0.4234025753	0.5772002993	C	0.9690279194	0.7856315188	0.6306324995
H	0.2695140733	0.5701576358	0.4831771314	C	0.5309666837	0.2856300716	0.8693653601
H	0.7304859267	0.4298423642	0.5168228686	C	0.5164013028	0.7440153938	0.2054492716
H	0.1235188015	0.5214661330	0.5104565370	C	0.4835986972	0.2559846062	0.7945507284
H	0.8764811985	0.4785338670	0.4895434630	H	0.6027882652	0.7805836636	0.2069894741
C	0.3087060583	0.4275856370	0.4618219946	H	0.3972107348	0.2194163364	0.7930105259
C	0.6912949417	0.5724143630	0.5381780054	C	0.0425100691	0.2302383931	0.2218886680
H	0.2498775016	0.4085885212	0.5112019038	C	0.4574922311	0.7302386435	0.2781105303
H	0.7501224984	0.5914114788	0.4887980962	C	0.9574889309	0.7697616069	0.7781113320
H	0.4024468309	0.4535686376	0.4895383828	C	0.5425077689	0.2697613565	0.7218894697
H	0.5975531691	0.5464313624	0.5104616172	C	0.5097395199	0.7675051739	0.3564836028
H	0.3399890999	0.3809008078	0.4285278793	C	0.4902604801	0.2324948261	0.6435163973
H	0.6600099001	0.6190991922	0.5714721207	C	0.6640218647	0.7808647700	0.0688900213
C	0.0895989727	0.4384689895	0.3742040901	C	0.3359781353	0.2191352300	0.9311099787
C	0.9104020273	0.5615310105	0.6257959099	H	0.7144324440	0.7878477879	0.0126913336
H	0.0237067141	0.4735395579	0.3348533079	H	0.2855675560	0.2121522121	0.9873086664
H	0.9762932859	0.5264604421	0.6651466921	H	0.7433357644	0.7626104043	0.1154565901
H	0.0296243279	0.4204164923	0.4234948788	H	0.2566652356	0.2373895957	0.8845434099
H	0.9703756721	0.5795835077	0.5765051212	H	0.6278897771	0.8330056811	0.0871136125
H	0.1157240104	0.3916983374	0.3392300660	H	0.3721102229	0.1669943189	0.9128863875
H	0.8842759896	0.6083016626	0.6607699340	C	0.6024087209	0.6570942841	0.0301390037
C	0.6902888917	0.4221051639	0.3047751381	C	0.3975912791	0.3429057159	0.9698609963
C	0.3097101083	0.5778948361	0.6952248619	H	0.5184668508	0.6184492174	0.0196715214
H	0.6247554180	0.3763261917	0.2870271144	H	0.4815331492	0.3815507826	0.9803284786
H	0.3752445820	0.6236728083	0.7129728856	H	0.6771603530	0.6356981870	0.0773742114
H	0.6853774865	0.4312450515	0.3696885838	H	0.3228396470	0.3643018130	0.9226257886
H	0.3146215135	0.5687549485	0.6303114162	C	0.4416414020	0.7555782525	-0.0113425775
H	0.7978300516	0.4079458025	0.2958382426	C	0.5583595980	0.2444217475	1.0113425775
H	0.2021699484	0.5920541975	0.7041617574	H	0.3993778015	0.8071855484	0.0044485863
C	0.7352637448	0.5502577119	0.2864543701	H	0.6006221985	0.1928144516	0.9955514137
C	0.2647362552	0.4497422881	0.7135456299	C	0.6110918180	0.8268796274	0.3451683651
H	0.8459195357	0.5389250132	0.2828445616	C	0.3889081820	0.1731203726	0.6548316349
H	0.1540804643	0.4610749868	0.7171554384	H	0.7069194913	0.8078317134	0.3217707072
H	0.7194455541	0.5612207475	0.3499211667	H	0.2930805087	0.1921682866	0.6782292928
H	0.2805544459	0.4387792525	0.6500788333	H	0.6405534436	0.8527419314	0.4033648273
H	0.7073905858	0.5979128877	0.2509344765	H	0.3594465564	0.1472580686	0.5966351727
H	0.2926094142	0.4020871123	0.7490655235	H	0.5657764089	0.8674326227	0.3035578159

H	0.4342235911	0.1325673772	0.6964421841	C	-0.1725290705	-0.0257018352	0.3333088061
C	0.3831282161	0.7965068094	0.3939149318	H	-0.1247556831	-0.1236740609	0.2129720974
C	0.6168717839	0.2034931906	0.6060850682	H	-0.1853789067	-0.0687561243	0.1303107981
H	0.4133582426	0.8204576622	0.4529995358	H	-0.2978302830	-0.0920559700	0.2041609495
H	0.5866407574	0.1795423378	0.5470004642	H	-0.3459215790	0.0389262267	0.2171552895
H	0.3094818250	0.7536577071	0.4020912826	H	-0.2194470302	0.0612209636	0.1500788895
H	0.6905191750	0.2463422929	0.5979087174	H	-0.2073916280	0.0979127369	0.2490654388
H	0.3304133760	0.8371166281	0.3552463659	H	-0.1171796775	-0.0730436625	0.3570209230
H	0.6695866240	0.1628823719	0.6447536341	H	-0.2833271551	-0.0338626891	0.3394125287
C	0.5781198574	0.7110811514	0.4121422899	H	-0.1360502260	0.0196800518	0.3702476329
C	0.4218811426	0.2889188486	0.5878577101	C	0.7191004753	1.0223585354	0.9085249663
H	0.6714962052	0.6899333193	0.3877561470	C	0.9241827894	1.0142281026	0.8239623425
H	0.3285037948	0.3100666807	0.6122438530	C	0.6778296872	0.9597431460	0.9591732975
H	0.5063049426	0.6671562181	0.4193334106	C	0.8087053232	1.0724146353	0.9618222733
H	0.4936950574	0.3328437819	0.5806665894	C	0.5895974909	1.0615311116	0.8742042944
H	0.6091344182	0.7336501098	0.4719303792	H	0.9749609427	1.0514559801	0.8663333682
H	0.3908655818	0.2663498902	0.5280696208	H	0.6099561115	0.9234029864	0.9227993685
C	0.3913155554	-0.0098963146	0.3613907195	H	0.7695140608	0.9298423073	0.9831769851
H	0.4543437646	-0.0392196410	0.4089702562	H	0.6235178304	0.9785325293	1.0104575858
H	0.4544025535	0.0015651306	0.3113664074	H	0.7498778942	1.0914119904	1.0112024402
H	0.3054217768	-0.0435804266	0.3374012644	H	0.9024467808	1.0464321717	0.9895391009
C	0.6086844446	1.0098963146	0.6386092805	H	0.8399897962	1.1190997613	0.9285288652
H	0.5456562354	1.0392196410	0.5910297438	H	0.5237070708	1.0264600649	0.8348535141
H	0.5455974465	0.9984348695	0.6886335926	H	0.5296214481	1.0795839386	0.9234941663
H	0.6945782232	1.0435804266	0.6625987356	H	0.6157229424	1.1083015200	0.8392297670
H	-0.0618683342	0.5958865400	0.1803654143	C	1.1482733999	1.0129564446	0.7548313891
H	-0.1027296863	0.6703678035	0.1186819678	C	1.1902898887	1.0778955954	0.8047755526
H	1.0618683342	0.4041134600	0.8196345857	C	1.2352650069	0.9497424586	0.7864543744
H	1.1027296863	0.3296321965	0.8813180322	C	1.1725290705	1.0257018352	0.6666911939
H	-0.0681433849	0.7159241162	0.2732431506	H	1.1247556831	1.1236740609	0.7870279026
H	1.0681433849	0.2840758838	0.7267568494	H	1.1853789067	1.0687561243	0.8696892019
C	0.2808995247	-0.0223585354	0.0914750337	H	1.2978302830	1.0920559700	0.7958390505
C	0.0758172106	-0.0142281026	0.1760376575	H	1.3459215790	0.9610737733	0.7828447105
C	0.3221703128	0.0402568540	0.0408267025	H	1.2194470302	0.9387790364	0.8499211105
C	0.1912946768	-0.0724146353	0.0381777267	H	1.2073916280	0.9020872631	0.7509345612
C	0.4104025091	-0.0615311116	0.1257957056	H	1.1171796775	1.0730436625	0.6429790770
H	0.0250390573	-0.0514559801	0.1336666318	H	1.2833271551	1.0338626891	0.6605874713
H	0.3900438885	0.0765970136	0.0772006315	H	1.1360502260	0.9803199482	0.6297523671
H	0.2304859392	0.0701576927	0.0168230149	C	-0.0457631689	0.2284513209	0.4445447828
H	0.3764821696	0.0214674707	-0.0104575858	C	-0.0163941331	0.2440132411	0.2945520402
H	0.2501221058	-0.0914119904	-0.0112024402	C	-0.1640236232	0.2808651811	0.4311101389
H	0.0975532192	-0.0464321717	0.0104608991	C	-0.1024097623	0.1570940884	0.4698617336
H	0.1600102038	-0.1190997613	0.0714711348	C	0.0583581825	0.2555786863	0.5113435476
H	0.4762929292	-0.0264600649	0.1651464859	H	-0.1027830417	0.2805799993	0.2930148723
H	0.4703785519	-0.0795839386	0.0765058337	H	-0.2144347494	0.2878485695	0.4873086866
H	0.3842770576	-0.1083015200	0.1607702330	H	-0.2433393150	0.2626120725	0.3845441837
C	-0.1482733999	-0.0129564446	0.2451686109	H	-0.1278939684	0.3330067633	0.4128869500
C	-0.1902898887	-0.0778955954	0.1952244474	H	-0.1548644638	0.1630516156	0.5255075556
C	-0.2352650069	0.0502575414	0.2135456256	H	-0.0184659751	0.1184500197	0.4803285954

H	-0.1771606327	0.1356973777	0.4226263773	H	1.1548644638	0.8369483844	0.4744924444
H	0.0082584543	0.2617293478	0.5677691467	H	1.0184659751	0.8815499803	0.5196714046
H	0.1006220328	0.3071856639	0.4955516718	H	1.1771606327	0.8643026223	0.5773736227
H	0.1448554086	0.2184430282	0.5219396607	H	0.9917415457	0.7382706522	0.4322308533
C	-0.0097413433	0.2675058774	0.1435151801	H	0.8993779672	0.6928143361	0.5044483282
C	-0.1110941007	0.3268806438	0.1548313032	H	0.8551445914	0.7815569718	0.4780603393
C	0.1168709452	0.2965074339	0.1060837728	C	1.0097413433	0.7324941226	0.8564848199
C	-0.0781213887	0.2110810079	0.0878568632	C	1.1110941007	0.6731193562	0.8451686968
H	-0.2069223841	0.3078335801	0.1782290442	C	0.8831290548	0.7034925661	0.8939162272
H	-0.1405574428	0.3527441208	0.0966355062	C	1.0781213887	0.7889189921	0.9121431368
H	-0.0657793205	0.3674339260	0.1964417413	H	1.2069223841	0.6921664199	0.8217709558
H	0.0866464229	0.3204589942	0.0469983475	H	1.1405574428	0.6472558792	0.9033644938
H	0.1905171180	0.2536577681	0.0979087748	H	1.0657793205	0.6325660740	0.8035582587
H	0.1695865608	0.3371170305	0.1447530728	H	0.9133535771	0.6795410058	0.9530016525
H	-0.1714975110	0.1899326126	0.1122433163	H	0.8094828820	0.7463422319	0.9020912252
H	-0.0063064249	0.1671561747	0.0806665539	H	0.8304134392	0.6628829695	0.8552469272
H	-0.1091386750	0.2336472436	0.0280676730	H	1.1714975110	0.8100673874	0.8877566837
C	1.0457631689	0.7715486791	0.5554552172	H	1.0063064249	0.8328438253	0.9193334461
C	1.0163941331	0.7559867589	0.7054479598	H	1.1091386750	0.7663527564	0.9719323270
C	1.1640236232	0.7191348189	0.5688898611	H	0.6548630106	0.6630542009	-0.0255065166
C	1.1024097623	0.8429059116	0.5301382664	H	0.3451369894	0.3369457991	1.0255065166
C	0.9416418175	0.7444213137	0.4886564524	H	0.4917455546	0.7617285532	-0.0677664884
H	1.1027830417	0.7194200007	0.7069851277	H	0.3551427015	0.7184434101	-0.0219408054
H	1.2144347494	0.7121514305	0.5126913134	H	0.5082544454	0.2382714468	1.0677664884
H	1.2433393150	0.7373879275	0.6154558163	H	0.6448572985	0.2815565900	1.0219408054
H	1.1278939684	0.6669932367	0.5871130500				

II C2/c				H	0.3776125443	0.1906603225	0.2351516965
Mg	1.0086828839	-0.0086743476	0.2500142490	C	0.3287626422	0.2737615557	0.4543439497
O	0.1597276686	0.1484404098	0.3205787523	H	0.2402699134	0.2079174412	0.4956554683
O	0.8312054432	-0.0180846824	0.3134740492	H	0.4347303871	0.3590236325	0.4811774412
C	0.1251340151	0.2310578418	0.3648506761	H	0.3611373300	0.1901970016	0.4253721690
C	0.9712306043	0.2076625838	0.3829379604	C	0.2219191155	0.4734928281	0.4453424999
H	0.9576433354	0.2872403212	0.4213578531	H	0.1669870759	0.5318878435	0.4113423799
C	0.8332208796	0.0841836117	0.3576258112	H	0.3292351391	0.5663121388	0.4678312542
N	0.2145969909	0.9797828926	0.1906832823	H	0.1409885810	0.4147613006	0.4902462491
C	0.2650547087	0.3595001139	0.4029215064	C	0.2622334250	0.8791630169	0.2354469123
C	0.6719230769	0.0718375879	0.3819412986	H	0.1606209742	0.6591016195	0.2945966665
C	0.1661483131	0.9126238489	0.1200720658	C	0.3915311805	0.4520237483	0.3473399733
H	0.0687940463	0.7943026152	0.1243826852	H	0.4970661655	0.5387929658	0.3737085938
H	0.2661514949	0.9060451459	0.0906446264	H	0.3491323696	0.5163347219	0.3100718810
H	0.1233067292	0.9864320425	0.0893427608	H	0.4251633504	0.3727638805	0.3158485936
C	0.6752597866	0.1427069130	0.4550825192	C	0.5529943224	0.8992123067	0.3820992898
H	0.7190746482	0.0873924569	0.4961939350	H	0.5519621301	0.8463022604	0.3298718667
H	0.5556297698	0.1245946546	0.4709337409	H	0.4341622962	0.8888183452	0.3946628979
H	0.7493420120	0.2705034650	0.4553844166	H	0.5820496427	0.8304622590	0.4226117245
C	0.3427883300	0.1372443234	0.1824174548	C	0.6233950061	0.1622091611	0.3261580074
H	0.3009457935	0.2110056921	0.1510784462	H	0.7059681907	0.2878926739	0.3245298845
H	0.4461388956	0.1334554611	0.1548055119	H	0.5053698615	0.1540280867	0.3393632724

H	0.6203838916	1.1136254213	0.2725920798	H	0.1245757785	0.5556531201	0.9709350305
Mg	-0.0086898609	1.0087082581	0.7500136320	H	0.7295183513	0.2506706347	0.0446385159
O	0.8515713539	0.8402835363	0.1794486120	H	0.2506522996	0.7295359679	0.5446408726
O	0.8402684627	0.8515986348	0.6794481883	H	0.2704833580	0.7493663971	0.9553862468
O	0.1484231384	0.1597530878	0.8205790667	C	0.8627621688	0.6572201171	0.3176114906
O	1.0180970709	0.1688065306	0.1865540632	C	0.6572058246	0.8627900705	0.8176103412
O	0.1687904269	1.0181213322	0.6865542183	C	0.1372305315	0.3428146009	0.6824161300
O	-0.0181014665	0.8312305500	0.8134738482	H	0.7890002466	0.6990632260	0.3489496400
C	0.7689551365	0.8748782296	0.1351759406	H	0.6990481130	0.7890275398	0.8489486335
C	0.8748612542	0.7689799447	0.6351752927	H	0.2109910064	0.3009710580	0.6510772037
C	0.2310415296	0.1251594336	0.8648505161	H	0.8665511788	0.5538700847	0.3452242041
C	0.7923538744	0.0287820789	0.1170887772	H	0.5538556664	0.8665783767	0.8452228802
C	0.0287659167	0.7923765503	0.6170883272	H	0.1334405254	0.4461646326	0.6548038392
C	0.2076454736	0.9712551256	0.8829382157	H	0.8093488929	0.6223957810	0.2648766595
H	0.7127751063	0.0423693380	0.0786673131	H	0.6223810451	0.8093756678	0.7648758046
H	0.0423513342	0.7127989947	0.5786680237	H	0.1906457740	0.3776389384	0.7351505775
H	0.2872240052	0.9576671262	0.9213577719	C	0.7262582425	0.6712574101	0.0456791674
C	0.9158297484	0.1667909268	0.1424014646	C	0.6712356737	0.7262812068	0.5456817741
C	0.1667740132	0.9158530216	0.6424008574	C	0.2737430143	0.3287831763	0.9543459332
C	0.0841682624	0.8332456289	0.8576257108	H	0.7921022841	0.7597556625	0.0043696138
N	0.0202237093	0.7854112808	0.3093465720	H	0.7597306067	0.7921262188	0.5043712683
N	0.7853975274	0.0202515151	0.8093454008	H	0.2078997107	0.2402868928	0.9956564599
N	0.9797691562	0.2146237569	0.6906821186	H	0.6409989071	0.5652918622	0.0188430155
C	0.6405158445	0.7349571767	0.0971034512	H	0.5652687984	0.6410211523	0.5188469334
C	0.7349406862	0.6405399709	0.5971041535	H	0.3590036616	0.4347501841	0.9811806391
C	0.3594830594	0.2650800326	0.9029219837	H	0.8098237959	0.6388816445	0.0746497417
C	0.9281796203	0.3280902930	0.1180844280	H	0.6388615580	0.8098459297	0.5746537972
C	0.3280722473	0.9282012389	0.6180845457	H	0.1901775459	0.3611584002	0.9253750740
C	0.0718202131	0.6719467846	0.8819416285	C	0.5265217137	0.7780936100	0.0546836943
C	0.0873802243	0.8338611125	0.3799581694	C	0.7780756874	0.5265473653	0.5546827546
C	0.8338467198	0.0874078760	0.8799570781	C	0.4734771575	0.2219442592	0.9453419851
C	0.9126100226	0.1661743640	0.6200709529	H	0.4681257655	0.8330222207	0.0886850643
H	0.2057018992	0.9312149038	0.3756487382	H	0.8330061186	0.4681501056	0.5886825186
H	0.9312011683	0.2057291634	0.8756470576	H	0.5318720560	0.1670139275	0.9113410040
H	0.7942885354	0.0688204296	0.6243809121	H	0.4337037575	0.6707782087	0.0321937407
H	0.0939571030	0.7338579269	0.4093865391	H	0.6707597925	0.4337297778	0.5321931521
H	0.7338436954	0.0939854316	0.9093851473	H	0.5662961128	0.3292597881	0.9678313194
H	0.9060321960	0.2661778507	0.5906432563	H	0.5852521669	0.8590272503	0.0097807704
H	0.0135714272	0.8767030627	0.4106865429	H	0.8590071993	0.5852795395	0.5097793990
H	0.8766882231	0.0135981957	0.9106852952	H	0.4147465977	0.1410115616	0.9902452352
H	0.9864177844	0.1233325559	0.5893417089	C	0.1208446522	0.7377734242	0.2645847104
C	0.8573143955	0.3247534962	0.0449419732	C	0.7377615583	0.1208735561	0.7645830035
C	0.3247345381	0.8573325703	0.5449430497	C	0.8791506734	0.2622625710	0.7354451369
C	0.1426872897	0.6752832717	0.9550835602	H	0.6590889436	0.1606487921	0.7945942002
H	0.9126318760	0.2809389659	0.0038319966	H	0.8393750584	0.3409360332	0.7054340549
H	0.2809188643	0.9126474653	0.5038322508	H	1.1136109471	0.6204088480	0.7725929513
H	0.0873711211	0.7190974542	0.9961943722	C	0.5479939736	0.6084736340	0.1526824525
H	0.8754276645	0.4443840738	0.0290901450	C	0.6084610985	0.5480151826	0.6526843044
H	0.4443646429	0.8754458028	0.5290911597	C	0.4520047734	0.3915604890	0.8473415907

H	0.4612283168	0.5029395206	0.1263117928	H	0.4179430301	0.1695768443	0.5774143134
H	0.5029263853	0.4612486111	0.6263142817	H	0.8304441625	0.5820733870	0.9226105221
H	0.5387722589	0.4970949057	0.8737112439	C	0.8378057931	0.3766195044	0.1738655518
H	0.4836794245	0.6508656609	0.1899514823	C	0.3766021195	0.8378298849	0.6738671014
H	0.6508565078	0.4837009526	0.6899521576	C	0.1621928060	0.6234192418	0.8261592228
H	0.5163172318	0.3491657356	0.8100726120	H	0.7121221354	0.2940477473	0.1754924998
H	0.6272548760	0.5748417891	0.1841733467	H	0.2940302992	0.7121458987	0.6754952076
H	0.5748296979	0.6272747014	0.6841763860	H	0.2878759496	0.7059922778	0.8245317423
H	0.3727443291	0.4251935053	0.8158510604	H	0.8459895569	0.4946454793	0.1606598658
C	0.1008050299	0.4470175498	0.1179278570	H	0.4946280207	0.8460133486	0.6606617367
C	0.4469993070	0.1008270831	0.6179266432	H	0.1540117812	0.5053940151	0.8393643884
C	0.8991951275	0.5530178602	0.8820987532	H	-0.1136142458	0.3796303397	0.2274322229
H	0.1537125018	0.4480501073	0.1701561365	H	0.3796133126	-0.1135870000	0.7274330877
H	0.4480317911	0.1537360371	0.6701544316	H	0.9513718135	0.3318689121	0.7796941387
H	0.8462865120	0.5519862454	0.8298709365	H	0.6681525098	0.0486544002	0.7203343077
H	0.1112005319	0.5658499997	0.1053635799	H	0.0486251352	0.6681655616	0.2203356269
H	0.5658315003	0.1112223714	0.6053627911	H	0.3409074259	0.8393880414	0.2054366140
H	0.8888002765	0.4341852032	0.8946625820	H	0.3318409790	0.9513838809	0.2796955619
H	0.1695562509	0.4179614635	0.0774163041				

III P-1 P $\bar{1}$				C	0.4620944872	0.7433580369	0.6223265036
Mg	0.4720002214	0.5091383926	0.7551417399	C	0.5379055128	0.2566419631	0.3776734964
Mg	0.5279997787	0.4908616074	0.2448582601	H	0.4616525626	0.8297742318	0.5846832762
O	0.2957297327	0.6735261255	0.6932948181	H	0.5383474374	0.1702257682	0.4153167238
O	0.7042702673	0.3264738745	0.3067051819	C	0.8412516263	0.2444154571	0.9135099292
O	0.6402598649	0.3549652453	0.8239261322	C	0.1587483737	0.7555845429	0.0864900708
O	0.3597401350	0.6450347547	0.1760738678	C	0.1595447077	0.9131180743	0.6287011417
O	0.6296944726	0.5035628840	0.6806279211	C	0.8404552923	0.0868819257	0.3712988583
O	0.3703055274	0.4964371160	0.3193720789	C	0.7607125288	0.5899282006	0.5962593359
O	0.4719543866	0.6842795501	0.8142048279	C	0.2392874712	0.4100717994	0.4037406641
O	0.5280456136	0.3157204499	0.1857951721	C	0.3863519785	0.3558508845	0.6299519754
N	0.2700965272	0.4959501678	0.8189179602	C	0.6136480215	0.6441491155	0.3700480246
N	0.7299034728	0.5040498322	0.1810820398	H	0.2669938635	0.4571378368	0.6349345321
C	0.5743043072	0.6782968133	0.8593631559	H	0.7330061365	0.5428621632	0.3650654679
C	0.4256956928	0.3217031867	0.1406368441	H	0.3755938636	0.2581254060	0.6026192770
C	0.7175278728	0.3860250783	0.8715305109	H	0.6244061364	0.7418745940	0.3973807230
C	0.2824721272	0.6139749217	0.1284694890	H	0.4605473763	0.3935688116	0.5977157730
C	0.3136079503	0.7664221027	0.6500405648	H	0.5394526238	0.6064311884	0.4022842270
C	0.6863920497	0.2335778973	0.3499594352	C	0.6503808841	0.8320503703	0.9492196977
N	0.4609531352	0.3049686880	0.6992372924	C	0.3496191159	0.1679496297	0.0507803023
N	0.5390468648	0.6950313120	0.3007627076	H	0.5984179446	0.7925043336	0.9924973701
C	0.6927363001	0.5382572952	0.8893873234	H	0.4015820554	0.2074956664	0.0075026299
C	0.3072636999	0.4617427048	0.1106126766	H	0.6340189305	0.9507345797	0.9626560861
H	0.7699688238	0.5489704652	0.9295942453	H	0.3659810695	0.0492654203	0.0373439139
H	0.2300311763	0.4510295348	0.0704057547	H	0.7804969452	0.7538947462	0.9477333100
C	0.6099242779	0.6122796664	0.6369544636	H	0.2195030549	0.2461052538	0.0522666900
C	0.3900757221	0.3877203336	0.3630455364	C	0.3275971895	0.4231551147	0.8878277599
C	0.5697517524	0.8362850799	0.8788247199	C	0.6724028105	0.5768448853	0.1121722401
C	0.4302482476	0.1637149201	0.1211752801	H	0.4291849049	0.3052730217	0.8818296975

H	0.5708150952	0.6947269783	0.1181703025	H	0.1438711235	0.3594632102	0.8055534515
H	0.2303996700	0.4136281424	0.9179317718	H	0.8561288765	0.6405367898	0.1944465485
H	0.7696003300	0.5863718576	0.0820682282	C	0.3641388854	0.2576175519	0.7450743938
H	0.3705363587	0.4945101818	0.9184288432	C	0.6358611146	0.7423824480	0.2549256062
H	0.6294636413	0.5054898182	0.0815711568	H	0.4420196876	0.1857319402	0.7882689144
C	0.3957066661	0.9639968275	0.8803936641	H	0.5579803124	0.8142680598	0.2117310856
C	0.6042933339	0.0360031725	0.1196063359	H	0.3237712127	0.1807192132	0.7161524778
H	0.3353636827	0.9668146396	0.8302017860	H	0.6762287873	0.8192807869	0.2838475222
H	0.6646363174	0.0331853604	0.1697982140	C	0.7396092132	0.7344367297	0.5541992744
H	0.3905493469	0.0802354615	0.8898809151	C	0.2603907868	0.2655632703	0.4458007256
H	0.6094506531	0.9197645385	0.1101190849	H	0.6478332618	0.7651266131	0.5126892789
H	0.3282146569	0.9426158897	0.9232304381	H	0.3521667382	0.2348733869	0.4873107211
H	0.6717853431	0.0573841103	0.0767695619	H	0.8532141587	0.7116192625	0.5279134853
C	0.1369192536	0.6528635994	0.8294105282	H	0.1467858413	0.2883807375	0.4720865147
C	0.8630807464	0.3471364006	0.1705894718	H	0.7060246032	0.8379891277	0.5885533561
H	0.1799019256	0.7255004489	0.8589909274	H	0.2939753968	0.1620108723	0.4114466439
H	0.8200980744	0.2744995511	0.1410090726	C	0.8974819446	0.5462900680	0.6492813087
H	0.0376781626	0.6472250266	0.8594543795	C	0.1025180554	0.4537099320	0.3507186913
H	0.9623218375	0.3527749734	0.1405456205	H	0.8732601582	0.6448196361	0.6857074175
H	0.0930945975	0.7088633041	0.7777253296	H	0.1267398418	0.3551803639	0.3142925825
H	0.9069054024	0.2911366959	0.2222746704	H	1.0102476494	0.5182139570	0.6209252900
C	0.6597559361	0.8720284172	0.8192746621	H	-0.0102476494	0.4817860430	0.3790747100
C	0.3402440639	0.1279715828	0.1807253379	H	0.9121817447	0.4437888234	0.6809935739
H	0.7845578262	0.7788900196	0.8152614467	H	0.0878182553	0.5562111766	0.3190064261
H	0.2154421738	0.2211099804	0.1847385533	C	0.7457022510	0.1895079135	0.9621064952
H	0.6633211579	0.9841299525	0.8299922142	C	0.2542977490	0.8104920865	0.0378935048
H	0.3366788421	0.0158700475	0.1700077858	H	0.6709654129	0.2821916401	0.9998262934
H	0.6004129981	0.8812434575	0.7679983325	H	0.3290345871	0.7178083599	0.0001737066
H	0.3995870019	0.1187565425	0.2320016675	H	0.8284838619	0.0852457267	0.9926177234
C	0.9541964436	0.2822682729	0.9584504244	H	0.1715161381	0.9147542733	0.0073822766
C	0.0458035564	0.7177317271	0.0415495756	H	0.6667241797	0.1562911445	0.9308553648
H	0.0211047468	0.3287482101	0.9260798365	H	0.3332758203	0.8437088555	0.0691446351
H	0.9788952531	0.6712517899	0.0739201635	C	0.8011801813	0.4513473943	0.5457533726
H	0.0428965149	0.1737749420	0.9843668818	C	0.1988198187	0.5486526057	0.4542466274
H	0.9571034851	0.8262250580	0.0156331182	H	0.8194533993	0.3451615204	0.5756123638
H	0.8905729467	0.3680098335	1.0005228057	H	0.1805466007	0.6548384796	0.4243876362
H	0.1094270533	0.6319901665	-0.0005228057	H	0.9123444576	0.4254755867	0.5163990641
C	0.6220817531	0.1754948588	0.6898655284	H	0.0876555424	0.5745244133	0.4836009360
C	0.3779182469	0.8245051412	0.3101344716	H	0.7045244733	0.4774736464	0.5069712792
H	0.6915338558	0.2164307692	0.6562275319	H	0.2954755268	0.5225263536	0.4930287208
H	0.3084661442	0.7835692308	0.3437724681	C	0.9404736308	0.1125718502	0.8620908977
H	0.6187479185	0.0718579209	0.6647477743	C	0.0595263692	0.8874281498	0.1379091023
H	0.3812520815	0.9281420791	0.3352522257	H	0.8624835502	0.0847146145	0.8276091237
H	0.6822952090	0.1412579750	0.7414190408	H	0.1375164498	0.9152853855	0.1723908763
H	0.3177047910	0.8587420250	0.2585809592	H	0.0207860346	0.0052185871	0.8913026603
C	0.2205025811	0.3990862171	0.7750435717	H	0.9792139654	0.9947814129	0.1086973397
C	0.7794974189	0.6009137829	0.2249564283	H	1.0154669212	0.1462921601	0.8281812234
H	0.1457701957	0.4742272901	0.7318054671	H	-0.0154669212	0.8537078399	0.1718187766
H	0.8542298043	0.5257727099	0.2681945329	C	0.1833673502	1.0105527736	0.5702678992

C	0.8166326498	−0.0105527736	0.4297321008
H	0.2648661147	0.0590407347	0.5865644904
H	0.7351338853	0.9409592653	0.4134355096
H	0.0672842596	0.1112014215	0.5569559574
H	0.9327157405	0.8887985785	0.4430440426
H	0.2314643600	0.9414429142	0.5216069285
H	0.7685356400	0.0585570858	0.4783930715
C	0.0357501468	0.8602668876	0.6051447627
C	0.9642498532	0.1397331124	0.3948552373
H	0.0741674269	0.7896994290	0.5563278791
H	0.9258325731	0.2103005710	0.4436721209
H	0.9196699588	0.9634801577	0.5945155406
H	0.0803300412	0.0365198423	0.4054844593
H	0.0181797080	0.7881530991	0.6463845534
H	0.9818202920	0.2118469009	0.3536154466
C	0.0983546046	0.0140713189	0.6953425965
C	0.9016453954	0.9859286811	0.3046574035
H	0.0786910840	0.9465042691	0.7380755853
H	0.9213089160	0.0534957309	0.2619244147
H	−0.0156263632	0.1199675525	0.6846671787
H	1.0156263631	0.8800324475	0.3153328213
H	0.1858860549	0.0528405397	0.7143738767
H	0.8141139451	0.9471594603	0.2856261233

Table S5

Optimized geometry of the isolated molecule (xyz coordinates, Å). Theory level: PBEsol/SSSP Precision

Mg	15.000000	15.073344	15.000000	C	14.584113	19.076518	18.787376
O	16.637468	15.083138	16.197902	C	12.625883	17.603751	18.310085
O	13.362532	15.083138	13.802098	C	13.497247	19.136888	16.539724
O	14.171134	16.367235	16.298460	C	15.415917	19.076518	11.212654
O	15.828896	16.367235	13.701570	C	17.374117	17.603751	11.689915
N	15.938044	13.321748	13.870374	C	16.502753	19.136888	13.460276
N	14.061956	13.321748	16.129626	H	18.044981	14.203348	18.928154
C	16.958533	15.955716	17.066329	H	19.720662	14.314702	18.324881
C	13.041497	15.955716	12.933671	H	18.419860	13.721533	17.249117
C	14.754403	17.109765	17.146890	H	18.620572	17.894685	18.372457
C	15.245597	17.109765	12.853140	H	19.781643	16.708813	19.008103
C	15.298919	13.181550	12.564000	H	18.093237	16.681134	19.573116
C	17.369092	13.548347	13.682654	H	20.369540	16.057090	16.640472
C	15.702740	12.147865	14.714210	H	19.157422	17.203783	16.002007
C	14.701081	13.181550	17.436000	H	19.083718	15.487171	15.530939
C	12.630938	13.548347	16.317346	H	11.955019	14.203348	11.071846
C	14.297290	12.147865	15.285790	H	10.279338	14.314702	11.675119
C	16.094305	16.952466	17.552633	H	11.580140	13.721533	12.750883
C	18.409276	15.873026	17.566107	H	11.379458	17.894685	11.627573
C	13.905725	16.952466	12.447367	H	10.218357	16.708813	10.991896
C	11.590724	15.873026	12.433893	H	11.906763	16.681134	10.426914
C	13.888315	18.240266	17.721068	H	9.630490	16.057090	13.359558
C	16.111715	18.240266	12.278932	H	10.842578	17.203783	13.997993
H	14.216944	13.027451	12.673548	H	10.916282	15.487171	14.469091
H	15.740401	12.334607	11.996568	H	14.886310	18.465855	19.653568
H	15.440374	14.111727	11.993928	H	13.895709	19.856732	19.151850
H	17.509564	14.472407	13.102131	H	15.478613	19.582552	18.390149
H	17.845284	12.702099	13.143776	H	12.120267	16.990236	17.549632
H	17.845459	13.686649	14.663714	H	11.930456	18.387353	18.652816
H	16.983707	18.539603	14.249437	H	12.869738	16.962323	19.173307
H	15.783056	13.027451	17.326452	H	14.384428	19.628410	16.107664
H	14.259599	12.334607	18.003432	H	12.797935	19.920948	16.874150
H	14.559656	14.111727	18.006072	H	13.016293	18.539603	15.750593
H	12.490436	14.472407	16.897899	H	15.113720	18.465855	10.346432
H	12.154716	12.702099	16.856224	H	16.104291	19.856732	10.848150
H	12.154571	13.686649	15.336286	H	14.521387	19.582552	11.609851
H	16.439945	12.179607	15.533994	H	17.879763	16.990236	12.450368
H	16.484392	17.645082	18.294417	H	18.069544	18.387353	11.347214
C	18.661917	14.441184	18.045745	H	17.130292	16.962323	10.826693
C	18.734365	16.846707	18.692352	H	15.615572	19.628410	13.892366
C	19.309169	16.172964	16.361193	H	17.202095	19.920948	13.125850
H	13.515608	17.645082	11.705583	H	15.882804	11.206053	14.151189
C	11.338083	14.441184	11.954255	H	14.117196	11.206053	15.848811
C	11.265635	16.846707	11.307648	H	13.560085	12.179607	14.466006
C	10.690831	16.172964	13.638807				