

Supporting Information

Tris(3-nitro-pentane-2,4-dionato- κ^2 O,O') complexes as a new type of highly energetic materials: theoretical and experimental considerations.

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1. Theoretical IR spectra

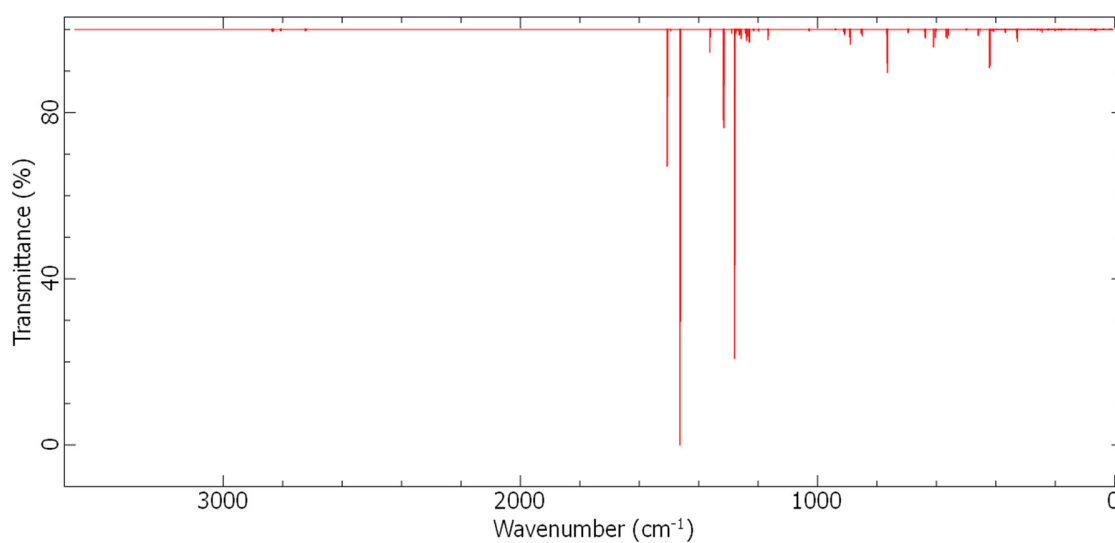


Figure S1. Theoretical IR spectrum of $\text{Cr}(\text{AcAc}-\text{NO}_2)_3$

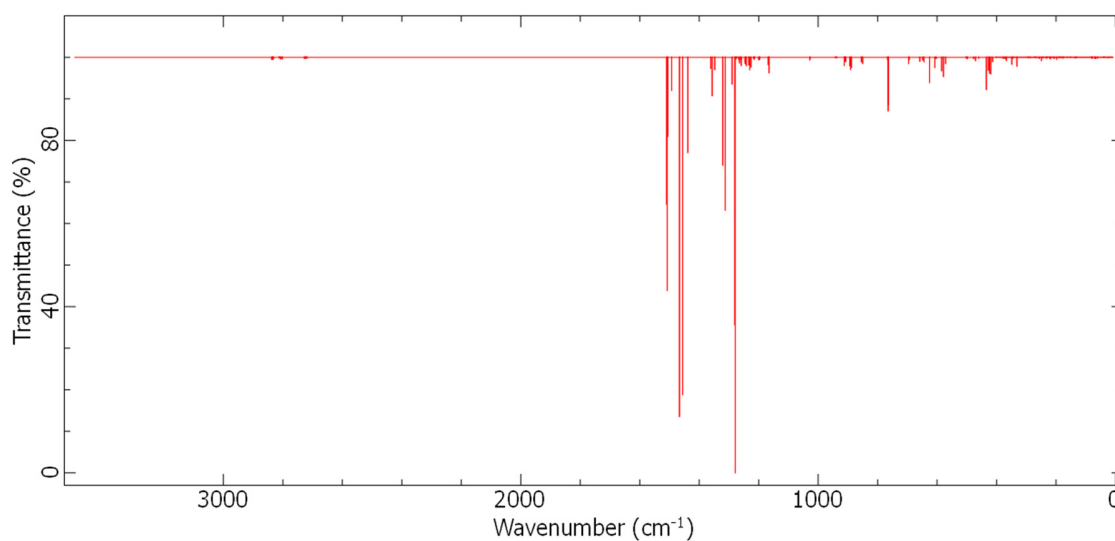


Figure S2. Theoretical IR spectrum of $\text{Mn}(\text{AcAc}-\text{NO}_2)_3$

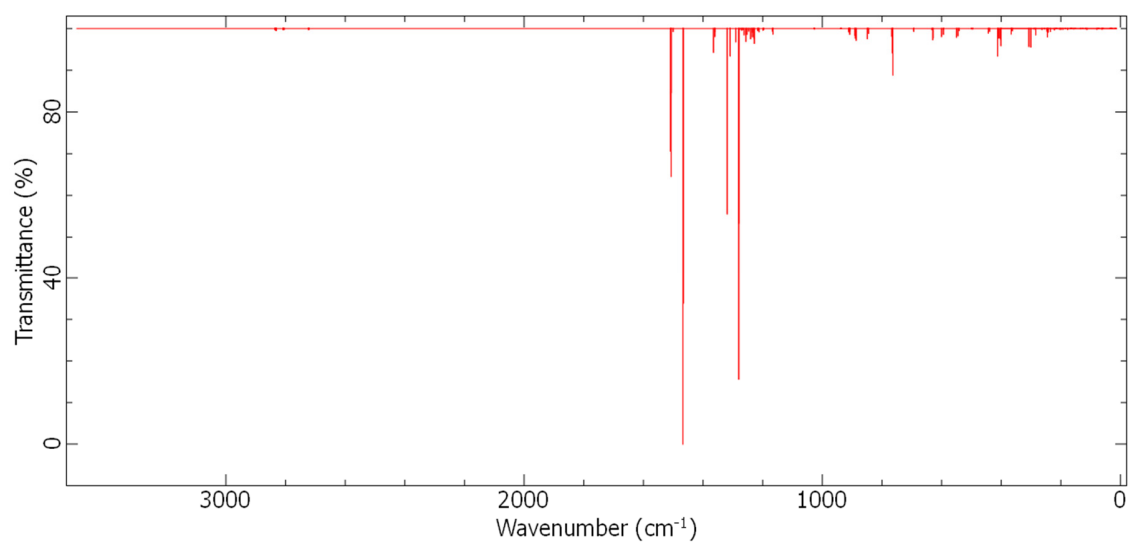


Figure S3. Theoretical IR spectrum of $\text{Fe}(\text{AcAc}-\text{NO}_2)_3$

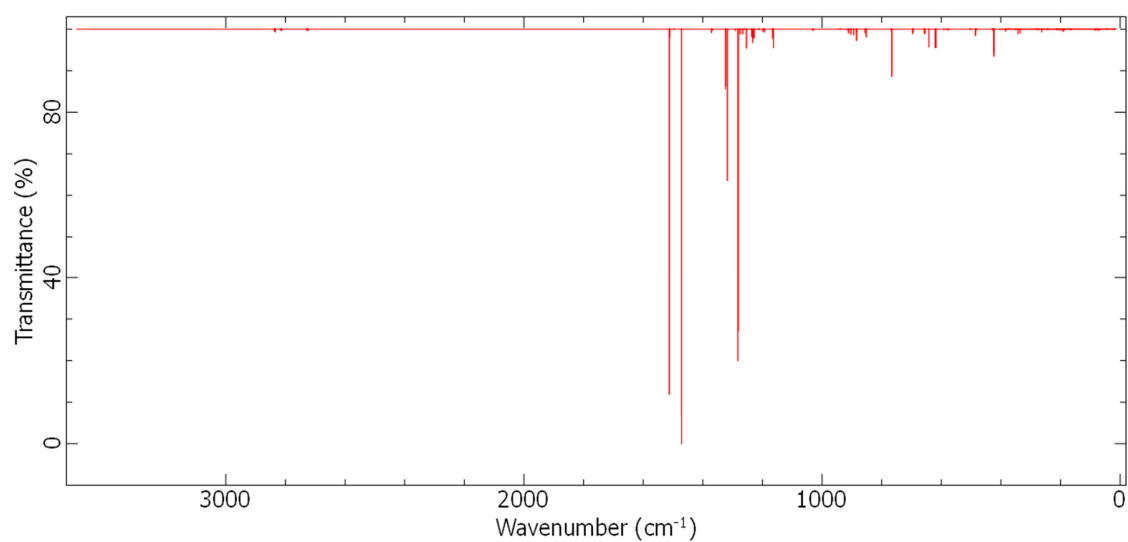


Figure S4. Theoretical IR spectrum of $\text{Co}(\text{AcAc}-\text{NO}_2)_3$

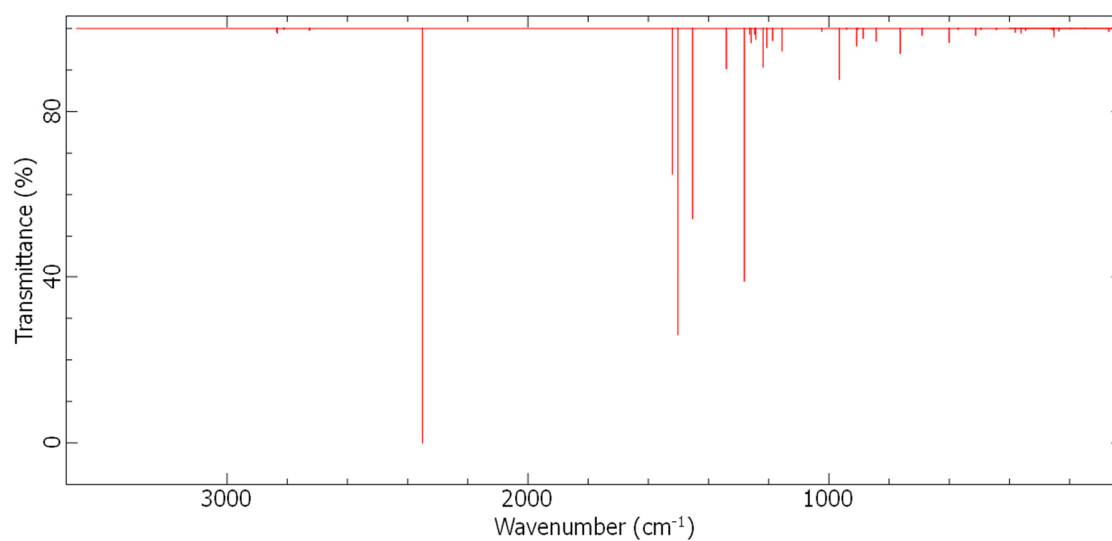


Figure S5. Theoretical IR spectrum of nitroacetylacetone

2. Hirshfeld map and fingerprint plot

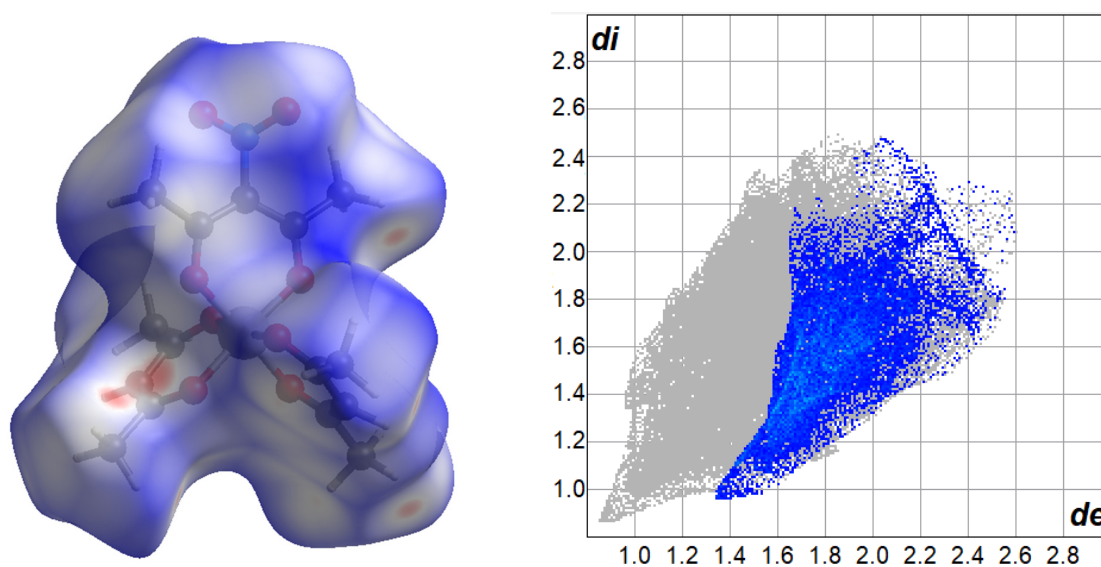


Figure S6. Hirshfeld surface mapped with d_{norm} (left) and filtered 2-D fingerprint plot showing O···H interactions (right) calculated and visualized for KUCAM crystal structure. The blue area in the filtered 2-D fingerprint plot indicate existence of O···H interactions in KUCAM crystal structure.

3. Cartesian (xyz) coordinates

Table S1. Cartesian coordinates for Cr(AcAc–NO₂)₃ complex

Cr	0.0581430000	-0.2118650000	0.0566640000
O	-0.7844780000	-1.6900230000	1.0088140000
O	-1.4332710000	-0.2822850000	-1.2053100000
O	1.1140920000	-1.4616460000	-1.0052840000
O	0.8399100000	1.2916300000	-0.9050310000
O	1.5444990000	-0.1670030000	1.3159330000
O	-0.9691630000	1.0793570000	1.0999290000
C	-1.9440040000	-2.1878080000	0.9195460000
C	-2.8686130000	-1.7754190000	-0.0811990000
C	-2.5547130000	-0.8645980000	-1.1278060000
C	-2.2613930000	-3.2162300000	1.9557220000
C	-3.4902300000	-0.5594880000	-2.2530550000
C	2.7537210000	-0.5129760000	1.1757620000
C	3.2112250000	-1.2285530000	0.0345050000
C	3.6385330000	-0.1622710000	2.3281810000
C	2.3522710000	-1.7218330000	-0.9863350000
C	2.8281870000	-2.5669470000	-2.1225780000
C	0.5799750000	2.5301560000	-0.8784840000
C	-0.3717240000	3.0867620000	0.0206260000
C	-1.0871820000	2.3354670000	0.9945740000
C	-2.0568640000	2.9495480000	1.9512620000
C	1.3868520000	3.3538610000	-1.8288670000

H	-1.5035170000	-3.1444060000	2.7449310000
H	-3.2709830000	-3.0965400000	2.3698830000
H	-2.2354440000	-4.2185290000	1.5039680000
H	-4.0865550000	-1.4247970000	-2.5676030000
H	-4.2061220000	0.2110140000	-1.9299450000
H	-2.8944280000	-0.1697440000	-3.0876670000
H	2.9984250000	0.0091730000	3.2024230000
H	4.3957270000	-0.9271900000	2.5404420000
H	4.1864610000	0.7630840000	2.0954710000
H	3.7730380000	-2.2035100000	-2.5472450000
H	3.0246750000	-3.5900740000	-1.7708300000
H	2.0394530000	-2.5826420000	-2.8841710000
H	-1.5078450000	3.4354920000	2.7712430000
H	-2.6696480000	3.7331190000	1.4879040000
H	-2.6859280000	2.1478000000	2.3564930000
H	1.6979120000	4.3170590000	-1.4050990000
H	2.2576710000	2.7602340000	-2.1331550000
H	0.7784890000	3.5877540000	-2.7151580000
N	-4.2045730000	-2.3565940000	-0.0724340000
N	-0.5961810000	4.5261640000	-0.0370880000
N	4.6351710000	-1.5233450000	-0.0484260000
O	-0.7829040000	5.1221770000	1.0105700000
O	-0.5857740000	5.0601140000	-1.1337150000
O	4.9821230000	-2.6006710000	-0.5030310000
O	5.4106200000	-0.6662150000	0.3428470000

O	-4.3288350000	-3.5230260000	0.2619670000
O	-5.1348170000	-1.6379270000	-0.3998530000

Table S2. Cartesian coordinates for Mn(AcAc–NO₂)₃ complex

Mn	-0.1821910000	-0.2287710000	0.0643710000
O	-1.5816100000	-0.0585530000	1.3858350000
O	-1.3769460000	-1.1904150000	-1.0873810000
O	1.2226840000	-0.3887720000	-1.2553110000
O	0.3884880000	-1.8755960000	0.8733370000
O	1.0321080000	0.7346330000	1.1800390000
O	-0.7410010000	1.4094630000	-0.7409820000
C	-3.6493600000	0.2236310000	2.4018960000
C	-2.8288610000	-0.1748890000	1.2164910000
C	-3.4000350000	-0.7008420000	0.0229410000
C	-2.6423970000	-1.2508880000	-1.0455600000
C	-3.2590090000	-1.9347680000	-2.2226110000
C	3.2994390000	-0.7511720000	-2.2269100000
C	2.3008630000	-1.0438100000	-1.1529730000
C	2.5150090000	-2.0181300000	-0.1390320000
C	1.5121910000	-2.4514020000	0.7720460000
C	1.6912580000	-3.6121990000	1.6955410000
C	2.5929270000	2.2589450000	1.9785130000
C	1.4890470000	1.9084070000	1.0338650000
C	0.9544600000	2.8190140000	0.0847470000
C	-0.1847910000	2.5476450000	-0.7214370000

C	-0.8180260000	3.5582300000	-1.6214050000
N	1.5809710000	4.1315300000	-0.0176530000
O	2.7958950000	4.1832180000	0.0769720000
O	0.8673290000	5.1038580000	-0.1946670000
N	3.8233920000	-2.6596910000	-0.0915540000
O	3.8856390000	-3.8477040000	0.1761460000
O	4.7970340000	-1.9600250000	-0.3177430000
N	-4.8548110000	-0.7403570000	-0.0643500000
O	-5.4720900000	0.2020160000	0.4039380000
O	-5.3816750000	-1.7012600000	-0.5997450000
H	-2.9964120000	0.2031240000	3.2832120000
H	-4.0228390000	1.2479860000	2.2544380000
H	-4.5309070000	-0.4115810000	2.5515960000
H	-3.6406570000	-2.9219570000	-1.9257990000
H	-4.1213520000	-1.3818870000	-2.6177630000
H	-2.4850010000	-2.0480510000	-2.9909820000
H	4.0234640000	-0.0132510000	-1.8485860000
H	3.8785640000	-1.6285610000	-2.5391320000
H	2.7592530000	-0.3156960000	-3.0767000000
H	0.8535840000	-3.6147520000	2.4025980000
H	1.7119560000	-4.5500930000	1.1231290000
H	2.6496600000	-3.5652180000	2.2303130000
H	3.5592120000	2.1147180000	1.4710270000
H	2.5666580000	3.3041040000	2.3097860000
H	2.5346180000	1.5744390000	2.8338590000

H	-1.5012970000	3.0288900000	-2.2960920000
H	-1.3777480000	4.2931980000	-1.0255120000
H	-0.0759600000	4.1299600000	-2.1939440000

Table S3. Cartesian coordinates for Fe(AcAc –NO₂)₃ complex

Fe	0.2155800000	-0.2867990000	0.0866520000
O	-0.5436630000	-1.9275740000	0.8904650000
O	-1.2498920000	-0.5153770000	-1.2680470000
C	-1.6889410000	-2.4622230000	0.8195720000
C	-2.6372250000	-2.0597520000	-0.1611360000
C	-2.3481640000	-1.1366750000	-1.2087720000
C	-1.9583820000	-3.5196780000	1.8400160000
C	-3.2859080000	-0.8745250000	-2.3439600000
H	-1.1843800000	-3.4463630000	2.6132690000
H	-2.9610330000	-3.4321070000	2.2787790000
H	-1.9209630000	-4.5117140000	1.3669210000
H	-3.8634390000	-1.7563490000	-2.6472920000
H	-4.0178250000	-0.1118390000	-2.0379610000
H	-2.6942590000	-0.4850100000	-3.1817790000
N	-3.9601020000	-2.6691320000	-0.1454430000
O	-4.0612160000	-3.8370990000	0.1908630000
O	-4.9047340000	-1.9671150000	-0.4679130000
O	1.5417530000	-1.1724490000	-1.0908780000
O	1.7118880000	-0.2150570000	1.3948290000
C	2.9653380000	-0.2804710000	1.2457730000

C	3.5555390000	-0.7057500000	0.0216070000
C	3.7647350000	0.0620290000	2.4618860000
C	2.8069850000	-1.1898150000	-1.0879150000
C	3.4363200000	-1.7354890000	-2.3282580000
H	3.1051340000	-0.0361960000	3.3329780000
H	4.6658390000	-0.5524370000	2.5778280000
H	4.1060020000	1.1054330000	2.3862340000
H	4.2856490000	-1.1284930000	-2.6683480000
H	3.8404120000	-2.7391660000	-2.1319740000
H	2.6615610000	-1.7921270000	-3.1021680000
N	5.0097880000	-0.7020780000	-0.0651250000
O	5.5582100000	-1.6015530000	-0.6796290000
O	5.6045690000	0.2111840000	0.4831590000
O	0.6779630000	1.4724530000	-0.7497370000
O	-0.9746670000	0.8208580000	1.2529230000
C	0.0856420000	2.5888380000	-0.7612010000
C	-1.0071050000	2.8710350000	0.1077070000
C	-1.4616510000	1.9808750000	1.1215620000
C	-2.5516530000	2.3246650000	2.0846690000
C	0.6552980000	3.5966540000	-1.7069860000
H	-2.1591260000	2.9938100000	2.8642650000
H	-3.3803950000	2.8656600000	1.6098120000
H	-2.9036660000	1.3925550000	2.5432460000
H	0.6330990000	4.6217990000	-1.3176450000
H	1.6805800000	3.2890890000	-1.9476250000

H	0.0560450000	3.6002160000	-2.6299640000
N	-1.6422470000	4.1770240000	-0.0075630000
O	-2.0137570000	4.7329000000	1.0126150000
O	-1.7703740000	4.6464560000	-1.1263980000

Table S4. Cartesian coordinates for Co(AcAc–NO₂)₃ complex

O	0.7185260000	-1.3910660000	-1.0908130000
Co	-0.0001090000	-0.0412450000	-0.0001930000
C	1.8717420000	-1.9010050000	-1.0059110000
O	1.4809260000	0.0351750000	1.1530300000
O	0.8546550000	1.2292450000	-1.0907100000
O	-0.8524080000	1.2309820000	1.0902450000
O	-0.7212730000	-1.3895840000	1.0905670000
O	-1.4811080000	0.0378660000	-1.1533140000
C	2.5519480000	-0.6297490000	1.0591820000
C	0.7568300000	2.4866070000	-1.0083750000
C	-0.7518690000	2.4881390000	1.0080200000
C	-1.8755750000	-1.8971060000	1.0060190000
C	-2.5534400000	-0.6249150000	-1.0592280000
C	2.8016570000	-1.5656060000	0.0174690000
C	2.1502570000	-2.9298540000	-2.0563980000
C	3.5506860000	-0.3090450000	2.1266470000
C	0.0032560000	3.1483030000	-0.0000890000
C	1.5486040000	3.2160500000	-2.0479600000
C	-1.5420310000	3.2192290000	2.0476750000

C	-2.8049520000	-1.5600290000	-0.0172980000
C	-2.1560140000	-2.9251720000	2.0567390000
C	-3.5515670000	-0.3025540000	-2.1267680000
N	-4.0974340000	-2.2340340000	-0.0034950000
O	-4.6108240000	-2.4629620000	1.0787460000
O	-4.6004450000	-2.5351220000	-1.0726900000
N	4.0928060000	-2.2422110000	0.0038740000
O	4.5950800000	-2.5443190000	1.0731220000
O	4.6058180000	-2.4722560000	-1.0783100000
N	0.0049660000	4.6068400000	0.0001580000
O	0.0141680000	5.1792710000	1.0766190000
O	-0.0027180000	5.1797160000	-1.0760820000
H	1.1915630000	-3.2275720000	-2.4987800000
H	2.7921860000	-2.4925130000	-2.8346340000
H	2.6878830000	-3.8021910000	-1.6635200000
H	4.5744860000	-0.2352420000	1.7376220000
H	3.2451230000	0.6307140000	2.6028630000
H	3.5609290000	-1.1142330000	2.8750840000
H	2.0767900000	4.0887910000	-1.6427010000
H	2.2554820000	2.5051590000	-2.4931410000
H	0.8699520000	3.5963080000	-2.8249710000
H	-0.8625720000	3.5975110000	2.8249480000
H	-2.0679730000	4.0934080000	1.6426100000
H	-2.2507400000	2.5099530000	2.4925260000
H	-2.6946560000	-3.7968700000	1.6637780000

H	-1.1979130000	-3.2242020000	2.4995370000
H	-2.7975910000	-2.4867980000	2.8346580000
H	-3.5633390000	-1.1079220000	-2.8749970000
H	-4.5752410000	-0.2266600000	-1.7378190000
H	-3.2441660000	0.6364770000	-2.6032320000

Table S5. Cartesian coordinates for nitroacetylacetone

O	-1.2207600000	1.9793900000	0.0610100000
O	1.2212100000	1.9741500000	-0.0298400000
C	0.0010900000	-0.0089500000	-0.0015100000
C	-1.2171700000	0.6805100000	0.0358800000
C	1.2576400000	0.7304400000	-0.0399300000
C	-2.5750000000	0.0818400000	0.0810000000
C	2.5939700000	0.0704500000	-0.1351500000
H	-2.8278800000	-0.3473800000	-0.8990900000
H	-2.6346000000	-0.7485200000	0.7959000000
H	-3.2905300000	0.8730200000	0.3371300000
H	3.3302800000	0.8455900000	-0.3809700000
H	2.8508400000	-0.3991200000	0.8251500000
H	2.6074100000	-0.7372800000	-0.8792600000
N	-0.0060800000	-1.4571400000	0.0077900000
H	-0.2338500000	2.2697100000	0.0284700000
O	0.9828800000	-2.0290200000	0.4360400000
O	-0.9986100000	-2.0347500000	-0.4076600000